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Directory

Topical Sessions =》 1. Carbon Nanomaterials

最终交流类型: Invited

The crack, contamination and wrinkle-free transfer of large-area graphene films and the related applications

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Owing to its fascinating properties, graphene has exhibited great potentials in the applications of high-performance electronics, flexible devices and encapsulation. The availability of graphene on a wide range of substrates forms the basis for large-area applications, such as graphene integration with silicon-based technologies, which requires graphene on silicon with outperforming carrier mobilities. In this regard, although currently, large-area graphene films have been successfully produced based on chemical vapor deposition methods, with outperforming quality and uniformity. Graphene films were only produced on limited archetypal substrates, such as metal foils. Reliable after-growth transfer techniques, that do not produce cracks and contamination are critical for layering 2D materials onto arbitrary substrates for further applications. During the transfer of graphene, with atomically thin and highly flexible nature, polymer-based transfer medium is usually introduced for avoiding the formation of cracks and wrinkles, which, however, introduces unavoidable contamination on graphene surface. In addition, traditional transfer routes, including etching and bubble-based delamination, involve the aqueous solution-based reactions or processing, which would induce the water-related p-doping in graphene and improve the complexity in the design of industrial equipments for batch transfer.

Here, in our group, based on the structural design of transfer medium and careful modulation of interfacial forces, we have achieved the crack, contamination and wrinkle-free transfer of graphene films over large area: (1) we achieved the mechanical delamination of graphene both from the Cu surfaces and from the polymer surface, based on the uniform oxidation of Cu substrates and the controllable tuning of the interaction between graphene and polymer, and all the transfer process were conducted without using water or organic solvent; (2) we showed that, by incorporating oxhydryl groups-containing volatile molecules, the supporting films can be deformed under heat to achieve a controllable conformal contact, enabling the large-area transfer of graphene wafers without cracks, contamination, and wrinkles onto silicon wafers, and the ultraclean surfaces provide the carrier mobilities of transferred graphene up to 14,000 cm2 V−1 s−1 at room temperature; (3) we achieved the preparation of high-performance water barrier films based on layer-by-layer transfer of A3-sized graphene films, and the water vapor transmission rate of double-layer graphene can be as low as 5×10-3 g/(m2·d), which is one order of magnitude lower than previously reported values; (4) we designed and built the transfer systems for the batch transfer of graphene films, including the automatic spin-coater, delaminator and laminator.

Keyword: graphene；transfer；contamination；crack；batch transfer

最终交流类型: Invited

Controlled Synthesis and Properties of Ultralong Carbon Nanotubes

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Carbon nanotubes (CNTs) have drawn intensive research interest in the past near 30 years due to their excellent properties and wide applications. Ultralong CNTs usually have perfect structures and lengths up to centimeters, even decimeters, showing extraordinary mechanical, electrical, and thermal properties. Ultralong CNTs are promising candidates for transparent displays, nanoelectronics, superstrong tethers, aeronautics and aerospace, etc. The controlled synthesis of ultralong CNTs with perfect structures is the key to fully exploit the extraordinary properties of CNTs. Over the past two decades, significant progress has been made in the study of ultralong CNTs, but there are also great challenges in controlled synthesis and mass production of ultralong CNTs, which limits their application.

In this talk, I will talk three aspects about ultralong CNTs.

(1) The growth mechanism of ultralong CNTs.
(2) The controlled synthesis of ultralong CNTs with ultrahigh yields.
(3) The structural coloration of CNT fibers and their properties.

Keywords: Carbon nanotubes, chemical vapor deposition, synthesis, fibers, properties

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最终交流类型: Invited

Controlled Growth of Horizontally Aligned Single-Walled Carbon Nanotube Arrays

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Single-walled carbon nanotubes (SWNTs), especially horizontally aligned SWNT arrays, have become one of the most promising materials for next-generation electronic systems due to their special nanostructures and excellent electrical properties. However, the synthesis of SWNT arrays still faces two major problems, purity and yield. Synthesis determines the future. For further promoting the practical application of carbon nanotubes, growth of SWNT horizontal arrays with controlled structures and high density is imperative. In the chemical vapor deposition (CVD) growth of carbon nanotubes, catalyst is of vital importance. We found that, carbide catalysts with high melting point can maintain their crystal structures at the growth temperature, so the nucleation of carbon nanotubes can be thermodynamically controlled to have the same symmetry with the catalyst crystal plane. Further optimization of growth kinetics can result in the enrichment of carbon nanotubes with specific chirality.[1] In order to increase the yield of SWNTs with controlled structures, we developed an approach of in-situ preparation and continuous loading of solid catalysts: floating solid catalyst CVD (FSCCVD).[2] The carbide catalyst nanoparticles were directly obtained in the carrier gas by decomposition and carbonization of catalyst precursor at high temperature. SWNT horizontal arrays can be obtained on ST-cut quartz substrates after the deposition of TiC catalyst nanoparticles, and the chirality of the grown SWNTs had the same symmetry as the carbide catalyst crystal plane. The enrichment of (16, 8) tubes with a purity of 74% was finally realized. This method can be further used to realize the direct growth of high-density arrays via a spatially confined strategy, which greatly increase the deposition efficiency of the catalyst nanoparticles and the growth efficiency of the SWNTs through a trapping effect. As a result, high-density of ~65 tubes/μm and high semiconducting purity of ~97% were obtained at the same time, benefiting from the titanium-based catalyst structures.[3] We are now trying to utilize the charge-transfer between catalysts and SWNTs with the assistance of illumination to selectively synthesize semiconducting tubes in horizontal arrays. From fine structure control to continuous growth, we provide new ideas for preparation of SWNTs with high-density and specific structures, and aims to realize wafer-scale, high-density SWNT arrays with controlled structures.

Keyword:single-walled carbon nanotubes, structural control, floating solid catalyst, high- density arrays, charge transfer

最终交流类型: Invited

Versatile Nanoemulsion Assembly of Tunable Mesoporous Carbonaceous Materials

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Mesoporous carbonaceous materials have attracted tremendous attention owing to their advantages of lightness, conductivity, high stability, tunable porosity and surface functionality. Impressively, large pores of mesoporous carbonaceous materials provide broadly accessible passageway for the mass transport of chemicals in the field of biomedical applications, gas separation, catalysis, sensing, and energy storage and conversion. To date, although substantial efforts have been devoted to synthesize mesoporous carbons with large internal volumes, controlled synthesis of functional mesoporous carbons with novel nanostructures and high nitrogen content remains challenging. Meanwhile, the formation

mechanism for these porous nanostructures is vague. Herein, we developed diverse novel mesoporous carbonaceous materials with tunable shapes via a nanoemulsion strategy.

In the synthesis, micelle composed of surfactants, swelling agents and dopamine precursor species is assembled at first via hydrogen bonds, Coulombic and/or other noncovalent interactions in the nanoemulsion system. Each micelle acts like a template for a single mesopore. Then, multiple micelles can be stacked like LEGO blocks accompanied by polymerization of dopamine molecules. After carbonization, micelles transform to mesopores resulting in mesoporous carbonaceous materials with various nanostructures. The resultant mesoporous carbonaceous materials show large open mesochannels, high accessible surface area (> 500 m2 g-1), and rich nitrogen dopants (> 6 wt %), affording them excellent electrochemical performance for energy storage.

Analyzing the formation mechanism, we found that by continuously adjusting the amphipathicity of surfactants or the concentration of swelling agents, the packing parameter and size of micelles changed. This change caused micellar structure transformations (e.g., from spherical to cylindrical and to lamellar one), resulting in carbonaceous materials with pore structures transforming from single-porous, to radial orientated, to flower-like, to multi-shelled hollow nanospheres, and to jellyfish-like mesoporous carbon hemispheres. Microscopically, the grow manners of micelles switched from isotropic self-assembly to interface anisotropic self-assembly. Overall, we believe this versatile nanoemulsion strategy and proposed mechanism explanation opens up new horizons for synthesis of mesoporous materials with novel nanostructures.

Keyword:Nanoemulsion Assembly, Mesoporous Carbonaceous Materials, Micellar Structure, Interface Assembly

最终交流类型: Invited

Atomically precise graphene nanoribbons for next-generation quantum electronics

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Atomically precise graphene nanoribbons (GNRs) have attracted much interest from researchers worldwide, as they constitute an emerging class of quantum-designed materials tailored by controlling their width and edge structure during chemical synthesis [1-3]. The major challenges toward their exploitation in electronic applications include reliable contacting, complicated by their nanometer size, and the preservation of their intrinsic physical properties upon device integration [4]. Here, we report on the device integration of armchair GNRs into various device architectures with different electrode materials [5]. First, we demonstrate an improved tunability of GNRs quantum dot (QD) behavior thanks to multiple nanometer-sized gates [6]. Second, beyond graphene-based contacts, we demonstrate the successful contacting and characterization of individual GNRs using single-walled carbon nanotubes (SWNT) electrodes and multiple gates. We observe well-defined quantum transport phenomena, including Coulomb blockade, excited states, and Franck-Condon blockade, indicating that a single GNR was contacted [7]. In addition, we demonstrate the encapsulation of GNRs in hexagonal boron-nitride and the contacting using metallic side contacts. These experimental realizations of advanced contracting and gating pave the way for the integration of GNRs in quantum devices to exploit their topologically trivial and non-trivial nature.

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Keyword: graphene nanoribbons, bottom-up synthesis, quantum dot, Coulomb blockade, quantum transport

最终交流类型: Invited

Moisture Power: A New Type of Clean Energy

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Graphene has outstanding electrical, thermal, and mechanical properties, plus high specific surface area, and environmental stability. The physical and chemical properties of graphene and its macroscopic structure depend on its controllable assembly and functional modification, which in turn affects its specific applications. We have developed new methods and technologies such as confined assembly to achieve the preparation of graphene with different dimensions of functionality, including zero dimensional graphene quantum dots, macroscopic one-dimensional graphene fibers, two-dimensional graphene films, and three-dimensional graphene skeleton structures. Based on the functional structures limited by these dimensions, they exhibit unique application potential in the fields of energy and environment. For example, graphene regulated by microstructure can be used as a high-performance energy storage electrode material; The ordered assembly structure of graphene with three-dimensional structure has efficient photothermal conversion efficiency, and has important application prospects in the production of clean water through photothermal treatment. This report will present the cutting-edge applications of graphene functional assembly materials in the field of spontaneous generation of electrical energy by moisture.

Harvesting energy from clean and renewable sources has boomed the development of diverse electrical generators to satisfy the growing demand of electricity in our daily life. Moisture enabled electric generator (MEG) is proposed as a means to produce electric power from air by absorbing gaseous or vaporous water molecules, which are ubiquitous in the atmosphere. In this regard, we designed and developed a series of graphene based MEGs with a heterogeneous structure and interface mediation between electrodes/materials with Schottky junctions. Benefiting from the functional groups-reconfiguration and inner protons asymmetrical distribution, the asymmetric porous graphene oxide membrane can proactively generate a sustained electrical voltage approaching 1.5 V. High voltage of up to 1000 V can be easily reached by simply scaling up the number of MEG units in series, enough to drive many commercial electronic devices such as liquid crystal displays (LCD) and light-emitting diodes (LED). This work provides insight for the design and development of MEGs that may promote the efficient conversion of potential energy in the environmental atmosphere to electricity for practical applications.

Keyword:graphene; moisture power; electric generator

最终交流类型: Invited

Lithium–sulfur batteries: From nanocarbon materials to machine learning

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Advance energy storage constitutes an importance part of the sustainable energy landscape. To meet the demand for electric vehicles and large-scale grid storage, developing next-generation high-energy-density secondary batteries is regarded as one of the most promising solutions. Among various new battery chemistries, the lithium–sulfur batteries have attracted enormous attention due to multiple advantages in specific energy, cost, resource, and operational flexibility. Nevertheless, its cathode material, sulfur, is intrinsically electron insulating, and the multi-electron conversion reactions between sulfur and lithium sulfides involve multiscale and multi-process coupling, bring in additional complexity to the working battery. To fully demonstrate the energy storage ability of sulfur necessitates deep understanding of the reaction mechanism, effective reaction regulating strategies, construction of highly efficient reaction interfaces, and holistic device integration and optimization.

In this talk, I will firstly introduce our recent understanding of the sulfur conversion processes with nanocarbon-based cathode hosts in lithium–sulfur batteries. The multi-phase sulfur conversion processes including the liquid–liquid polysulfide interconversion and the liquid–solid lithium sulfide deposition, as well as their impacts on the battery capacity and battery cycling, will be concentrated. In particular, the liquid–liquid polysulfide interconversion has been probed to largely determines the cathode reaction kinetics while mediating the spatial distribution of liquid–solid lithium sulfide deposition is crucial for achieving good cycling stability. Then, I will discuss how the extrinsic parameters such as the electrolyte properties (e.g. dielectric constant) and battery operational conditions (e.g. current density) affect the sulfur conversion reactions on nanocarbon-based hosts and what are the major limitations that carbon nanomaterials confront when serving as sulfur hosts. Next, I will introduce our efforts in modifying the nanocarbon-based sulfur hosts with additional reaction mediators to improve the regulation effectiveness of nanocarbon for sulfur cathodes. Finally, I will introduce our very recent efforts in understanding the degradation of practical lithium–sulfur batteries using machine learning. This talk is aiming to rationalize the design strategies of working lithium–sulfur batteries and these insights may contribute to developing better batteries.

Keyword: Lithium–sulfur batteries, Carbon nanomaterials, Interface regulation, Reaction mediators, Machine learning

最终交流类型: Invited

Circularly Polarized Raman Spectroscopy of Two-Dimensional Materials

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Raman spectroscopy is a powerful tool for the characterization of materials. The peak positions correspond to the energies of specific phonons, which give information on the composition and the lattice structures of materials. The intensity is determined by the optical transitions and the coupling between electrons and phonons. Generally, a linearly polarized laser is used for excitation. However, circularly polarized Raman scattering can provide more information that is not accessible by linear polarization.

In this talk, we will introduce our recent work on circularly polarized Raman scattering of two-dimensional (2D) materials. 2D materials are layered crystals of atomic thickness with intralayer chemical bonding but interlayer van der Waals interaction, which possess superior optical, electrical, mechanical and thermal properties. Raman scattering has been widely used to characterize the fine structures of 2D materials, such as layer number, defects and type of edges. In our work, we use circularly polarized laser for the excitation of Raman scattering in layered MoS2, ReS2 and graphene. By measuring the helicity of Raman scattered light, we can characterize the relative contribution of the two kinds of electron/exciton−phonon interactions, that is, deformation potential (DP) or the Fröhlich interaction (FI). We will also show that the oblique ange of vertical graphene arrays can be measured using helicity-resolved Raman spectroscopy.

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Keyword: Raman scattering, circular polarization, two-dimensional materials, electron-phonon coupling, graphene

最终交流类型: Invited

The Preparation and Medical Applications of Fullerenes and Metallofullerenes

王春儒
中科院化学所

This presentation will introduce the discovery, preparation, characterizations, as well as the applications of fullerene materials. As is well known that fullerenes are rare in the earth but extensively distributed in the cosmos. In 1985, three scientists, i.e., Kroto, Curl, and Smalley, found the fullerene C60 for the first time while they imitating the cosmos environments in laboratory, and they finally obtained the Nobel prizes of Chemistry in 1996. In the last 30 years, scientists have developed a dozen of techniques to prepare the fullerenes and metallofullerenes. Regarding their applications, it will be focused on several aspects as followings: First, based on the phase transition feature of fullerene and metallofullerene crystals, as well as the universal leaking structure of tumor blood vessels, a novel tumor therapeutic strategy was introduced in which the fullerene and metallofullerene nanocrystals were used to selectively destroy the tumor vascular structures rapidly. This tumor therapy technique was revealed to widely used in various tumors such as liver, kidney etc.. Secondly, due to the high ROS scavenging activity, watersoluble fullerenes and metallofullerenes have been applied to protect against chemotherapy injury, treat pulmonary fibrosis and inflammation-related diseases, revealing that the excellent ROS scavenging capability of water-soluble fullerenes derivatives brings broad medical applications. As an example, we explored the anti-oxidative hydroxylated [70] fullerene nanoparticles (HFNPs) to reverse insulin resistance in diabetes. HFNPs could alleviate insulin resistance both in palmitic acid (PA)-induced cells and in db/db diabetic mice, which significantly normalize glucose uptake and reduce blood glucose. Of note, we demonstrated that HFNPs resist insulin resistance by doubly regulating oxidative stress and endoplasmic reticulum stress based on proteomic profiling. In addition, we further confirmed that HFNPs repress the activation of phosphorylated c-Jun N-terminal kinase (JNK), resulting in re- activating insulin receptor substrate (IRS) signaling pathway and inhibiting gluconeogenesis, and thus alleviate insulin resistance.

Keyword: Fullerenes, Metallofullerenes, tumor, diabets

最终交流类型: Invited

Emergent optoelectronic properties of graphene-based junctions

Mario Hofmann
National Taiwan University

While fundamental research has elucidated the properties of individual nanostructures, most experiments and applications focus on mesoscopic collections of nanostructures. Such assemblies exhibit optoelectronic properties that are distinctly different from traditional bulk materials, exhibiting fascinating properties such as critical pathways and structure-related degrees of freedom.

I will detail our progress in enhancing the understanding of emergent properties that occur when the morphology of nanostructure assemblies is controlled. To this end, I will introduce a novel approach to simulating electronic transport in nanostructure assemblies with arbitrary morphology. . By exploiting complex network theory, a tool was developed that allows simulating realistic conduction in nanostructured films, composites and other geometries. The presented approach has been applied to identifying novel morphologies and critical properties for future applications. Our tool opens a route to study the phenomenon of which “emergence” – a collective behavior that is not observed in individual members [2]. A simple example of this process is found in percolative transport through assemblies of carbon nanostructures and the sensitivity of the percolative transport on mechanical deformation allow the realization of nanoelectromechanical transducers that were exploited for bolometric infrared sensing.

Beyond percolation, we have identified a new conduction process that we term “subthreshold percolation”. The self-selective carrier transport is experimentally confirmed in lateral 2D all-carbon junction networks and enables wearable and ubiquitous sensors with unprecedented optoelectronic performance.

Morphology-dependence extends beyond DC carrier transport and I will demonstrate the impact of neighbor-neighbor interactions on plasmonic properties of nanostructures. The increased hot-electron yield under such collective effects makes plasmonic assemblies promising for photocatalytic applications such as CO2 reduction.

Finally, I will demonstrate the efficient transduction of light into current in complex junction structures. Unlike traditional photosensors or solar cells, conversion proceeds through direct rectification of the light's electric field as evidenced by clear polarization control and wavelength-dependent photovoltage [1]. Graphene-junction based rectennas showed a tenfold increase in photon-electron coupling and open exciting avenues towards optical quantum computing

Keyword： Graphene junctions, emergence, percolation, optoelectronics

最终交流类型: Keynote

Synthesis of Some Topological Molecular Carbons

Jishan Wu
National University of Singapore

We report the bottom-up synthesis of some challenging molecular nanocarbons with well-controlled edge structure and topology. This includes: (1) long rylene ribbons,1 (2) macrocyclic polyradicaloids with alternatively fused six- and five-membered rings;2 (3) kekulenes, expanded keulenes and cycloarenes;3-4 (4) twisted carbon nanobelts with persistent chirality;5-8 (5) single-layer/bilayer graphene fragements,9 and (6) a γ-graphyne spoked wheel molecule.10 Their unique electronic properties and their applications for photonics will be also discussed.

Keywords: molecular carbon, nanographene, carbon nanobelt, edge structure, topology

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最终交流类型: Invited

Bulk Synthesis of Single-Walled Carbon Nanotubes with Narrow Chirality Distributions

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Bulk synthesis combined with post-growth sorting techniques is the prevailing approach for obtaining single-chirality single-walled carbon nanotubes (SWNTs). To improve the sorting efficiency and reduce costs, the initial SWNT materials should consist of only a few specific (n, m) species. Chemical vapor deposition (CVD) growth of SWNTs using solid supported heterogeneous catalyst has demonstrated significant potential in chirality selection. Impressive achievements have been made in the selective synthesis of (6, 5) or (9, 8) SWNTs at low reaction temprature and high pressures. The growth rate of these SWNTs generally follows the screw dislocation theory, facilitating the enrichment of near armchair SWNTs. So far, bulk synthesis of other SWNT species with a narrow chirality distribution remains challenging.

In this lecture, we will start with the understandings to the SWNT growth mechanisms on solid support catalyst, with a focus on the crucial role played by the metal-support interaction in activating and influencing catalyst performance. Additionally, various parameters of the CVD reaction, the carbon precursor, reaction temperature, and pressure, are investigated for their impact on the chirality distribution of synthesized SWNTs. Building upon these insights, we have designed and developed a series of solid supported catalysts specifically tailored for the preferential growth of SWNTs with specific (n, m) indices. The chirality distribution is evaluated using absorption and photoluminescence spectroscopy. For instance, using a magnesia supported rhodium catalyst, predominant synthesis of ultrasmall (5, 4) nanotubes is achieved by CO CVD, in which both the catalyst composition and the reaction parameters are crucial for the growth results. In contrast, a rhodium catalyst supported by mesoporous alumina only affords the growth of SWNTs with a relatively wide chirality distribution, highlighting the importance of the metal-support interaction in catalytic CVD synthesis of SWNTs. The resulting SWNTs, with their precisely controlled chirality distribution, enable the high-purity separation of single-chirality SWNTs, thereby opening up exciting possibilities for advanced applications in the field of SWNTs.

Keyword: Single-walled carbon nanotubes; Chirality selective; Bulk synthesis; Catalyst design

最终交流类型: Invited

The Principle and application of carbon nano cold cathode X-ray technology

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Carbon nanotubes are a new type of carbon material that consists of single-layer or multi-layer graphite sheets curled into a tubular structure, with a diameter from several to tens of nanometers. These tubular fibers also vary widely in length, from a few micrometers to several centimeters. The aspect ratio (length/diameter) of carbon nanostructures is very large, making carbon nanotubes the most ideal material for electron field emission.Multi-structured carbon nanotubes are especially suitable for electron field emission, which can provide a powerful and stable electron flow, and make one of the important applications of cathode field emission X-ray. The cold cathode X-ray technology generates X-rays from the cold cathode electron source of carbon nanostructure (CNX), which releases electrons from the CNX tip to bombard the target. Due to the particularity of carbon nanostructures, the cold cathode electron source can instantly excite a stable electron beam at room temperature and in a weak electric field. Cold cathode X-ray tubes have incomparable advantages over hot cathode tubes, such as fast instantaneous response, low power consumption, small size, light

weight, easy protection, and long life. In 2011, the smallest cold cathode X-ray machine (tube voltage65kV, tube current1mA, focus 0.5mm) was successfully developed in the world, weighing 1.8kg, using only one AA battery to continuously shoot more than 100 X-ray films without special protection, so far used normally. In recent years, more than ten kinds of cold cathode X-ray products have been developed, including wireless minicomputer, high-energy minicomputer, portable tomographic imagers, self-propelled cable detector, and subminiature CT, which have been applied to power cables, nuclear power pipelines, power plant pipes, aerospace and other fields. Also, medical X-ray diagnostic equipment and security inspection equipment have been developed. The cold cathode X-ray source currently developed has a maximum tube voltage of 200kv and a maximum tube current of 30mA, and adopts two insulating packaging methods: solid seal and oil seal.

Keyword:Carbon nanotubes; Cold cathode X-ray; Electronic source

最终交流类型: Invited

Gas Adsorptions on Carbon Nanotubes: Theoretical Investigations and Field Emission Gas Sensing Applications

董长昆
Wenzhou University

The structural and electronic properties of various types of carbon nanotubes (CNT) with different gas atoms and molecule are investigated theoretical by first-principles density functional theory and experimentally by the field emission energy distribution (FEED) measurement. With molecular and atomic hydrogen, oxygen and nitrogen adsorptions on vacancy defects, the defective CNT shows the half-metal properties, but molecular chemisorption could convert the electronic property to semiconductor. The physisorption of H2 is unstable for the endothermic process, while the weaker nitrogen chemisorption is able to keep oxygen away from adsorbing as the protective agent. CNT work function drops with chemisorptions of molecular or atomic hydrogen, while oxygen behaves opposite. The adsorption of atomic nitrogen may fill in the missing carbon atom to “repair” the defect and reduce the work function by 0.83 eV. Atomic O or N chemisorption could break C-C bond to form doping type structure. C-C bonds are weakened from H chemisorption, favoring hydrogen storage. There is a total amount of about 1.0 e charge transfer between N or O atom

and carbon atoms, and the catalytic activity is expected to be higher with N adsorption around the cap top. The work functions vary with the adsorption of different atoms. Work functions increase to above 5.0 eV with the adsorption of N and O, and drop below 4.8 eV for H adsorption. The FEED measurement confirmed the reductions of electron tunneling energy barriers in H2 and N2 ambiences.

For nitrogen-doped CNTs, the C-N bonds may break up with serious defects for high N concentrations of above 23.3 at.%. CNT remains metallic and the work function drops after doping due to the upward shift of Fermi level, leading to the increase of the electrical conductivity. Meanwhile, N doping enhances the oxygen reduction activity stronger than N adsorption because of higher charge transfers. Catalyst Ni or Fe embedment enhances the adatom-SWNT interactions significantly with the increases of the adsorption energies, and promotes further the work function reduction with H adsorption. The Bader charge transfer analysis implies that the cap possesses higher oxygen reduction activities than the tube, and the density of states analysis shows that Ni or Fe embedment deepens the C-adatom hybridizations.

Based on the field emission enhancement with gas adsorption on multi-walled carbon nanotubes (MWNT), an innovative low pressure gas sensing technique is developed accordingly. Hydrogen, nitrogen, and air pressures in the range of 10-3-10-7 Pa could be detected from the high cryatallinity MWNT field emitters. On the contrary, the defect MWNT emitter is applicable for the helium detection, attributed to the charge aggregation on defect carbon atoms after helium adsorption. Such miniature CNT sensors are promising for in-situ pressure and leak detections in compact space and vacuum electronic device applications.

Keyword: Carbon nanotube; Gas adsorption; Field emission; Pressure sensing; Helium detection

最终交流类型: Oral

Simultaneously Enhanced Mechanical and Thermal Properties of CNT Fibers by Raising Effective Tube Portion

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Although individual carbon nanotubes (CNTs) are superior to polymer chains on the mechanical and thermal properties, those of CNT fibers (CNTFs) remain inferior to the many advanced synthetic fibers. The degradation on CNTFs is believed to originate from the failure of embedding CNTs effectively in superstructures, that is, the alignment or compaction. Conventional techniques always resulted in a mild improvement of target properties while degrading others. In this talk, a double-drawing technique as well as an annealing method we developed will be discussed, which rearrange the constituent CNTs and enhance the interfacial interaction. Consequently, with the newly developed techniques, the mechanical and thermal properties of the resulting CNTFs can simultaneously reach their highest performances with specific strength ~3.30 N/tex, work of rupture ~70 J/g, and thermal conductivity ~354 W/(m·K) despite starting from low-crystallinity (IG:ID ~ 5) and thick raw materials. The processed CNTFs are more versatile than comparable carbon fiber, Zylon and Dyneema. In the end, with all the experimental evidence, we find that, despite of the known dependence of fiber properties on CNT alignment and stacking, new evidence of the load transfer efficiency on individual CNTs measured with in situ stretching Raman highlights the importance of (i) straightening of CNT bundles, which increases the proportion of effective bundles jointly sharing the load, and (ii) the higher barrier of slippage activation within bundles, which originates from the effective tube length increase within effective bundles.

The high performance with low-crystallinity CNTs demonstrates that the limiting feature of CNTFs is their mesoscale arrangement rather than atomic-scale vacancies. The resulting simultaneous optimization properties result in an attractive overall performance, continuing the impressive line of improvement seen within CNTFs worldwide in recent years. We anticipate further advancement in material properties using the double-drawing technique, which is applicable to other CNT ensemble, including forests, films, fibers, and aerogels.

Keyword: carbon nanotubes; fibers; mechanics; thermal conductivity; strength

最终交流类型: Invited

Synthesis of a Monolayer Fullerene Network

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Each discovery of new carbon materials, such as fullerenes, carbon nanotubes, graphene and graphyne, has always triggered a research upsurge. However, due to lack of effective and reliable synthesis methods, the preparation of new carbon materials has been a great challenge.

We prepared a new single-crystal 2D carbon allotrope, namely monolayer quasi-hexagonal-phase fullerene (C60), with a large size via a technique of combination of bottom-up and top-down. By adjusting the ratio of magnesium to C60, two closely aligned magnesium intercalated polymer single crystals, quasi hexagonal (qHP) and quasi tetragonal (qTP) phase, were synthesized through a facile reaction at atmospheric pressure. Using an organic cation slicing strategy, monolayer polymeric C60 was exfoliated from the quasi-hexagonal bulk single crystals, along with few-layer polymeric C60 from the quasi-tetragonal bulk single crystals. Both atomic-scale 2D polymeric C60 materials exhibit high crystallinity and a unique topological structure. Characterizations of single crystal X-ray diffraction and scanning tunneling electron microscopy show that adjacent C60 is connected by carbon-carbon bridged single bond and [2+2] cycloaddition bridged bond in one layer of qHP C60, forming a new two-dimensional topological structure. In contrast to graphene and free C60, the monolayer qHP C60 has been shown to be a semiconductor with a band gap of about 1.6 eV and has promising applications in 2D electronic and optoelectronic devices. Good thermodynamic stability was also demonstrated in the monolayer qHP C60 demonstrates. In addition, due to the asymmetric structure, the monolayer qHP C60 has remarkable in-plane anisotropy and other excellent properties, and is expected to have potential applications in the fields of nonlinear optics and functional electronic devices. Moreover, the unique conjugated system, lattice and porous skeleton structure all make such new carbon material potentially suitable for applications in superconductivity, quantum computing, spin transport, energy storage and catalysis.

This research adds a new member to the family of carbon materials. The method of constructing two-dimensional topological structure using zero dimensional clusters provides a new prospect for exploring new carbon materials.

Keyword: carbon materials, fullerene, two dimensional materials, polymeric fullerene, semiconductor

最终交流类型: Invited

Reconfigurable Low-Dimensional Field Effect Devices

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As the silicon-based field effect transistor (FET) approaches its fundamental physical limit, the semiconductor industry will enter the post-Moore era, in which a reconfigurable field effect device could enable more complex functions in a less complicated circuit. Low-dimensional materials, such as carbon nanotubes (CNTs) and two-dimensional (2D) materials, have demonstrated great promise for future electronic devices because of their excellent gate electrostatics and high mobility. [1,2] Adding to these superior properties, we have recently found more interesting traits that are perfect for constructing reconfigurable devices. One example is the reconfigurable CNT barristor, realized by asymmetrically modulating the Schottky barrier in a CNTFET utilizing a drain-induced self-gating effect. [3] The CNT barristor works as a rectifier, reconfigurable for a forward rectifying mode or a backward rectifying mode by applying an appropriate voltage on its global gate. Another example of the reconfigurable CNT device is a mixed-dimensional CNT-MoS2 FET, realized by constructing a heterostructure between an individual semiconducting CNT and a MoS2 sheet. [4] The device shows a gate-controllable reconfigurability that can be set as a n-n junction, a p-n diode, or a band-to-band tunneling (BTBT) transistor. For constructing better 1D-2D hybrid devices using 2D semiconductor channels, we have explored the potential of using 1D semimetallic CNTs as nanoscale electrodes, and quantitatively studied the behavior of semimetal-semiconductor (Sm-S) contacts. We found that the contact-induced Fermi-level shift in semimetal greatly modulates the electrical contact behavior between 1D semimetal CNTs and 2D semiconductors. [5,6] A reconfigurable WSe2 transistor with semimetal CNT contacts exhibits excellent ambipolar transfer characteristics and abundant reconfigurable functions: as an FET, its threshold voltage is reconfigurable; as a diode, it can work in p-p, p-n, n-p or n-n regimes under different gate voltage. [7] These reconfigurabilities of low-dimensional devices may provide a clue for future design of practical reconfigurable devices and circuits.

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Keyword:reconfigurability, carbon nanotube, 2D material, 1D-2D heterostructure, semimetal-semiconductor contact

最终交流类型: Invited

On-surface construction of organic structures enabled by dopants

黄立

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On-surface chemistry has become a quickly developing field and provides an important route for synthesizing complex organic compounds benefiting from extraordinary controllability over the reaction process. By introduction of certain dopants in specially-designed precursors, specific reaction sites could be activated for the formation of novel organic structures. Here, we present such controllable reactions with the help of N or S dopants. (1) We demonstrate the selective activation of four quasi-equivalent C-H bonds in a specially-designed nitrogen-containing polycyclic hydrocarbon (N-PH) on Ag(100). Experimentally depositing N-PH on Ag(100) followed by a sequential-annealing process reveals the hierarchical dehydrogenation of the four C(sp3) atoms through non-contact atomic force microscopy. Further annealing leads to the formation of N-doped graphene nanoribbons with partial corannulene motifs. Density functional theory calculations of the vibrational modes of N-PH molecule reveal that the four ortho C(sp3) atoms in the N-heterocycles are more active than the other C(sp2) atoms. The adsorption of N-PH on Ag(100) further differentiates the activity of the four C(sp3) atoms into two groups, resulting in a hierarchical dehydrogenation. Our work provides a new route of designing precursor molecules with ortho C(sp3) atom in a N-heterocycle to realize surface-induced selective dehydrogenation in quasi-equivalent sites. (2) We show the construction of vinylene linkage by direct connection of methyl groups with the help of S dopant. Based on specially-designed monomers containing ortho methyl thiophenes, we successfully achieved the building of vinylene linkages via selective C-H bond activation in methyl groups on gold surfaces. Non-contact atomic force microscopy studies verify the vinylene linkage by bond-resolved imaging. Further density functional theory calculations and control experiments reveal that the strong interactions between S dopant and the gold surface decrease the energy barrier of the methyl C-H dissociation, which leads to selective C-H activation and the formation of

C=C bond linked polymers. Our work provides a novel method to selectively active methyl C-H bonds to achieve carbon double bond polymerization.

Keyword： selective C-H activation, on-surface synthesis, graphene nanoribbons, non-contact atomic force microscopy, scanning tunneling microscopy

最终交流类型: Invited

Pressure-Induced Phase Transitions of Group IVA Elements

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In the periodic table, the elements of the IVA group such as C and Si can form a variety of chemical hybrid bonds due to their special electronic configuration (s2p2) in outer shell, and then show the rich allotropic structures, including zero-dimensional fullerene, and three-dimensional graphite and diamond. Due to the significant difference in chemical structures, a variety of novel physical properties of IVA elements have attracted intensive attentions. However, their internal correlation, mutual transformation and physical mechanism between these different allotropes of carbon or silicon are still unresolved, and there are still many fundamental and scientific issues worthy of further research efforts. Herein, this work focuses on pressure-induced phase transitions of the most common elements in the IVA group, such as C and Si, as shown in Figure 1. Using diamond anvil cell to apply ultrahigh hydrostatic pressure and laser heating technology, the controlled transformation from carbon-based graphite to ultra-thin diamond is realized. In principle, the final thickness of ultrathin diamond should ideally depend on the layer number of graphene. The characteristic Raman vibrational modes and high-resolution transmission electron microscopy images with high signal-to-noise ratio were further obtained, and the controlled preparation and luminescence characteristics of NV-, NV0 and SiV- color centers in ultrathin diamond structures were explored as well. In the Si system, many novel phases displayed under extreme conditions, including the metallic Si-II, Si-XI, and the semiconducting Si-XII, Si-IV and Si-III. By optimizing the pressure and temperature conditions, the ratio of Si-III to Si-XII are quantitatively modulated through the kinetic strategy. In addition, the pure Si-IV phase was obtained after elongating the decompression period. These experimental methods and achievements can offer the significant insights to develop novel phases of functional

nanomaterials, and further explore their potential applications in nanodevices and nanomechanics.

Keyword: IVA elements, phase transitions, diamond anvil cell, allotropy

最终交流类型: Invited

A study on the controlled growth mechanism and manipulation of carbon nanotubes by in situ TEM

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Due to their tiny size, high growth temperature and complex growth environment, it has been quite difficult to reveal the growth mechanism of carbon nanotubes (CNTs) accurately. Here we study the growth process and mechanism of CNTs under near-atmospheric pressure by using an in situ transmission electron microscope (TEM) method. When cobalt was used as a catalyst, we found that orthorhombic Co3C phase nanoparticles remained unchanged during CNT growth. We further studied the growth of single-wall CNTs (SWCNTs) from a high melting-point CoW alloy catalyst, and the active catalytic phase was identified as a cubic η-carbide phase. When truncated octahedral Pt nanoparticles were used as a catalyst, we found that the graphene layers were initially formed preferentially on the (111) surfaces, which further joined together to form an annular belt and a hemispherical cap followed by the elongation of the SWCNT. Based on the observations, an annular belt assembling nucleation model was proposed.

We further demonstrate that the local chirality and electronic property of a CNT can be changed by in situ TEM manipulation. Upon heating and mechanical strain applied, a transition trend toward a larger chiral angle region was observed and explained in terms of orientation-dependent dislocation formation energy. A metal-to-semiconductor transition was realized to create nanotube transistors with a semiconducting nanotube channel covalently bonded between a metallic nanotube source and drain.

Keyword： Growth mechanism, nucleation, Manipulation, Carbon nanotube, in situ TEM

最终交流类型: Keynote

Designer graphene nanostructures with non-trivial electronic and magnetic properties

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National University of Singapore

Imprinting magnetism and non-trivial topology and harnessing their interplay in graphene nanostructures create a significant paradigm shift in realizing non-trivial collective quantum behaviors and exotic quantum phases in low-dimensional organic quantum materials. Recent advances in on-surface synthesis have made it possible to fabricate these atomically precise graphene quantum nanostructures with exotic electronic and magnetic effects from the on-surface bottom-up synthesis approach, while also characterizing them at the sub-molecular resolution. During this talk, I will highlight the versatility of this on-surface synthetic strategy, showcasing highly correlated magnetic graphene quantum nanostructures [1-3], molecular superlattices with flat electronic bands [4], and organic quantum corrals with topology-controlled quantum resonance states [5]. We then employed bond-resolved scanning tunneling microscopy and spin excitation spectroscopy to unambiguously resolve the molecular backbone and reveal the strongly correlated open-shell characters in these graphene nanostructures. Furthermore, we demonstrate that the nickelocene magnetic probe can sense highly correlated spin states in nanographene. The ability to create such atomically precise molecular quantum materials with strong electronic and spin correlations not only presents exciting opportunities for realizing non-trivial quantum magnetism and electronic phases in organic materials, but also marks an essential step towards the realization of high-density, ultrafast spintronic devices, and quantum information technologies

Keyword：Strong correlation, spin entanglement, on-surface synthesis, STM/AFM, graphene nanostructures

最终交流类型: Invited

The past, present and future of carbon nanocages

胡征
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The past, present and future of carbon nanocages

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In the past 40 years, fullerene, one-dimensional carbon nanotubes, two-dimensional graphene and graphdiyne have been discovered, and nanocarbon materials have become one of the most concerned frontier fields today. Our research group has long been committed to the physical and chemical research of energy nanomaterials, and has long-term accumulation in the design and energy application of new nanocarbon materials, especially in the research of mesoscopic carbon nanocages. Mesoscopic carbon nanocages are becoming a new platform for developing advanced energy conversion and storage functions due to the characteristics of microporous-mesoporous-macroporous connectivity, efficient coordinated transportation of materials/charges, and efficient utilization of active species. This lecture will focus on: (1) the preparation science of carbon nanocages, (2) the construction of supported catalysts (from highly dispersed to single atoms) and confined catalysts with nanocages or applied as metal-free catalysts for energy conversion, (3) the application of nanocages as electrode materials for energy storage (supercapacitors, lithium-sulfur batteries, etc.), and (4) the opportunities and challenges faced by carbon nanocage research.

Keyword： carbon nanocages， meso-structured, energy conversion and storage

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最终交流类型: Keynote

Growth and Application of 1D van der Waals Heterostructures Based on Single-Walled Carbon Nanotubes

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Single-walled carbon nanotubes (SWCNTs) with diverse optical and electronic properties (metallic or semiconducting) depending on chiral indices (n, m) have been the critical nano-material in nanoscience and nanotechnology[1]. The controlled modulation of properties can be possible either by employing the inner space of the SWCNTs to encapsulate various materials or by externally wrapping the SWCNT template with additional atomic layers [1]. Here, the latter case is discussed as a one-dimensional (1D) van der Waals (vdW) heterostructure based on SWCNT [2].

A typical 1D vdW heterostructure is composed of SWCNT, boron nitride nanotube (BNNT), and molybdenum disulfide nanotube (MoS2NT), coaxially grown by serial chemical vapor deposition (CVD) steps [2,3]. We can also remove SWCNT from SWCNT@BNNT by a gentle oxidation process [3]. By comparing the optical properties of BNNT@MoS2NT and SWCNT@BNNT@MoS2NT, we found strong photoluminescence (PL) from monolayer MoS2NT and quenching of PL by coupling to SWCNT through thin BNNT [4]. The prominent population of free charges and inter-tube excitons is proved by ultrafast optical spectroscopy [5].

In order to study the pristine optical and device properties, micro-meter long 1D vdW heterostructure SWCNT@BNNT@MoS2NT is prepared between Si pillars [6]. After transferring to a custom-made TEM grid, we can study optical properties and TEM characterizations from the same hetero nanotube. After transferring to SiO2 substrates and lithographically fabricating metal electrodes, we examined various device characteristics. The naturally p-doped SWCNT and n-type MoS2NT become a radial semiconductor–insulator–semiconductor (S-I-S) tunneling heterojunction diode [6]. We can expect various devices from 1D heterostructure based on SWCNTs such as field-effect transistors (FET) and photovoltaic devices [7].

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Keyword： Single-walled carbon nanotubes, One-dimensional heterostructure, van der Waals heterostructure, CVD growth, Optoelectronic device

最终交流类型: Keynote

Electrical control in the chemical vapor deposition synthesis of carbon nanotubes and graphene

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MIT

Chemical vapor deposition (CVD) is widely used for the efficient growth of low dimensional materials. Typically, the synthesis parameters such as gas flow rate, temperature, pressure etc. are being optimized in order to achieve desirable results such as high-quality materials. Up to now, gas phase electro-chemical reactions have not been widely considered in CVD. In this talk, our explorations of using applied voltages to control the CVD synthesis results will be presented. We have found that applying an electric field between the copper substrate and a counter electrode has significant impacts on the growth of graphene. Electrochemical effect and ionic collision effect are observed in different conditions. Switching electric field can also be used to twist the chirality of carbon nanotubes. It is anticipated that electrical control during CVD synthesis could open up new ways to assist the synthesis of low dimensional materials in the future.

Keyword:electrical control, carbon nanotube, graphene

最终交流类型: Oral

Surface functionalization of vertical graphene significantly boosts the energy storage capability for symmetric supercapacitors

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江西师范大学

Vertical graphene (VG) sheets, which consist of few-layer graphene vertically aligned on the substrate with three-dimensionally interconnected porous network, make them become one of the most promising energy storage materials, especially for supercapacitors. Nevertheless, the intrinsic hydrophobic nature of pristine VG sheets severely limited its application in aqueous supercapacitors. Here electrochemical oxidation strategy is adopted to increase the hydrophilicity of VG sheets by introducing oxygen functional groups so that the aqueous electrolyte can fully be in contact with the VG sheets to enhance charge storage performance. This work demonstrated that the introduction of oxygen functional groups not only greatly improved the hydrophilicity but also generated a pseudocapacitance to increase the specific capacitance. The resulting capacitance of electrochemically oxidized VG for 7 min (denoted as EOVG-7) exhibited three orders of magnitude higher (1605 mF/cm2) compared to pristine VG sheets. Through assembled two EOVG-7 electrodes, a symmetric supercapacitor demonstrated high specific capacitance of 307.5 mF/cm2, high energy density of 138.3 μWh/cm2 as well as excellent cyclic stability (84% capacitance retention after

10000 cycles). This strategy provides a promising way for designing and engineering carbon-based aqueous supercapacitors with high performance.

Keyword: vertical graphene, electrochemical oxidation, surface functionalization, areal specific capacitance, symmetric supercapacitors

最终交流类型: Invited

On-surface Synthesis of Tetraphenylethylene Macrocycles Exhibiting Extended Conjugation

Nian Lin
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Creating conjugated macrocycles has attracted extensive research interest because their unique chemical and physical properties, such as conformational flexibility, intrinsic inner cavities and aromaticity/antiaromaticity, make these systems appealing building blocks for functional supramolecular materials. Here, we report the synthesis of four-, six- and eight-membered tetraphenylethylene (TPE)-based macrocycles on Ag(111) via on-surface Ullmann coupling reactions. The as-synthesized macrocycles are spontaneously segregated on the surface and self-assemble as large-area two-dimensional mono-component supramolecular crystals, as characterized by scanning tunneling microscopy (STM). We propose that the synthesis benefits from the conformational flexibility of the TPE backbone in distinctive multi-step reaction pathways. Combined in-situ spectroscopic and computational analysis identifies extended conjugation in the macrocycles. Interestingly, macrocycles undergo structural symmetry breaking which realigns the frontier molecular orbitals. This study opens opportunities for exploring the electronic properties of TPE-based macrocycles.

Keyword: on-surface synthesis, macrocycle, extended conjugation, STM

最终交流类型: Invited

Silk-Nanocarbon Hybrid Fibers/Textiles for Smart Wearables

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清华大学

Flexible and wearable electronics are attracting wide attention due to their potential applications in wearable human health monitoring and medical care systems. It is of great importance to explore low cost and scalable preparation approaches for high performance flexible and wearable electronics. Nanocarbon materials have combined superiorities such as good electrical conductivity, intrinsic and structural flexibility, light weight, high chemical and thermal stability, ease to be chemically functionalized, as well as potential mass-production, enabling them to be promising candidate materials for flexible and wearable electronics. Besides, silkworm silk, with five thousand years’ usage history, is a popular natural material for clothes or wearing accessories. We have been working on the rational design and controlled fabrication of flexible electronics based on silk, carbon nanotubes and graphene materials towards applications in human health monitoring and human-machine interfaces. In this talk, I will introduce our work on combing nanocarbons with natural silk materials to produce E-fibers/textiles. We realized the fabrication of silk-nanocarbon based fibers, inks and textiles and studied their performance in wearable physical and chemical sensing for health management. The applications of the obtained materials and devices in human health monitoring, human motion tracking, and human-machine interfaces were demonstrated. We hope these efforts may promote the development of next generation high performance and biocompatible smart wearables, and may also help to extend the application of silk materials from traditional textile industry to next-generation smart textiles.

Keyword: Nanocarbon, Silk fibers, Electronic fibers/textiles, Smart wearables, Health management

最终交流类型: Oral

CORRELATING THE ATOMIC STRUCTURE OF SOLID CATALYSTS TO THE NUCLEATION AND GROWTH BEHAVIOR OF SINGLE-WALL CARBON NANOTUBES BY ENVIRONMENTAL TEM

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Solid catalysts with high melting point and specific shape or symmetry have been considered to be effective for the structure-controlled growth of single-wall carbon nanotubes

(SWCNTs). However, the key roles of the catalysts on the nucleation mode and growth kinetics of SWCNTs have rarely be evidenced experimentally, because of the small dimensions of SWCNTs and catalyst nanoparticles and the complex catalytic growth environment. Here we report the unconventional nucleation and growth behaviors of SWCNTs from two kinds of solid catalysts by means of close-cell environmental transmission electron microscopy (TEM)[1, 2]. The active catalytic phase of Co-W-C alloy catalyst was investigated and precisely identified as a cubic η-carbide phase. We have also in situ observed the catalyst-tube interfacial dynamics during CNT growth, demonstrating an undefined orientation dependence for the solid catalyst (Fig.1). Using a truncated octahedral Pt catalyst, we have studied the atomic-resolved nucleation process of SWCNTs under atmospheric pressure and proposed an annular belt assembly nucleation model. Finally, possible chirality control strategies are proposed for SWCNTs based on the above in-depth growth mechanism understandings from high melting point alloy and well-faceted catalysts.

Keyword: carbon nanotube, growth mechanism, in situ TEM, alloy catalyst

最终交流类型: Oral

Designing composite lithium anodes for solid-state batteries

赵辰孜
清华大学

Solid-state lithium batteries are viewed as one of the most viable future technologies, with enhanced safety and energy density characteristics compared to the conventional lithium-ion batteries. However, the solid-state lithium batteries still suffer from the limited cycle life and uneven Li electrodeposits. The stable cycling of energy-dense solid-state batteries is highly relied on the kinetically-stable solid-state Li alloying reactions. The Li metal precipitation at solid–solid interfaces is the primary cause of interface fluctuations and battery failures. In this talk, we introduce the composite lithium anode as a model system to quantify the Li kinetics evolution and transition from the alloying reaction to the metal deposition in solid-state batteries, identifying that there is a carrier transition from Li atoms to Li vacancies during lithiation processes. And the rate-determining step is charge transfer or Li atom diffusion at different lithiation stages. Accordingly, we design a high-performance solid-state lithium battery with carbon-reinforced ionic-electronic composite anodes. When the interconnected carbon is compounded with a sulfide-based solid electrolyte, a three-dimensional electron-ion conduction network can be achieved, affording a large number of sites and scalable spaces for the lithium diffusion, nucleation and growth. The composite layer can achieve a long cycle life (> 5000 times) and stable electrochemical plating with a high areal capacity (> 8 mAh cm−2). The application of high-areal-capacity (4 mAh cm−2) pouch cell provides an efficient and effective strategy for practical solid-state lithium batteries.

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Keyword: Solid-state batteries, lithium metal anodes, carbon-based anodes, solid–solid interfaces, pouch cells

最终交流类型: Invited

Interface Design for Stable Lithium Metal Anode

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北京理工大学

Lithium metal anodes has been placed great expectations on as a promising anode candidate for next-generation energy storage systems, such as such as lithium–sulfur, lithium–air, solid state batteries. However, the unstable interfaces between lithium anode and electrolyte definitely induce the undesired and uncontrollable growth of lithium dendrites, which results in the stable hazards and limited cyclic life of the rechargeable batteries.

Several strategies have been proposed herein towards the construction of interface for dendrite-free and stable lithium metal anode. First, in-situ chemical/electrochemical reactions has been applied to built on lithium meal anode a stable solid electrolyte interphase (SEI). Both the chemical compositions of the SEI and their spatial distributions have shown tremendous influence on the stability of lithium metal interface. On the other hand, artificial interface design based on polymer matrix have been explore as well. The general idea is to utilize both the properties of rigid inorganic components and the soft organic components, and realize the rational design of functional composite interface for lithium metal anodes. The composite electrolyte interface with tunable mechanical properties and enhanced lithium ion transportation properties benefit the uniform plating of lithium metal anodes.

Keyword:lithium metal anode, carbon composite anode, solid electrolyte interphase

最终交流类型: Invited

Interlayer Drag Effects in Graphene-based Electronic Double-layer Systems

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中国科学技术大学

A closely spaced but electronically isolated electronic double-layer system is fascinating to study interlayer quasiparticle interactions and to reveal intriguing interlayer correlated states. Recent progresses in the development of graphene and other two-dimensional (2D) electronic systems have sparked renewed interest in the field of strong interlayer interactions and corresponding novel quantum phases. In particular, the highly tunable electronic properties of constituent 2D layers, together with the accessibility of ultra-small interlayer separation, enable the investigation of the drag effect in previously inaccessible strong-coupling regimes.

In this talk, I will present our recent work on the interlayer drag experiments in several graphene-based electronic double-layer systems, including: 1) Revealing a fingerprint feature of drag effect between massless and massive fermions in heterostructures consisting of monolayer graphene and bilayer graphene separated by hBN spacer [1]. 2) Discovery of a new type of quantum interference effect in inter-layer Coulomb drag, with the interference pathway comprising different carrier diffusion paths across the two constituent graphene layers [2]. 3) Demonstration of a giant and highly-tunable drag effect between graphene and superconducting LaAlO3/SrTiO3 heterointerface, and a brand-new Josephson-Coulomb drag mechanism is proposed to account for such effect, rooting in the interactions between the substantially enhanced dynamical quantum fluctuations of the superconducting phases in Josephson junction arrays and the normal electrons [3]. Our findings establish a novel platform, i.e., electronic double-layer systems, to exploit novel inter-layer quantum effects, and offer unforeseen opportunities for new-principle electronic devices.

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Keyword: Interlayer drag effects, Interlayer quantum interference effect, Josephson-Coulomb drag

最终交流类型: Invited

Milligram-scale production and photoelectrical property detection of single-chirality carbon nanotubes

刘华平

中国科学院物理研究所

Single-wall carbon nanotubes (SWCNTS) are considered as ideal materials for the fabrication of high-performance electronic devices in the post-molar era due to their extremely high carrier mobility, tunable band gap and nanoscale size. However, even slight difference in the structures of different SWCNTs induces huge difference in their optical and electrical properties [1-3]. The mixture structure of the as-grown SWCNTs hinder their applications in device applications. Therefore, mass production of single-chirality SWCNTs have long been the goal in SWCNT area. However, the large-scale preparation of single-chirality SWCNTs, both growth and separation, still faces great challenges.

Most recently, we found a simple, yet effective, method to increase the yield of gel chromatography separation of single-chirality SWCNTs by enabling significantly higher concentrations of raw nanotubes solution. With this technique, milligram-scale separation of multiple single-chirality SWCNTs have been achieved. To increase the concentration of SWCNTs, we developed a strategy for dispersing a highly concentrated individualized SWCNT solution by redispersion, in which the SWCNT solution was first ultrasonically dispersed, followed by ultracentrifugation and reultrasonic dispersion. With this technique, the dispersible initial concentration of SWCNTs increased from 1 to 8 mg/mL, and the corresponding concentration of the resulting individualized SWCNT solution increased from 0.19 to ~1.02 mg/mL [4]. In combination with the binary surfactant system [5], the separation yields of multiple single-chirality species, including (6, 4), (6, 5), (11, 1), (7, 5), (7, 6), (8, 3), (8, 4) and (9, 1), were increased by approximately six times to the milligram scale in one separation run with gel chromatography, reaching milligram scale. We further explored the structural dependence of photoelectronic properties of SWCNTs, and found that their optical and electrical properties depend on their chiral structures, which is rooted in the difference of their bandstructures [1].

Keyword: Carbon nanotubes; single chirality; purification and separation; electrical properties

最终交流类型: Invited

Graphene Epitaxy: from Misorientation-Free to Misorientation-Engineered Graphene Films

孙禄钊
Beijing Graphene Institute, China

Chemical vapor deposition (CVD) is considered the most promising method, and great progress has been achieved over the last decade. Currently, this field is being pushed to new heights that pursuit structure control (e.g. orientation, layer, stacking order, contamination, doping, etc.) and low-cost production (e.g. increasing the production capacity and growth rate)1,2. In this talk, I will introduce our recent works on controlled growth of high-quality graphene films via CVD approach, especially on controlling the crystallographic orientation of graphene. By designing and preparing single-crystal Cu(111) foils, we have opportunities in realizing the epitaxial growth of large-area single-crystal misorientation-free graphene film3. We designed and constructed a pilot-scale CVD system suitable for producing A3-size graphene films, which works well and output high-quality graphene films with high capacity. In another hand, we explore the possibility on controlling the layer number and stacking order, which is motivated by the emerging twistronics. Here I will present our state-of-the-art hetero-site nucleation method for growing twisted bilayer graphene (tBLG)4. Gas-flow perturbation and switching of the graphene edge termination play crucial roles in triggering the formation of interlayer twist. We also established a slip-line-guided growth principle to explain and predict the crystal orientation distribution of graphene on a variety of metal facets, further enabling the controllable synthesis of single-crystal graphene and grain boundary engineering of bi-crystal graphene on designed metal facets5, which opens a new avenue for

manipulating the crystal orientations, grain boundary structures, and even twisted angles of bilayer 2D materials in a bottom-up manner.

Keyword: Graphene, Chemical vapor deposition, orientation control, single crystal

最终交流类型: Invited

Investigating the magnetism in surface-supported metal-organic frameworks by scanning tunneling microscopy

王炜华
中国科学院物理研究所

In metal-organic frameworks the transition-metal atoms are accommodated in ligand fields with identical spatial symmetry and bonding configuration, which dictates the charge, orbital and spin of the transition-metal atoms. Therefore, surface-supported metal-organic frameworks provide us platforms to manipulate the electronic and magnetic properties of single transition-metal atoms and to explore the novel physical properties of metal-organic frameworks by scanning tunneling microscopy (STM).

We have prepared Ni-TPyP frameworks with dinuclear coordination centers on Au(111) substrate by self-assembly, in which each dinuclear coordination center consists of two Ni atoms sitting above (denoted as top-Ni) and below the molecular plane. The spatial distributions of the nonbonding and antibonding orbitals associated with the top-Ni atoms are revealed by dI/dV maps, and their energy separation, the ligand-field splitting parameter, is directly measured by STM [1]. We further manipulated the electronic and magnetic properties of top-Ni atoms by hydrogen adsorption. Specifically, by fitting the spin-flip spectra in a vertical magnetic field, we find the spin state of top-Ni atoms is tuned from $S = 1/2$ to $S = 1$ by attaching one H atom and $S = 3/2$ by attaching two H atoms [2]. This work demonstrates atomic-scale control over the electronic and magnetic properties of coordinated metal atoms in a surface-supported MOF.

We also report a new strategy to prepare high-quality early-transition-metal-based conjugated metal-organic frameworks on metal surfaces. As revealed by low-temperature STM, while deposition of Cr atoms and 2,3,6,7,10,11-hexaaminotriphenylene precursors produces irregular branches, crystalline $Cr_3(HITP)_2$ frameworks are obtained by substituting Cr atoms for Ni atoms in $Ni_3(HITP)_2$ or $Fe_3(HITP)_2$ templates on Au(111) substrate [3]. The $Cr_3(HITP)_2$ framework shows a flat-band state near the Fermi level that shifts to higher energy with an increased magnetic field. These results are explained by negative orbital magnetism associated with the flat band with a non-zero Chern number.

Keyword: metal-organic framework, scanning tunneling microscopy, spin, conjugation, flat band

最终交流类型: Keynote

Graphene Industry: Synthesis Determines Its Future

LIU ZHONGFAN
Peking University

With 19 years history of graphene materials, there still exist lots of technical challenges towards graphene industry, including: 1) Low-cost mass production technology; 2) Batch peeling-transfer technology; 3) Transition from single-layer graphene component to macroscopic materials with retained intrinsic performances; 4) Dispersing technology into matrix materials; 5) Irreplaceable killer applications. Beijing Graphene Institute (BGI), established in 2018 and currently having over 360 employees, aims to solve these challenging issues by paying particular emphasis to mass production of high-quality CVD graphene materials and manufacturing equipments. BGI is devoted to providing the best graphene materials and related equipments to the market as well as the graphene-related R&D services to enterprises.

The current R&D emphasis on CVD graphene materials at BGI is laid on three different directions: 1) high-quality graphene films and wafers for general purpose; 2) graphene-skinned materials (GSM); 3) purpose-oriented graphene materials focusing on thermal managements, electrothermal conversion and electromagnetic applications. The star products already put into market are A3-size graphene films with cm grain boundaries, 4- and 6- inch single crystal graphene wafers, superclean graphene films with best thermal and electrical performances, graphene-skinned glass & fibers, graphene-skinned aluminum oxide fibers, etc. The graphene-skinned glass fibers have been used for deicing applications with extremely high electrothermal conversion efficiency up to 94%. At BGI, we are also working for the customized graphene growth depending on the special needs and requests from customers. There is a great space in this area, which is particularly important before graphene films and wafers find their practical application market in next ten years.

Keyword: graphene

最终交流类型: Invited

Electronic transport properties of single clusters and molecules

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Nanjing University, China

Electrical transport is an important method for studying the physical effects of single clusters and molecules where we have made some initial progress: 1. We have reported the fabrication of a single-electron transistor device based on a silicon cluster connected to a gold break junction with a nanometer scale separation1. We can see a Coulomb blocking gap up to 300 meV, which has the potential to operate at room temperature. We also investigated the Zeeman effect of this silicon cluster and obtained a Landé g factor of 2.3, which is consistent with the theoretical prediction. 2. Based on the single-molecule electrical transport platform, we have also reported a Gd@C82 single-molecule electret2. A coercive field ~50 mV/A-1 causes the molecular system to switch between the two transmission channels, producing a ferroelectric hysteretic loop. Using density functional theory, we attribute these two states to permanent electric dipoles in two different directions generated by Gd atoms at two different locations within the C82 cage. The two dipoles are separated by a transition energy barrier of 11 meV. When the coercive force field provides the energy needed to overcome the transition barrier, the electric field can drive the dipole to reorient, resulting in a conductive switch. 3. Recently, we have tried to demonstrate an all-electrical solution by constructing the interferometer in a three-terminal single-molecule transistor (Fig. 1)3. A two-dimensional interference pattern composed of Fano and Breit-Wigner resonances is observed, unveiling and distinguishing different phases of the backbone and side channels. When substituting the side group with a single atom, the phase difference between the two channels at the Fano resonant energy decreases from ~70º to ~46º, which is consistent with a less pronounced backbone-side separation and reveals the sub-nanometre details of the molecules. All the observations are corroborated by density functional theory calculations.

Keyword: Electrical transport, single clusters, Zeeman effect, single-molecule electret, single-molecule interferometer

最终交流类型: Oral

Isomer/enantiomer-pure [60]bisPCBM for Organic Electronics

John Dennis
Xian Jiaotong-Liverpool University

The as-produced isomers mixture of [60]bisPCBM was purified into in individual 19 isomers, and the chiral isomers were separated into enantiomer pairs.

Single-enantiomer field-effect transistors showed the potential to discriminate CPL with a fast response time and a very high photocurrent dissymmetry factor (gph = 1.27 ± 0.06).

UV-Vis absorption spectroscopy and cyclic voltammetry reveal the HOMOs, LUMOs, and HOMO–LUMO gaps of the purified isomers vary from (-5.673 – -5.444 eV), (-3.901 – -3.729 eV), and (1.664 – 1.883 eV), respectively.

13NMR spectroscopy shows all 19 isomers are cyclopropafullerenes. Seven isomers have C1 molecular point-group symmetry, four are Cs, six are C2, one is C2v, and one is C2h. From a correlation between HPLC retention time and the relative positions of the addends enabled all isomers were unambiguously assigned to their respective HPLC fractions.

[60]bis-PCBM (major isomer) was employed in perovskite solar cells which achieve better stability, efficiency, and reproducibility than PCBM. [60]bisPCBM additionally resists moisture ingress and passivates pinholes. A PCE of 20.8% was obtained (cf PCBM 19.9%). The PCE of unsealed devices dropped by > 10% in ambient air after 44 d at 65 °C, and by 4% after 600 h under continuous full-sun illumination and maximum power point tracking indicating excellent stability.

The 19 isomers were also characterised by ultraviolet photoelectron spectroscopy, thermal gravimetric analysis, differential scanning calorimetry, single crystal structure analysis. Higher molecular symmetry yields higher crystallinity. Isomers with higher crystallinity tend to form a multi-crystalline phase giving increased energetic disorder and lower charge transport and photovoltaic performance than more amorphous isomers. Low dimensionality of charge transport seems also to associate with higher symmetry and crystallinity. As a result, the best transistors and photovoltaic devices are realised using more amorphous isomers.

These results represent a very substantial advanced in the knowledge of single isomer/enantiomer fullerene derivatives in organic electronics.

Keyword: Fullerenes, organic electronics, single-isomer, molecular characterisation, device characterisation

最终交流类型: Invited

Flexible Energy Storage based on Conjugated Carbon Nanomaterials

赵扬
Beijing Institute of Technology

The development of new energy storage devices is constantly exploring in the directions of scale diversification, lightweight flexibility and micro- and nano-integration. Carbon nanomaterials with conjugated structures can provide an ideal material platform for the further development of such devices. However, when the electrode structure is constructed with conjugated carbon-based materials as the basic element, the difference in the component mechanical properties of the components in the assembly structure will cause internal stress, resulting in covalent molecular skeleton fracture, molecular conformation transformation (such as bending, stretching or twisting) or intermolecular ordered structure collapse and other problems. This would lead the intramolecular and intermolecular electron transport path to be blocked, and then the performance of the energy storage device is reduced or even failed. Therefore, precisely regulating the internal stress of the conjugated carbon assembly structure and revealing the influence mechanism of stress dissipation on energy storage performance are of great significance for improving energy storage performance and stability and developing the next generation of flexible energy storage devices. Therefore, based on conjugated carbon materials, we carried out structural design of electrode materials at different scales of intramolecular, intermolecular, assembly microstructure and macroscopic interface, developed mechanical adaptation electrode interface, dynamic dissipation microstructure of internal stress, and normal internal stress models, and realized accurate regulation of electron transport characteristics of conjugated intramolecular, intermolecular and interface. The strain-activated in situ mechanism is explained, the construction of highly conductive and flexible electrode materials is successfully realized, and its application in flexible energy storage fields such as intelligent and biocompatible is explored. This report will describe our progress in multi-dimensional processing methods for carbon-based materials, patterned preparation, and new flexible energy storage devices.

Keyword: Conjugated carbon, Flexible, Energy storage

最终交流类型: Invited

Carbon Nanotube Electron Blackbody

姜开利
清华大学

An optical blackbody is an ideal absorber for all incident optical radiation, and the theoretical study of its radiation spectra paved the way for quantum mechanics (Planck’s law). Herein, we propose the concept of an electron blackbody, which is a perfect electron absorber as well as an electron emitter with standard energy spectra at different temperatures. Vertically aligned carbon nanotube arrays are electron blackbodies with an electron absorption coefficient of 0.95 for incident energy ranging from 1 keV to 20 keV and standard electron emission spectra that fit well with the free electron gas model. Such a concept might also be generalized to blackbodies for extreme ultraviolet, X-ray, and γ -ray photons as well as neutrons, protons, and other elementary particles.

Keyword: carbon nanotube; blackbody; electron blackbody; blackbody radiation

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最终交流类型: Invited

Precise Synthesis and Application of Single-Walled Carbon nanotubes

胡悦
温州大学

The array density and semiconducting selectivity of single-walled carbon nanotubes (SWNTs) are the major bottlenecks that limit their application in the field of nanoelectronics. The key to solving the real-world application of SWNTs in nanoelectronics is obtaining a high-density semiconducting SWNT horizontal arrays with a structurally uniform and mature fabrication process. This is also the challenging issue currently being researched in the control and preparation of SWNTs. Our goal is to prepare a high-density semiconducting SWNT horizontal arrays from a material preparation perspective, guided by the application of SWNTs in nanoelectronics, in order to solve the problem of their application in future nanoelectronic devices and computer chips. 1) By designing and regulating the catalyst efficiency, control preparation of high-density SWNT horizontal arrays has been achieved. 2) Based on the difference in selectivity between metal/semiconducting SWNTs, the controlled

preparation of semiconducting SWNT horizontal arrays and SWNT Schottky junctions was achieved through free-radical reactions.

Keyword: Single-Walled Carbon Nanotubes; Catalyst; Horizontal Array; High-Density; Semiconducting

最终交流类型: Invited

On-surface synthesis of carbon-nanomaterials and characterization using multi-domain scanning probe microscopy

王兵
University of Science and Technology of China

The rapid development of on-surface synthesis provides a powerful means for the accurate bottom-up design of carbon-based nanostructures, which opens the door to measure and control the carbon-based spin states for future quantum computing. Due to the complex and varied structures of carbon-based materials and their complicated interactions with the surrounding environment, it is urgently needed to develop a multi-domain characterization technique that can comprehensively probe the geometric, electronic, vibrational and spin state with chemical bond precision. Along this line, I will introduce our recent progresses in developing the joint tip-based STM-AFM-TERS method, which enables us to univocally determine the heterogeneities of pentacene species on surface (1), and reveal the intramolecular isotope effects (2). With this method, we have also revealed the unique spin states and topological states in several synthesized nanostructures, such as, the T-shape fused pentacene dimer with spin-vibration interactions, the tunable Kondo resonance the second-layer topological graphene nanoribbons (3), and wide bandgaps by embedding the periodic divacancies into graphene nanoribbons (4, 5).

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Keyword: Carbon nanoribbons; On-surface synthesis; Tip-based microscopic techniques; Isotope effects.

最终交流类型: Keynote

The macroscopic synthesis and applications of Fullerenes

谢素原
Xiamen University

Carbon ranks fourth in the total mass of all elements in the universe. It is widely distributed in the earth's crust, but its content in the crust is only ~0.027 wt%. There are a class of all carbon molecules, namely Fullerenes! The Fullerenes, including C60, C70 and other Cn (n^{3}20 but ^{1}22), were discovered by Kroto, Smalley and Curl in 1985 when they studied Interstellar dust. Because of the spherical cage structures that are subject to disorder in crystallographic identification, the most precise method to characterize Fullerenes so far is the X-ray diffraction analysis on the co-crystals of Fullerene guest and supermolecule host. This presentation will focus on the research about supermolecule host decapyrrylcorannulene (DPC) and its co-crystals with fullerene guests. This host-guest system with involvement of DPC facilitates the structural identification of a series of Fullerenes and their derivatives that have never been characterized heretofore. In addition, this presentation will introduce the synthesis and industrial production of Fullerenes, and the application of Fullerenes in organic electronics (organic and perovskite solar cells) and catalytic performances, exemplified by the electron acceptor of Fullerenes and selective hydrogenation by C60-Cu/SiO2 catalyst involving in a reaction of coal/syngas-to-ethylene glycol.

Keyword: Keyword: Fullerenes；The macroscopic synthesis；Organic electronics；Catalyst

最终交流类型: Invited

Precisely Engineering of the Electronic and Magnetic properties of Nano-graphene

蔡金明
昆明理工大学

The excellent properties of graphene predict its promising application prospects. We are committed to realizing the all-round development of graphene from the four aspects of education, research, production and application. In combination of ultra-high vacuum-molecular beam epitaxy-low temperature/variable temperature scanning probe microscope system and density functional theory, we explored the precise structure of graphene and its relationship with the electronic and magnetic properties at the atomic scale. Based on a profound understanding of the mechanism of graphene, we prepared highly oriented graphene thermal conductive film and aerogel by means of chemical synthesis. The prepared graphene thermal film has been applied to mobile phone terminals, the aerogel also shows excellent mechanical properties and adsorption characteristics, which can be used for sensor devices and adsorption materials.

Keyword: graphene, nanoribbon, band engineering, magnetic properties

最终交流类型: Invited

Precision Synthesis of Helicene-Based Chiral Nanographenes

王小野
南开大学

Chiral organic optoelectronic materials have attracted enormous interest in recent years because of their potential applications in information encryption, 3D display, bio-imaging, and quantum communication etc. Organic conjugated molecules with a helical structure are expected to become chiral optoelectronic materials with excellent performance due to their intrinsic helical chirality. However, such materials still face problems such as poor luminescent efficiency and low dissymmetry factors.

To address these problems, we first proposed that under the condition of maintaining the distribution of frontier molecular orbitals (FMO), chiral helicene-based nanocarbons with excellent luminescence properties can be obtained via the helical π-extension of highly luminescent chromophores.[1] We have therefore achieved a perylene-based chiral nanocarbon molecule with luminescent quantum efficiency of over 90%. Furthermore, we developed B,N-doped double helicenes via the helical π-extension of a highly luminescent B,N-doped polycyclic arene.[2] These new double helicenes exhibit a wide range of chiroptical responses in the visible light region, and the maximum absorption dissymmetry factor (gabs) reaches 0.033, which is the highest value in the visible region for helicene molecules. In addition, these molecules exhibit tunable circularly polarized luminescence properties and high photoluminescence quantum efficiencies of over 90% in the red-NIR region. These results provide new ideas for the future design of chiral organic optoelectronic materials.[3]

Keyword: nanographene, helicene, optoelectronic materials

最终交流类型: Oral

HORIBA Raman spectroscopy application in the field of carbon material analysis

王春阳
HORIBA

Raman spectroscopy, as a fast, nondestructive, high-resolution spectroscopic characterization technique, is an important tool for studying the lattice structure, fundamental electronic and phonon properties of materials and related device structures and properties. Raman spectroscopy is widely used to characterize various carbon materials such as pyrolytic graphite, graphene, carbon nanotubes, etc. It can provide information on defects, crystal disorder, edge structure, stress, doping, graphene layers, carbon tube diameter, and metallic semiconductivity. This presentation will introduce the application examples of HORIBA Scientific Raman spectroscopy technique for carbon material characterization.

Keyword: Raman, carbon material, SHG

最终交流类型: Invited

Gold Extraction by Graphene and Its Reuse Exploration

苏阳
清华大学深圳国际研究生院

Gold is the most valuable element in e-waste. Currently, only less than 20% of e-waste has currently been recycled primarily for a lack of technologies with sufficient efficiency and economic viability to recover valuable elements within it[1-3], Therefore, developing materials capable of extracting gold from complex sources, especially electronic waste (e-waste), can turn the e-waste recycling challenge into a profitable business and provide an efficient solution for global gold sustainability. Here we report an exceptionally high gold extraction capacity of chemically reduced graphene oxide (rGO), reaching ~1.8 g/g when extracting gold from its 10 ppm solution at 25 oC, one order of magnitude higher than other reported gold adsorbents, and an ability to extract gold from ppt concentrations. During extraction, rGO reduces >95% gold ions to metallic gold, avoiding elution and precipitation necessary in post-adsorption processing. Moreover, this reductive adsorption of gold by rGO is found different from (predominately) electrostatic adsorption of other metal ions, hence, exploiting the protonation process of rGO, a precise gold extraction without adsorption of the other 14 elements normally present in e-waste is achieved [4]. Next, we explore the reuse of the extracted gold for highly efficient solar thermal water purification. Exploiting graphene's strong adsorption to the solar spectrum and the plasmonic photothermal effect of the recycled gold, the resulting recycled gold/rGO material shows a water evaporation rate of ~3.6 kg m-2 h-1. Furthermore, we demonstrate such material has good washability allowing its repeated use for water purification and excellent adaptability for the purification of aqueous effluents with complicated contaminates. The demonstration of graphene for recycling gold and its subsequent reuse for water purification provides a new pathway for the circular and sustainable development of gold and water resources.

Keyword: Keyword: Graphene, Sustainability, Gold extraction, Water purification

最终交流类型: Oral

Tailoring carbon nanotubes quickly into graphene nanoribbons along axis-direction

Qingsong Huang
Sichuan University

The current methods for preparing graphene nanoribbons (GNRs) can be divided into two categories: bottom-up and top-down. Bottom-up approaches include epitaxial growth of GNRs on silicon carbide steps, synthesis by special organic monomers on specific substrates, chemical vapor deposition on specially shaped templates, and so on. Most of these methods can achieve precise control of nanoribbon width and structure through monomer structure design or substrate width control. Top-down approaches include preparing several layers of GNRs by longitudinally unzipping MWCNTs in solution by strong oxidizing agents, preparing GNRs by etching CNTs with metal nanoparticles, and etching carbon materials with plasma to prepare GNRs, etc. These top-down methods greatly improve the amount of GNRs preparation efficiently. However, the process of preparing GNRs by etching CNTs remains challenging along axis only. It looks impossible to ensure that all etching is carried out along the axial direction of carbon nanotubes. Therefore, it makes sense to develop a method for the preparation of GNRs by etching CNTs along the axial direction in large quantities and super-fast. Here, we prepared GNRs by in-situ etching CNTs with rutile nanoparticles in dynamic magnetic flux template (DMT). CNTs are etched along the axial direction only by rutile nanoparticles under the constraint of DMT. This method provides a reference for the top-down controllable preparation of graphene nanoribbons.

Keyword: Carbon Nanotubes, Graphene nanoribbons, Quiclk Tailoring , Axis-direction

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最终交流类型: Keynote

On-Surface Chemistry: Towards Precise Synthesis

迟力峰
Soochow University, China

On-surface chemistry is a new precise synthesis method that has developed in the past decade. The on-surface reactions occur on single-crystal surfaces by activating precursor molecules to promote their subsequent migration and coupling, aiming at preparing functional molecules and polymers that can hardly be prepared via traditional solution

chemistry. Atomic precision is achievable by designing the chemical structure of precursor molecules, tuning the interactions between adsorbate and substrate, forming pre-assembled molecular patterning, and single-molecule manipulation. Representative achievements include the synthesis of structural-adjustable graphene nanoribbons, linear polyenes, graphdiyne nanowires, and metal-organic hybrids. In this report, I will summarize the past works in this field by focusing on the synthesis of functional molecules and polymers through the dehalogenation or dehydrogenation of precursors. The characterization tools mainly used include scanning tunneling microscopy, non-contact atomic force microscopy, scanning tunneling spectroscopy, and single-molecule manipulation. The development of on-surface chemistry provides new strategies and approaches for designing and expanding atomic-level precise preparation and property characterization of new molecular materials.

Keyword: Keyword: On-surface chemistry; non-contact atomic force microscopy; scanning tunneling microscopy; single-molecule manipulation

最终交流类型: Invited

Rational design of low dimensional carbon nanomaterials

杜世萱
中科院物理所

Low dimensional carbon nanomaterials have attracted significant attention due to their unique physical phenomena arising from quantum confinement and their high tunability of properties through external fields and interfaces. Understanding the correlation between structure and properties is crucial for advancing the discovery and design of high-performance low dimensional carbon nanomaterials. In this presentation, I will discuss DFT calculations of the formation mechanism and design strategies employed to achieve superior properties in novel two-dimensional and one-dimensional carbon-based materials, including partially hydrogenate graphene, carbon-based organic topologic insulators and nanoribbons.

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Keyword: Low dimensional materials, DFT calculation, graphene nanoribbon, hydrogenated graphene

最终交流类型: Invited

Memristive Devices Based on Two-Dimensional Materials for Neuromorphic Computing

孙林锋
北京理工大学

To overcome the traditional von Neumannbottleneck in modern computer system, neuromorphic computation is essential forconstructing artificial neural networks, which could offer a platform forprocessing complicated issues, like image classification, pattern recognition,decision-making, etc., in a straightforward way. Great efforts have been paidto mimic neuromorphic computing using various materials and devices structures.However, neuromorphic computation has remained technically challenging to bedemonstrated without using numerous transistors and capacitors. Recentlytwo-dimensional materials have attracted the attentions of research communitiesdue to their unique physical properties. This talk will introduce some of ourrecent works on the memristive behaviors of novel two-dimensional materials forinformation storage and neuromorphic computing devices, overcoming thelimitation of scalability and power consumption in conventional CMOS-basedneuromorphic devices.

Keyword: Two-dimensional Materials, Neuromorphic Computing, Memristor

最终交流类型:

Gold Extraction by Graphene and Its Reuse Exploration

Huiming Cheng
Institute of Metal Research, CAS, China

Gold is the most valuable element in e-waste. Currently, only less than 20% of e-waste has been recycled primarily for a lack of technologies with sufficient efficiency and economic viability[1-3], Therefore, developing materials capable of extracting gold from complex sources, especially electronic waste (e-waste), can turn the e-waste recycling challenge into a profitable business and provide an efficient solution for global gold sustainability. Here we report an exceptionally high gold extraction capacity of chemically reduced graphene oxide (rGO), reaching ~1.8 g/g from its 10 ppm solution at 25 oC, one order of magnitude higher than other reported gold adsorbents. During extraction, the rGO reduces >95% gold ions to metallic gold, avoiding elution and precipitation necessary in post-adsorption processing. Moreover, this reductive adsorption of gold by rGO is found different from (predominately) electrostatic adsorption of other metal ions, hence, exploiting the protonation process of rGO, a precise gold extraction without adsorption of the other 14 elements normally present in e-waste is achieved [4]. Furthermore, we explore the reuse of the extracted gold for highly efficient solar thermal water purification. By using graphene's strong adsorption to the solar spectrum and the plasmonic photothermal effect of the recycled gold, the resulting recycled gold/rGO material shows a water evaporation rate of ~3.6 kg m-2 h-1. Then we demonstrate that this material has good washability allowing its repeated use for water purification and excellent adaptability for the purification of aqueous effluents with complicated contaminates. The demonstration of graphene for recycling gold and its subsequent use for water purification provides a new pathway for the sustainable development of gold and water resources.

Keyword:Keyword: Graphene, Sustainability, Gold extraction, Water purification

最终交流类型: Invited

二维范德华薄膜的界面工程和高温智能器件应用

刘锴
清华大学

伴随着半导体产业开启亚 10 nm 节点时代，现代信息技术和人工智能的高速发展使纳米电子器件在高度集成化的同时也面临复杂的使用环境。一方面，纳米晶体管器件的高度集成化伴随着越来越集中的局域发热，使器件常常工作在局部高温环境中；另一方面，在可穿戴电子器件、汽车电子和航空航天等领域，纳米电子器件常常需要适应 125 °C 以上高温、高湿度等复杂的工作环境。因此，发展耐受苛刻环境甚至极端

环境的纳米电子材料和器件势在必行。由一维或二维纳米材料通过范德华界面作用形成的低维范德华薄膜材料，具有纳米级甚至原子级厚度、无悬挂键的表面和宽范围的带隙，有望突破物理极限产生变革性的器件原理和技术。在本报告中，报告人将介绍近年来在 MoS2 等低维范德华薄膜材料的界面性质研究、新型纳米异质结构制备以及新原理高温纳米电子器件应用等方面的探索工作。通过这些研究，有望为高温等极端环境下新型纳米电子材料和器件的研发探索出新的思路。

Keyword:**:** 二维材料；范德华；界面工程；高温电子器件

最终交流类型: Invited

Atomic scaled evolution of catalysts for single-walled carbon nanotubes growth

李彦
北京大学

Catalysts play important roles in the chemical vapor deposition of single-walled carbon nanotubes (SWCNTs). Intermetallic Co7W6 catalysts and mono-metallic catalysts have shown distinct difference in growth selectivity of SWCNTs. It is important to reveal the mechanistic difference, especially the behavior of catalysts. Electron microscopic techniques, particularly the in-situ techniques enable us to study the growth mechanism and compare the behavior of catalysts at atomic scale. We found that the growth of SWCNTs by Co catalysts associates to the partial carbonization of catalysts as well as carbon dissolving and precipitation. However, the Co7W6 nanocrystals were stable at the temperature of 1100 °C under carbon feeding condition and no carbon dispersion within the nanocrystal happened. Due to the less efficient carbon diffusion and supply on the surface of catalysts than that in a vapor-liquid-solid process, SWCNTs normally nucleate on larger catalyst nanocrystals in vapor-solid-solid process. These results can help us to further understand the mechanism of the selective growth of SWCNTs, benefiting the rational design of catalysts.

Keyword: single-walled carbon nanotubes, catalysts, environmental transmission electron microscope, chemical vapor deposition.

最终交流类型: Invited

Targeted Design and Large-Scale Preparation of Atomic-Level Catalysts

邹如强
北京大学

As metals are reduced to the atomic level, they assume the form of single atoms or double atoms dispersed on the carrier surface. This leads to a substantial enhancement in the stability of metal sites due to their strong interaction with the substrate, resulting in a near 100% utilization efficiency of metal atoms, showcasing the catalytic charm induced by the size effect. However, the field of Single-Atom Catalysts (SACs) faces two critical challenges: the rational design of single-atom localized structures at the atomic level and the realization of high single-atom loading and large-scale synthesis of SACs.

To address these challenges, we are developing an atomic-level catalyst database specifically for the selective catalytic reduction of NO_x using NH_3. Our approach involves employing machine learning techniques to predict and screen potential highly active atomic-level catalyst configurations, followed by catalyst preparation, in-situ characterization, and first-principles calculations to explore structure-activity relationships and catalytic mechanisms. Initially, we conducted DFT calculations, with a particular focus on Cu_1/CeO_2 SACs, to screen the type and configuration of single atoms. Theoretical calculations revealed that the construction of Cu single atoms promoted the adsorption of reactant molecules and kinetically facilitated the SCR process.

Moreover, we are dedicated to developing and optimizing low-cost large-scale preparation processes. To this end, we propose an electron-driven strategy for synthesizing SACs with high loadings and yields, successfully applying it to Cu_1/CeO_2 SACs. This single-atom synthesis method is easily scalable to industrial levels, allowing us to achieve kg-level synthesis with high single-atom loading.

Our ultimate goal is to achieve the targeted design of atomic-level catalysts through the integration of machine learning and theoretical calculations, surpassing the traditional trial-and-error development approach. We want to provide a reference paradigm for the design and development of catalytic materials, opening up new possibilities for efficient and sustainable catalysts.

Keyword: Atomic-level catalysts, SACs, DFT calculations, Large-scale synthesis

Topical Sessions =》 2. Inorganic and porous Nanomaterials

最终交流类型: Invited

Precise control on pore structures in porous materials

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Precise control on pore structures in porous materials。

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Porous materials is an important branch of inorganic synthetic chemistry, which has shown the extensive applications in gas separation and storage, catalysis, electrode materials, energy chemistry and many other fields. The core scientific issues of porous materials include the following aspects: pore size distribution and its regulation, pore structure microenvironment, multifunctional synergies in confined pore space, stability and machinability, development of new porous materials, etc. Different applications have different requirements on porosity for porous materials. This paper focuses on the precise regulation of nanopore properties in the chemistry of porous materials, including 1) developing the template effect of nanopore in MOF materials, and opening up the research on MOF-based carbon materials [1-4]. 2) Regulating the layer spacing of two-dimensional materials for molecular scale accurate sieving, and further introduce the chiral environment in layer space for high value-added chiral separation [5-7]; 3) Creating dynamic metastable hydrogen-bonded ionic frameworks (HIF) for reversible guest molecules capture and release at mild conditions, via mimicking the behavior of combustible ice [8-10].

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Keyword： MOF, HOF, 2D carbon nitride, pore structure control, dynamic structure

最终交流类型: Invited

Coupled Colloidal Nanocrystal Molecules

崔家斌

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The electronic coupling between atoms through hybridization of atoms yields the richness of molecules with diverse physical properties. Colloidal quantum dots (CQDs) have been demonstrated as artificial atoms more than two decades ago and found their applicability in various optoelectronic applications owing to their unique size dependent optical properties1. Since then efforts were made to achieve the electronic coupling and wavefunction hybridization with the CQDs with a vision of contributing to quantum information technologies. Electronic coupling has been resolved among molecular beam epitaxy grown QDs at cryogenic temperatures, which still leaves large space for further investigation. Hence, we utilize solution processable colloidal semiconductor quantum dots as artificial atoms for the formation of coupled nanocrystal molecules (CQDs). Starting from highly developed core/shell CdSe@CdS CQDs as artificial atom building blocks, we describe the procedure to form the coupled homodimer CQD molecules 2. While the chemical bond is the basis for combining atoms in molecules, connecting CQDs has to occur through adjoining of their crystal faces to form a continuous crystal via oriented attachment3-6. We observed a red shift in the band edge transition which appears as the signature of electronic coupling after the rectification of all the other effects that can cause in the same. To understand the coupling effect in the fused structure, we teamed up with theoretical and spectroscopic approaches which provided a clear view of the mechanism. The change in core size and shell barrier tuned the delocalization of electron wavefunction and those directly reflected in the optical properties as predicted by our theoretical calculation. This response seems quite interesting to us to establish a general strategy for formation of CQD dimers with wide variety of particle engineering their wavefunction. Such novel CQD architectures hold significant potential for applications, as two color emitters, as ratiometric sensors, and as electric field sensors along with the already well established commercial applications in displays and in bio-tagging.

Keyword：QDs, Coupled nanocrystal molecules, Oriented attachment

最终交流类型: Invited

Self-assembly and opto-electronic properties of nanostructures

巩建晓

National Center for Nanoscience and Technology, China

Through the accurate structural design at nanoscale, developing new materials with unique properties and advanced functions, exploring the intrinsic relationship between structure and properties and applying them to solve difficulties in multiple fields is the focus of interdisciplinary research including materials, physics, chemistry, biology, etc 1-2. Our work focuses on the nanoscale structural and optoelectrical properties control, including noble metal, semiconductor and magnetic nano systems, etc 3-5. Through accurate structural design, we developed series of optoelectrical nanomaterials with complex structures through synthesis and self-assembly, revealed the formation mechanism, realized accurately control of their optics, carrier transport and phase transition, which provide experimental and theoretical guidelines for the development of new optical device, solid-state semiconductor device and their applications in different fields like sensing, imaging and energy. For nanocrystals synthesis, we are combing defects engineering and multifunction design to

explore the structural-property relationship. For example, through introducing twinning plane defects in to Cu2S nanocrystals by an in-situ oxidation synthetic approach, phase transition behavior and carrier transportation of the Cu2S nanocrystals were effectively manipulated. This led to a new type of superionic conductor (Cu2S nanocrystals with twinning plane defects) stabilized at room temperature, as a comparison, the superionic phase of bulk Cu2S could only be stabilized above 104°C 3. One the other aspect, we are intensively working on the self-assembly methodology that could be used to achieve structural design of materials across multiple length scales at high accuracy and yield, with which we explore the related electronic and optical properties.

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Keyword： Self assemble nano materials, Nano optics, Nano transport

最终交流类型: Invited

Polyoxometalates intercalated layered double hydroxides

宋宇飞

北京化工大学

Polyoxometalates intercalated layered double hydroxides

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Polyoxometalates (POMs), a class of discrete anionic metal-oxygen clusters composed of early transition metals (V, Mo, W, etc.), have been widely used as acid catalysts in esterification, transesterification, alkylation, dehydration reaction, etc. Benefitting from tunable Brønsted or Lewis acidity, thermal stability and pseudo-liquid behavior, POMs exhibit excellent acid catalytic activity and selectivity.

Layered double hydroxide (LDHs) represent an important class of 2D layered materials with the general formula of [M2+1−xM3+x(OH)2]x+(An−)x/n·mH2O. Compared with other oxides (hydroxides), LDHs show the advantage of tunable chemical composition, thickness, and precursors of metal oxides, thereby can be widely used as electrocatalysts, photocatalysts and thermo-catalysts.

As a class of functional materials, polyoxometalates (POMs) intercalated layered double hydroxides (LDHs) have adjustable construction units and rich structural types, which not only have the functional properties of POMs and LDHs, but also have great significance for solving the problem of POMs heterogenization in industrial catalytic process. The project focuses on the research direction of "POMs intercalation assemblies and functional materials".

1) New methods of POMs intercalation have been proposed, namely main laminate modification method and peel assembly method, which breaks through the limitation of charge and size of multi-acid intercalation materials produced by traditional methods.

2) Through the design and regulation of POMs intercalation structure, a series of POMs intercalation materials with novel structure are constructed.

3) we have carried out the upstream and downstream research from basic research to industrial application of POMs intercalation materials.

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Keyword： Polyoxometalates, layered double hydroxides, intercalation, confinement

最终交流类型: Invited

Surface Chemistry Enabled Direct Patterning of Colloidal Nanocrystals

张昊

清华大学

Colloidal inorganic nanocrystals with intriguing size-dependent properties have shown promising applications in thin-film optoelectronics, sensing, imaging, and clinical therapy. Despite the rapid progress in individual nanocrystal based optoelectronic or sensing devices, methods for patterning nanocrystals in a scalable and controllable manner is required for integrated optoelectronics at system-level, such as high-definition displays and photodetector arrays. Among the existing patterning methods, conventional photolithography combines the advantages of high-resolution, scalability, fast speed, and parallel patterning capabilities. However, the complexity introduced by the use of photoresists, such as the poor solvent orthogonality and degraded properties of nanocrystals in charge transport or optical properties have strongly impeded the use of photolithography in nanocrystal patterning.

In this talk, we will discuss our recent work on surface chemistry enabled direct patterning of colloidal nanocrystals, without the need of conventional photoresists. These direct patterning strategies employs photosensitive ligands and the ensuing light triggered reactions at nanocrystal surface. Decomposition, cross-linking or (partial) stripping of nanocrystal ligands occurs in the light exposed region of nanocrystal thin films, leading to substantial changes in the colloidal stability of nanocrystals compared to those in the unexposed region. Consequently, high fidelity nanocrystal patterns with resolution of ~5 μm (the limit of our masks) can be obtained. The patterning methods are widely applicable to nanocrystals of metals, semiconductors and oxides, whose optical and electrical properties are easily tunable by adopting different light sensitive surface ligands. For instance, luminescent quantum dots and perovskite nanocrystals largely maintain their optical properties after direct photopatterning via cross-linking pathways. Electroluminescent light emitting diodes of patterned quantum dot and perovskite nanocrystal thin films show comparable device performance with those fabricated without patterning processes. These patterning approaches are also compatible with previously reported surface treatment strategies. We expect these strategies can complement and outperform ink-jet printing and other approaches for fabricating high-definition light emitting pixels, photodetectors and sensing arrays.

Keyword： colloidal nanocrystals; photopatterning; surface ligands

最终交流类型: Invited

2D Conjugated Polymers

陈龙

吉林大学

In this presentation, our recent works on synthesis of 2D covalent organic frameworks (COFs) and 2D Conductive metal-organic frameworks (2D c-MOFs) will be introduced. Firstly, we developed a two-in-one molecular design strategy for facile synthesis of 2D imine based COFs. The integration of two different functional groups (e.g. formyl and amino groups) in one simple molecule affords various bifunctional building blocks. Furthermore, the versatility of this two-in-one strategy was verified by many examples. This two-in-one molecular design strategy dramatically reduces the difficulty of COF synthesis, and is anticipated to be applicable for the synthesis of various COFs by using different building blocks, various linkages and topologies. Furthermore, an efficient and universal approach via in-situ vapor-assisted transformation of the monomer films to the corresponding COF films was developed based on these “two-in-one” designed A2B2 monomers.

On the other hand, 2D c-MOFs have exhibited potential applications in chemiresistive sensors, electrodes for energy storage, electrocatalysts, and electronic devices. Our recent works on design and synthesis of new 2D c-MOFs as well as the exploration of new potential applications of 2D c-MOFs in spintronics will be introduced.

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works on design and synthesis of new 2D c-MOFs as well as the exploration of new potential applications of 2D c-MOFs in spintronics will be introduced.

Keyword：2D Polymers, Organic Frameworks, Conjugation, Charge Transport, Spin Valves

最终交流类型: Invited

All-physical production and extreme performances of quantum-sized materials

张勇

National Center for Nanoscience and Technology

Intrinsic characteristics (of crystals) are crucial to their material properties. It requires that both interior and surface of the material are intrinsic, i.e., single crystal, no defect, no doping for the inner lattices and entirely exposed, no ligand, no functionalization for the surface lattices [1]. When the material is in quantum scale, the surface lattices and inner lattices could be equivalent in quantity. Unlike the inner lattices, the surface lattices are in asymmetric environments and nonequilibrium conditions (i.e., broken lattice, dangling/unsaturated bond, dynamic change). Evidently, the surface is more complex and abundant than the interior of the material in terms of structures and properties [1]. Our research interests focus on the extreme change of the material and the related phenomena/rules, particularly on the extreme change of the material size and the accompanying new effects. We propose the dual synergy ball-milling strategy and push the limit into quantum scale [2]. We report the all-physical top-down method and realize the intrinsic, universal, and scalable production of quantum-sized materials directly from their bulk [3,4]. Quantum-sized intrinsic materials enable the simultaneous realization of ultrahigh nonlinear response and ultralow power excitation [3,4]. We demonstrate the relationship between the nonlinear saturation absorption and the material size across the nanoscale [5-7]. Similar relationship between other properties (e.g., electrocatalysis, carrier dynamics, solar cells) and the material size is presented [8-10]. We construct the heterostructures incorporating quantum-sized materials and plasmonic structures/two-dimensional materials, show their potentials in controlled/synergetic electrocatalysis, and improve the catalytic performances of quantum-sized materials in hydrogen evolution reaction [8,11]. These works would guide the future research and development in quantum-sized materials.

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Keyword： quantum-sized materials, all-physical production, intrinsic characteristics, nonlinear saturation absorption, electrocatalysis

最终交流类型: Poster

Dynamic and flexible Hydrogen-bonded ionic framework

刘聪妍

中国科学技术大学

Porous frameworks containing void spaces can accommodate guest molecules owing to their high specific surface area and surface energy. Compared to amorphous materials, crystalline porous materials are conducive to understanding the relationship between structure and property due to their long range and ordered structure, and then guide the design and synthesis of new materials. Because of their pore size, adjustable functionality and diverse structures, crystalline porous materials have attracted great attention and have been successfully applied to a wide-range of research fields, such as gas adsorption and separation, energy storage, sensors and catalysis. According to the types of intermolecular interaction, crystalline porous materials can be divided into metal-organic frameworks (MOFs), covalent-organic frameworks (COFs) and hydrogen-bonded organic frameworks (HOFs), etc. HOFs are assembled from organic or metal-organic components through hydrogen bond interaction. Compared with MOFs and COFs that based on coordination bond or covalent bond, HOFs that based on hydrogen bond have some advantages such as structural diversity, easy to recrystallize and regeneration, because hydrogen bond is reversible and flexible. Different from traditional HOFs comprising neutral molecules, ionic HOFs (iHOFs) are composed of cations and anions, in which hydrogen bonds and electrostatic interactions work together for establishing the framework. The introduction of electrostatic interaction strengthens the stability of the frameworks. But the building blocks of traditional HOFs and iHOFs are restricted to organic molecules or ions. In fact, inorganic ions can also form abundant hydrogen bonds, which are suitable for constructing the hydrogen-bonded frameworks. In terms of composition, building blocks can be organic, inorganic, or organic and inorganic ions, and iHOF does not include all of these factors. We define the hydrogen-bonded ionic framework (HIF), which describes the structure assembled through hydrogen bonding and electrostatic interactions, no matter organic or inorganic ionic components. Due to the specific features of hydrogen bonds, dynamic and flexible HIFs can be developed.

We report the first example of elastic HIF of $\{(CN_3H_6)_2[Ti(\mu_2\text{-}O)(SO_4)_2]\}_n$, which was assembled by 1D negatively charged inorganic $[Ti(\mu_2\text{-}O)(SO_4)_2]_n^{2n-}$ chains and positively charged organic guanidinium cations via hydrogen bonds with electrostatic interactions together. The HIF single crystal features a prism morphology with an aspect ratio up to 300 and exhibits a two-dimensional (2D) isotropic reversible bending response under mechanical stimulation, even at liquid nitrogen temperature (77 K). The revealed mechanism by crystallographic analyses manifests the flexible and dynamic hydrogen bonds and electrostatic interactions, and 1D channels in the HOF crystal are critical structural factors responsible for the elastic behavior of the HIF.

Hydrogen bonds are dynamic since they are weak interaction. Our research group reported a reversible structural transformation of $[B(OCH_3)_4]_3[C(NH_2)_3]_4Cl\cdot4CH_3OH$ upon MeOH capture and release, as an example of achieving dynamic behavior of gas hydrates at ambient conditions. Recently, the dynamic HIF structure transformation was applied to CO2 capture. We reported the first example of mimicking CO_2 hydrate structure with CO_2 as guest molecules using a simple guanidinium sulfate co-crystallized with CO2 into a stable clathrate (CO_2@Gua_2SO_4). The clathrate exhibits unique advantages towards carbon capture. First, Gua_2SO_4 exclusively captures CO_2 without water or nitrogen interference, swiftly overcoming the fatal weakness of any physisorption processes. Second, the CO_2 released through structure disassembly could be triggered at ambient conditions, requiring little energy input for absorbent regeneration, while defeating the parasitic energy dilemma of chemisorption. Third, Gua_2SO_4 is stable and non-corrosive, a highly desirable feature when compared with ethanol amine, ammonia and other basic solutions that are commonly used in carbon capture. Fourth, a stable CO_2@Gua_2SO_4 in powder form is also beneficial for storage and transportation of CO_2, benefiting from its remarkably high volume per weight capacity.

HIF is constructed based on hydrogen bond and electrostatic interaction, which is dynamic and flexible. It can be applied in a wide range of fields, including elastic crystals, proton conduction, CO_2 capture, et al.

Keyword： Dynamic, Flexible, Hydrogen-bonded ionic framework (HIF), Electrostatic interaction, CO2 capture.

最终交流类型: Keynote

Intermediates Formed Prior to Nucleation and Growth of Colloidal Semiconductor Quantum Dots (QDs)

余睃

Sichuan University

The synthesis of colloidal semiconductor quantum dots (QDs) and magic-size clusters (MSCs) has been performed as an empirical art, with the latter considered as a side product of the former. Regarding the growth relationship, different opinions are expressed in the literature. For a relatively full picture of the growth relation, it is critical to understand the chemical reactions that are involved in the pre-nucleation stage prior to nucleation and growth of binary II-VI metal chalcogenide (ME) QDs. I will introduce the two-pathway model (Yu) that we developed recently to elaborate the growth relationship of QDs and MSCs. This model invokes an important reaction intermediate that forms in the prenucleation stage. This intermediate is so-called the precursor compound (PC) of the MSC. In addition to the innovative concept that absorbing MSCs evolve from their corresponding PCs which are relatively optical absorption transparent, this model suggests that there are two reaction pathways existing. Pathway 1 depicts that the self-assembly of M and E precursors is followed by the formation of the M-E covalent bond inside each assembly that results in one ME PC. It is the E precursor rather than the M precursor that dictates quantitatively the self-assembly. The LaMer model of the classical nucleation theory (CNT) partially describes Pathway 2, which concerns the formation of monomers from M and E precursors directly. The two pathways are inter-connected via the decomposition of the PC to monomers. We have demonstrated that high feed concentrations and high feed M to E molar ratios facilitate Pathway 1. From prenucleation-stage samples, various ME MSCs are obtained, such as CdS MSC-311 and MSC-322, CdSe MSC-361, MSC-391, and MSC-415, and CdTe MSC-371, MSC-417, MSC-448, and MSC-488. Also, ZnS MSC-269 and ZnSe MSC-299 are synthesized, together with CdTeSe MSC-399 and MSC-422. I will also talk about our latest advances on the direct and indirect pathways of MSC transformations, focusing on the isomerization of CdTeSe MSCs. Our study brings a deeper understanding of the difference between nanochemistry and traditional organic and inorganic chemistry. It is our belief that the synthesis of colloidal nanocrystals is transforming from an empirical art to a science.

Keyword： Magic-Size Clusters (MSCs), Quantum Dots (QDs), Precursor Compounds (PCs), Induction Period (IP), Two-Pathway Model (Yu)

最终交流类型: Oral

Continuous and Step-wise Spectral Shifts During Transformations in Colloidal Semiconductor Magic-size Clusters

栾超然

四川大学

Discrete, step-wise shifts in optical absorption are commonly expected to occur when colloidal semiconductor magic-size clusters (MSCs) transform from one type to another. Here, we show that the shift can also be continuous, with two model systems which are CdTe MSCs and CdTeSe MSCs. The MSCs are labeled by their absorption peak positions in wavelength of nanometer. When CdTe MSC-448 isomerizes to CdTe MSC-488 and when CdTeSe MSC-399 isomerizes to CdTeSe MSC-422 at room-temperature, the absorption shift from 448 to 488 nm for the former and from 399 to 422 nm for the latter is monitored in situ and in real time. Continuous (Pathway 1) and/or step-wise (Pathway 2) behavior is observed. Based on experimental evidence, we propose that Pathway 1 is a direct shape change, with a relatively large energy barrier. For a chemically-induced MSC transformation via Pathway 1, ligand exchange occurs on MSCs (Step 1a); then intra-cluster reconstruction of the “mother cluster’ (Step 1b) causes the isomerization of the MSCs. Pathway 2 is indirect, assisted by MSC precursor compounds (PCs) that are relatively transparent in optical absorption. Pathway 2 has three key steps, which are from MSC-1 to PC-1 (Step 2a), PC-1 to PC-2 (Step 2b), and PC-2 to MSC-2 (Step 2c). For a chemically-induced MSC transformation via Pathway 2, ligand exchange occurs on the monomer (Mo) first (Step 2b-1); then the Mo substitution on the PCs (Step 2b-2) results in the MSC transformation which is inter-cluster. When Step 2b is the rate-determining step, an isosbestic point appears in the absorption spectra. Our findings unambiguously suggest that when a change occurs directly on a “mother cluster”, the absorption shift is uninterrupted, similar to that of quantum dots (QDs) when they grow in size. Thus, when a spectral shift is interrupted, the change shall not occur on the “mother cluster” directly but via its PC. Our study encourages a reconsideration of the step-wise spectral shift observed during the transformation of colloidal semiconductor nano-species including MSCs, nanowires, and nanoplatelets (NPLs).

Keyword： Magic-Size Clusters (MSCs), Chemically-induced Transformation, Continuous and Step-wise Spectral Shifts, Precursor Compounds (PCs), Two-Pathway Model (Yu)

最终交流类型: Keynote

MOFs to Create Advanced Polymers

Takashi Uemura

The University of Tokyo

Metal-Organic Frameworks (MOFs) composed of metal ions and organic ligands have been extensively studied. The characteristic features of MOFs are highly regular channel structures with controllable pore sizes approximating molecular dimensions and designable surface functionality. Here I discusses the mutual contributions of MOFs and polymers, in hybrid systems. Understanding their reciprocally enhanced relationships provides new insights for further development of MOF-polymer associated system.

Use of their regulated and tunable channels for a field of polymerization allows multi-level controls of resulting macromolecules and nanographenes[1]. In addition, construction of nanocomposites between MOFs and polymers provides unprecedented material platforms to accomplish many nanoscale functions[2]. We have also developed direct insertion of polymers into nanochannels of MOFs, which enables powerful macromolecular recognition and separation technologies with exceptionally high selectivity[3].

Designing nano-sized pores of MOFs with a regular arrangement of reactive/interactive/responsive entities offers the possibility of universal polymer production and purification that cannot be accomplished by conventional methods.

Keywords MOF, polymer, nanographenes, recognition, seperation

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最终交流类型: Invited

Metal-organic framework-based electrocatalysts with atomic controllability

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中国科学技术大学

The fine design and regulation of catalysts play critical roles in the development of catalysis. The microenvironment, which gives rise to unique spatial structures and electronic properties around catalytic sites, has been proven to dramatically regulate catalytic behavior in enzymes and homogeneous catalysis. However, understanding the microenvironment modulation (MEM) of catalytic sites remains challenging and very limited in heterogeneous catalysis mainly due to the lack of structural precision and/or tailorability of traditional solid catalysts. Among diverse materials, metal–organic frameworks (MOFs), a class of porous crystalline solids featuring definite and tailorable structures, have been intensively studied as heterogeneous catalysts in recent years. The atomically precise and well tunable structures of MOFs make them an ideal platform for rationally regulating the microenvironment surrounding catalytic sites. Accordingly, their well-defined structures hold great promise for elucidating how the microenvironment modulation affects the resulting catalytic performance. In this talk, I will present our recent research results in the enhanced catalysis over MOF-based materials via microenvironment modulation.

Keyword： metal-organic frameworks; heterogeneous catalysis; microenvironment modulation

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最终交流类型: Invited

Scandium-based Materials Chemistry and Luminescence

黄岭

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Scandium (Sc) sits at a very unique position in the periodic table, i.e., the very top of the rare earth column and the very beginning of the transition metal row. This has imparted Sc very special chemical and physical properties and Sc-based nanomaterials have then aroused gradually increased research enthusiasm since the first report by our group. 1 Our recent studies have shown that the final product can be monoclinic Na3ScF6:Yb/Er or hexagonal nanoparticles of NaScF4:Yb/Er, which solely depends on the volumetric ration of the organic solvents of oleic acid and octadecene. Moreover, the hexagonal NaScF4:Yb/Er generates decent upconversion red emission while those of Y- and lanthanide-based nanomaterials give strong green emission.1

Furthermore, during the synthesis of Sc2O3:Tb nanoparticles from Sc(OOH)3:Tb through high-temperature annealing, , we noticed that the codoped Tb3+ could be in-situ oxidized into Tb4+, which does not generate luminescence. This unique chemistry only occurs in Sc-based nanomaterials. 2

Intriguingly, the codoped Eu3+ in the nanoparticles of Sc2O3:Eu synthesized via thermal co-precipitation method can be in-situ reduced into Eu2+ by the oleyamine, which is used as an organic solvent. By taking advantage of the co-existence of Eu2+/Eu3+, we have fabricated a colorimetric nanoscaled thermometer with excellent sensitivity and accuracy, where the temperature-sensitive luminescence variation of Eu2+ works as a probe while that of Eu3+ works as an internal standard since the intensity of it does not change with temperature. 3

Most importantly, our experimental results have shown that the WO43- groups in the Sc2(WO4)3 can be deviated away from the normal crystallographic position, i.e., intrinsic WO43-, which forms the extrinsic WO43- and further generate an energy reservoir through energy level overlap with that of intrinsic WO43-. This energy reservoir can release the stored excitation energy upon heating and transfer to the codoped rare earth ions, so that thermally enhanced luminescence can be obtained. 4

Herein, we summarize our advances on Sc-based luminescent nanomaterials and their potential applications, which indeed show the uniqueness of Sc as a rare earth element.1-4

Keyword：Scandium, Rare Earth, Materials Chemistry, Upconversion Luminescence, Defect

最终交流类型: Oral

Extended surface band triggered bright and narrow green emissive sulphur nanodots for versatile applications

Lian Xiao

Nanyang Technological University

Fluorescent sulphur nanodots (S-dots) have been attracting increasing attention in novel applications by virtue of their combined merits such as heavy metal free nature, earth abundance, high annual production, and antibacterial property etc. However, the large band gap limitation of bulk sulphur and top down synthesis approach make it a fundamental challenge to realize the bright and narrow green light emission, which strongly hinders the sulphur nanodots based exploitations and applications. Here, for the first time, we develop a strategy to achieve a new extended surface band inside the band gap of bulk sulphur. Comprehensive spectroscopy study and theoretical calculations indicate that the oxidized sulphur account for the new surface band generation. The long phase coherence length and high density of states of the extended surface band contribute to the realization of large absorbance with molar absorption coefficient ~2.2 * 104 cm-1M-1@ 511 nm, photoluminescence quantum yield (PLQY) up to ~ 58.3% and narrow band width with full width at half-maximum ~ 33 nm. The simple and facile post treatment results in simultaneously the purification and further improvement of the green light emission properties of sulphur nanodots by eliminating the randomly distributed detrimental surface defects. Specifically, the photoluminescence quantum yield further increased up to 62.1% accompanied by the decreased non radiative recombination rate and strongly supressed re-absorption in longer wavelength range (>530 nm). All these features benefit to the sulphur nanodots based versatile applications in the fields of biomedicine e.g., bio imaging, optoelectronics e.g., micro laser etc., as presented in this work. It can be also envisioned that more sulphur nanodots based applications will appear in the near future. Our results not only pave the way for luminescent sulphur nanodots development, but also demonstrate the feasibility to tune the light emission via the generation of extended surface band on the nanomaterial surface.

Key Words sulphur nanodots, photoluminescence, green light emission

最终交流类型: Invited

Crystalline Assembly Catalysts Combining Oxidation-Reduction Molecular Junctions for Artificial Photosynthesis

兰亚乾

华南师范大学

Through simulating natural photosynthesis, it is an effective way to alleviate the greenhouse effect by coupling photocatalytic CO2 reduction and water oxidation reactions to realize artificial photosynthesis. Assembling of oxidative and reductive units to build photocatalysts with precise structural information, such as metal-based clusters, metal-organic frameworks (MOFs) or covalent-organic frameworks (COFs), is not only expected to complete artificial photosynthesis, but also conducive to uncovering the active sites and catalytic mechanisms. In recent years, our research group has designed and synthesized a series of crystalline assembly photocatalysts combining oxidation-reduction units. (i). Synthesis of redox covalent bond frameworks to realize artificial photocatalysis; (ii). Synthesis of redox heterometallic cluster-based metal-organic frameworks, using accurate crystal structures to determine the structure-activity relationship from molecular level; (iii). Synthesis of molecular oxidation-reduction junctions, adjusting the spatial arrangement of the oxidative and reductive units to explore new migration modes of photogenerated charge. These works provide new strategies for building more efficient crystalline catalysts for artificial photosynthesis.

Keyword： Crystalline catalyst, Molecular junctions, Artificial photosynthesis

最终交流类型: Oral

Polar Surface Chemistry of Atomically-thin Metal Oxide Nanosheet

刘朋昕

上海科技大学

Polar facets are a special class of high-energy facets with electrostatic fields perpendicular to the surface generated by dipole moments. Early surface science and theoretical calculation studies have found that magnesium oxide (111), a polar facet, has a metal-like electronic state that activates a variety of small molecules. However, this understanding has not been verified in the real material system, and the difficulty lies in (1) how to prepare self-supporting (111) single crystal magnesium oxide materials exposed by crystal planes; (2) how to recognize the reconstruction and defects of the atomic structure of polar surfaces; (3) The stability of the polar crystal plane is unknown. We study the prepared (111) face-exposed magnesium oxide single crystal nanosheet, and explore the special chemical properties caused by the special electronic structure of polar crystal faces from the perspective of surface species and reactivity with small molecules.

We used used single-crystalline MgO(111) two-dimensional nanosheets as support and explore the SOMC of Ir(COD)(acac) (COD, cyclooctadiene; acac, acetylacetonate) on its surface[56]. The supported species are either only single atoms at low loading or a combination of monomers, dimers, trimers and small clusters at high loading. Interestingly, Ir trimers are structurally similar, with a distance of 3.0 Å between adjacent Ir atoms, which formed congruent equilateral triangles. This observation, together with other results showed the chosen support can provide uniform binding sites for the supported species. The calcined MgO(111) nanosheets are terminated by threefold coordinated O anions (O3c2–) in a threefold symmetry. Hence, the single crystallinity of the support and the exposed ordered crystalline plane are ideally suited to minimize the surface heterogeneity for anchoring atomically dispersed species.

Since the polar MgO(111) surface exposes very basic oxygen surface sites, we tentatively propose that they likely assists the formation of styrene, either by participating at the hydrogen abstraction from the phenylethyl iridium intermediates or by dehydrogenating ethylbenzene.

Keyword：Polar Surface, 2D material, Single atom Catalyst, Atomically Dispersed Catalysts, Surface Coordination Chemistry

最终交流类型: Invited

Tuning the Photodetector Performance by the Perovskite Defect States

Xiangxing Xu

南京师范大学

Perovskite semiconductors are eminent materials that have been widely used in photoelectric detection, light-emitting diodes, solar cells, lasers, quantum information devices because of their excellent photoelectric properties such as tunable band gap, large absorption coefficient and high carrier mobility. The defect/trap state energy levels of traditional semiconductors are generally located within the bandgap, while perovskite defect states can locate within the valence and conduction bands. Although perovskites have partial defect tolerance, defect states remains a major obstacle to improving device performance in most cases and a major task is eliminating defect states. However, the presence of a large number of surface interfaces in perovskite quantum dots or their nanocomposite systems inevitably leads to high-density defect states. Our investigation on perovskite based photodetectors showed that the defect states of perovskite has special regulatory functions on the photoelectric performance of the devices. By injecting charge carriers into the defect states through the synergistic effect of light and electricity, ambipolar (positive and negative) photoresponses were achieved in CsPbX3-ITO(X=Cl,Br,I) and CsPbX3-ZnO nano heterojunction (NHJ) devices[1,2]. In lateral drain-source structured ITO/CsPbX3-ITO-NHJs/ITO and ITO/CsPbX3-ZnO-NHJs/ITO devices, the transition between the positive photoconductivity (PPC) and negative photoconductivity (NPC) was successfully controlled by the drain-source voltage, electrode gap, perovskite QD composition and size. The later device also exhibits excitation wavelength dependent PPC-NPC transform. High responsivity, on−off ratio, and detectivity were achieved. A general mechanism combining exciton, charge separation, transport, and most critical the voltage driven electron filling of the defect states with drain–source voltage above a threshold is proposed to understand this unusual ambipolar transform. In the carbon dot doped MAPbX3(X=Cl/Br/I) composite crystals, photodetectors with both narrowband and broadband response features were achieved by utilizing the capture and recombination of charge carriers via defect states[3]. Utilizing rather than eliminating the function and role of perovskite defect states in optoelectronic devices provides a unique approach for developing new perovskite based optoelectronic devices such as photodetectors, optoelectronic switches, and memories.

Keyword：perovskites, photoresponse, defect states, heterojunction

最终交流类型: Invited

Advancing Reverse Osmosis Membranes with Porous Cages and Nanoparticles

Dan Zhao

National University of Singapore

Porous cages, including metal-organic cages (MOCs) and porous organic cages (POCs), are discrete porous molecules with well-defined apertures and cavities. They offer unique advantages such as solubility, which enables solution-based processing, making them ideal additives for complex systems like membranes. In this presentation, I will discuss our recent

research on utilizing porous cages as water channels in reverse osmosis (RO) membranes. Specifically, we focus on zirconium metal-organic cages (Zr-MOCs) as molecular fillers for thin-film nanocomposite (TFN) membranes, along with the strategic modification of polyamide selective layers using mono amino compounds. The optimized TFN membranes exhibit significantly increased water flux without compromising salt rejection, highlighting the potential of porous cages in TFN membranes. Additionally, we explore the effectiveness of nanoscale porous organic cages (POCs) in achieving selective ion rejection and fast water permeation comparable to aquaporins. The nanoscale pores of POCs allow water molecules to flow in single-file, branched chains, leading to high water permeation and nearly perfect cation and anion rejections. This discovery underscores the promising role of POCs as molecular fillers in TFN membranes. Furthermore, we investigate the influence of nanoparticles on TFN membrane performance. Two series of TFN membranes, one incorporating hydrophobic porous zeolitic imidazolate framework (ZIF-8) nanoparticles and the other with nonporous amorphous ZIF-8 (aZIF-8), are prepared and compared. The TFN membranes containing hydrophobic ZIF-8 nanoparticles exhibit a substantial increase in water permeance while maintaining comparable salt rejection to traditional thin-film composite (TFC) membranes used in brackish water reverse osmosis (BWRO). On the contrary, the addition of aZIF-8 nanoparticles shows minimal enhancement in water permeance. By analyzing the physicochemical properties of the materials and membranes, we attribute this disparity to the presence or absence of internal hydrophobic pore structures in the nanoparticles, which act as additional water channels while effectively blocking NaCl passage during BWRO. Through these investigations, we contribute to the understanding and advancement of reverse osmosis membranes by harnessing the potential of porous cages and nanoparticles, opening avenues for improved water treatment technologies.

Keywords Metal-Organic Cages, Porous Organic Cages, ZIF-8, Water Channels, Reverse Osmosis

最终交流类型: Invited

Ultramicroporous titanium-organic nanohybrid material for deuterium separation

汪苏靖

中国科学技术大学

Separating deuterium from hydrogen isotope mixtures is of essential importance to develop nuclear energy industry, as well as other isotope-related advanced technologies. Conventional industrial processes for deuterium purification such as electrolysis of heavy water, chemical exchange and cryogenic distillation have to face inevitable limitations such as complex, low efficiency, time- and energy-consuming operating conditions, which calls for alternative methods to approach the requirements of a sustainable deuterium production. Among them, kinetic quantum sieving (KQS) using porous materials to preferentially separate heavier deuterium over protium has aroused a great interest. It features either notably elevated separation efficiencies or desirable deuterium capacities, even approaching a good balance of efficiency and capacity in the case of some advanced porous materials, standing among the most promising alternative technologies for hydrogen isotope separation. Recent research shows that a quantum sieve encompassing a wide range of practical features in addition to its separation performance is highly demanded to approach the industrial level. Here, the rational design of an ultra-microporous squarate pillared titanium oxide hybrid framework has been achieved, of which we report the comprehensive assessment towards practical deuterium separation. The material not only displays a good performance combining high selectivity and volumetric uptake, reversible adsorption-desorption cycles, and facile regeneration in adsorptive sieving of deuterium, but also features a cost-effective green scalable synthesis using chemical feedstock, and a good stability (thermal, chemical, mechanical and radiolytic) under various working conditions. Our findings provide an overall assessment of the material for hydrogen isotope purification and the results represent a step forward towards next generation practical materials for quantum sieving of important gas isotopes.

Keyword： titanium-organic hybrid, deuterium separation, quantum sieving, stability

最终交流类型: Invited

On Surface Synthesis of Covalent Organic Framework Structure

王栋

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The exotic properties associated with graphene and other 2D layered inorganic materials have attracted great interests from a variety of research fields. Two-dimensional covalent organic frameworks (2D COFs), which are covalently constructed from planar aromatic building blocks based on the principles of reticular chemistry, are a class of porous crystalline material with the highly ordered porous architectures and pre-designable electronic skeletons. 2D COFs feature the extended conjugation within a 2D layer and periodically columnar arrays aligned with an atomic precision in vertical direction, which is hardly achievable in other molecular architectures. In this context, high crystallinity and closely eclipsed stacking alignment of aromatic moieties render 2D COF as an ideal plat-form for charge carrier transport. With the improved crystallinity and controllable orientation, substrate supported 2D COF film would enable fabrication of advanced architectures for electronic devices, which however remains unexplored so far.

Herein, we report the on surface synthesis of high quality 2D COF thin film. We have developed a general method for constructing COF monolayers and thin films on substrate surfaces based on gas-solid and liquid-solid interfacial reactions. We proposed a method to improve 2D polymer orderliness by remotely modulating the molecular conformation through the effect of steric hindrance. We developed a chemical vapor deposition method, and prepared highly ordered 2D polymer films with controllable number of layers by modulating the kinetic process of the reaction. We further demonstrate that it is possible to fabricate COF thin film for optoelectric device. Two types of field-effect transistors with horizontal and vertical structures were constructed by directly growing COF films on the surfaces of hexagonal phase boron nitride and monolayer graphene, respectively, and their in-plane transverse charge transport properties and electronic properties in the π-π stacking direction were investigated. We have constructed COF-based electrochromic devices, and the highly ordered structure of COF significantly enhances their performance such as response speed.

Keyword：Covalent organic frameworks; on surface synthesis; optoelectronic devices

最终交流类型: Oral

Extremely stable amidoxime functionalized covalent organic frameworks for uranium extraction from seawater with high efficiency and selectivity

韩冰

Uranium extraction from seawater is a hot topic attracting more and more attention in the past few decades for the sustainable production of nuclear power. The development of adsorption materials with excellent uranium binding functional groups are prerequisite for the highly efficient recovery of seawater uranium. Amidoxime functionalized materials are the most promising adsorbents with the high affinity towards uranium. Nevertheless, such adsorbents always suffered from unsatisfying selectivity in extracting uranium under seawater condition, where vanadium is the most competitive interfering ions reducing the adsorption performance. Moreover, the binding chemistry of vanadium in amidoximated adsorbents is not yet clear. Herein, an amidoxime functionalized polyarylether-based covalent organic framework (COF-HHTF-AO) was synthesized. Owing to the rigid skeleton with suitable dimension, amidoxime in COF-HHTF-AO is verified with open-chain form rather than cyclic imide dioxime. COF-HHTF-AO shows remarkable chemical stability and excellent crystallinity. In uranium spiked aqueous solution, COF-HHTF-AO exhibited maximum adsorption capacity up to 550.1 mg/g. What's more, COF-HHTF-AO exhibited excellent reusability with the original adsorption efficiency maintaining up to ~82.4% after 5 cycles, owing to the rigidity of the COF skeleton. The distribution coefficient (Kd) of COF-HHTF-AO towards U(VI) was calculated to be 5.2×10^5 mL/g in real seawater containing 100× excess of UO_2^{2+} and competitive metals, which is 2.9 times higher than vanadium. Impressively, the adsorption capacity of COF-HHTF-AO towards uranium in natural seawater reached up to 5.12 mg/g, which is 1.61 times higher than that for vanadium. Detailed computational calculations revealed that the different adsorption behavior of uranium and vanadium on COF-HHTF-AO originates from their different interaction mechanisms with amidoxime groups. The driving force of adsorption between uranyl and COF-HHTF-AO is coordination interaction, which is much stronger than the hydrogen bonding between vanadium and COF-HHTF-AO. Combining enhanced adsorption capacity, excellent selectivity and ultrahigh stability, COF-HHTF-AO serves as a promising adsorbent for uranium extraction from the natural seawater.

Keyword： Covalent-organic framework, amidoxime, seawater uranium extraction, adsorption, selectivity

最终交流类型: Oral

Construction of subnanometer polyoxometalate assemblies and the electron delocalization effect at the sub-nanoscale

刘清达

清华大学

Polyoxometalates (POMs) clusters are discrete transition metal oxides with atomic precise structure, unique electronic structure and excellent redox properties for catalysis, which are ideal building blocks for the construction of subnanometer functional materials. We have fabricated a series of subnanometer POM assemblies based on the self-assembly of amphiphilic POM building blocks at the interface of insoluble phase. The morphology, electronic property and structure-property relationship of these assemblies have also been systematically investigated. The assembly behavior of POM clusters can be dominated by interactions at the molecular level, based on which a series of single-cluster nanowires, single-cluster nanorings and their three-dimensional superstructures have been fabricated with up to 15 kinds of POM clusters. By stepwise tuning of interactions at the molecular level, the configurations between clusters can be varied, leading to the morphology change from nanowires to nanorings. We have also realized the temperature-responsive reversible self-assembly of POM clusters driven by hydrogen bonds between clusters, which can spontaneously arrange into 2D single cluster superlattices at 25 °C and transform into single-cluster nanowires below 0 °C. Electron delocalization in subnanometer materials can efficiently lower the energy barrier for reactions and electron transfer, giving rise to significantly enhanced activity in catalysis and external field coupling. For the first time we fabricate a new class of 2D graphene-like matters, named "clusterphene", by using rare earth substituted Keggin type POM clusters as building blocks. Due to the electron delocalization in the clusterphene layer, the catalytic activity and stability of clusterphene toward olefin epoxidation is greatly enhanced, with a turnover frequency 76.5 times that of the unassembled clusters. Another type of 2D polyoxoniobate-based clusterphenes have also been reported using {Nb24O72} cluster building blocks and metal ion linkers, featuring in-plane electron delocalization properties and significantly enhanced photocatalytic activity toward benzyl alcohol oxidation. Moreover, we have developed Ag-POM nanowire heterostructures following the visible light-induced strategy, where notably enhanced activities in electrochemical sensing and catalytic gasoline desulfurization are obtained contributed by its unique electronic structure. These results provide atomically precise models for the in-depth investigation of their structure-property relationships, and may enlighten the design and precise synthesis of cluster-based materials.

Keyword：Subnanometer Materials; Self-assembly; Polyoxometalate; Non-covalent Interactions; Electron Delocalization

最终交流类型: Invited

Mass Transport Based on Covalent Organic Frameworks

冯霄

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Crystalline porous materials with nano-and sub-nanometer pores, such as covalent organic frameworks (COFs), constructed by the spatial connection of rigid molecular units, have great potential for confined substance transport. We focused on COFs to address the trade-off among water, ion, and gas transport in the catalytic layer of fuel cells.[1] To realize synergistic transport of multiple substances, we proposed “fast nucleation and slow growth” strategies to synthesize nanochannels, fabricating gradient 2D COF membranes, engineered geometry and functionality variations along the individual channels define and boost the overall function, and finally achieving highly oriented nano-channel construction.[2] Meanwhile, we developed “side-chain induced-dipole facilitated stacking” strategy, in conjunction with the monomer's structural rigidity and the concept of low steric hindrance in molecular design, to enhance the thermodynamic stability of interlayer stacking and prevent the formation of dispersed structures, creating a record for the maximum pore size of COF.[3] We developed a COF-to-COF transformation methodology to prepare microtubular COFs, leading to enhanced mass transfer properties, as proved by the adsorption measurement and chemical catalytic reactions.[4] Then we clarified the effects of size and hydrophobicity/hydrophilicity on water phase transition and diffusion, and showed that the unique one-dimensional penetrative channels with alternative hydrophobic/hydrophilic functionalities aligned on the pore walls in 2D COFs can significantly lower the energy barrier for water permeation and diffusion, then proposed a pore-confinement encapsulation strategy, and achieved fast ion transport at complex interfaces.[2, 5-12] Based on the above work, we developed a new open framework ionomers system, groundbreaking notion

transcends the constraints of traditional chain ionomers by augmenting the mass transfer efficiency within the catalytic layer. Remarkably, the mesoporous apertures and appendant sulfonate groups enabled the proton transfer and promoted oxygen permeation, overcoming the challenge of synergistic transport of multiple substances at the three-phase interface, and greatly improving the power density of proton exchange fuel cells.[1,13]

Keyword： covalent organic frameworks, porous materials, mass transport, fuel cell

最终交流类型: Invited

MOFs based materials for efficient hydrogen production and utilization catalysis

李光琴

中山大学 Sun Yat-Sen University

Developing hydrogen energy is crucial for the transformation of energy structure. However, there are challenges in terms of low catalytic efficiency and high cost of catalyst in hydrogen production and hydrogenation reaction. Porous materials such as metal-organic frameworks (MOFs) possess a large surface area, abundant host-guest properties, and can be tailored at the molecular level, which serve as ideal model materials for the study of catalytic reactions. Therefore, our group has designed and developed a series of MOFs based porous nanocomposites to conduct water electrolysis for hydrogen production and hydrogenation. We have developed structural engineering, defective ligand, and other strategies to regulate the coordination environment and electronic structure of MOFs to enhance the activity and stability in electrocatalytic oxygen evolution reaction (OER) [1-3], and optimize the hydrogen adsorption free energy for obtaining high performance in hydrogen evolution reaction (HER) [4-5]. Moreover, high performance of hydrogenation catalysis is the key to efficient utilization of hydrogen. To address the issues of hydrogenation selectivity and stability, we have proposed a locking effect strategy for preparing stable MOFs based catalysts and developed the coupling hydrogenation system for nitrogen oxide with electrolytic water, which achieved high efficiency and specific hydrogenation catalysis for hydrogen utilization.[6-10] Tuning the electronic structure of MOFs based materials can effectively modulate the interaction between reaction intermediates and active sites, leading to an appropriate adsorption free energy, thus enhancing catalytic efficiency and stability,

meanwhile reducing the cost of catalyst, which provides a novel guidance for future development and design of high-performance catalysts.

Keywords: MOFs; water electrolysis; hydrogen production; hydrogenation; electronic regulation.

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最终交流类型：Oral

Series of Research on Chiral Colloidal Semiconductor Nanocrystals

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Chirality means the ones that are not superimposable on their mirror images. It is a fantastic phenomenon ubiquitous in nature and the universe, ranging from small molecules to nanoscale proteins, sugars, and DNA to meter-scale eyes, flowers, animal shells, and the vast galaxy. Chirality has always been one of the most important research topics, with its profound significance in the origin of life.1

An essential property of chiral materials is their optical activity. The earliest study of chirality dates to 1811 with the observation of the optical activity in quartz, and then this subject achieved tremendous success in both experiment and theory. Notably, with the recent flourishing of nanotechnology, chiral nanomaterials composed of noble metals or semiconductors are marching into this fascinating family, and they display tunable optical activity in UV−visible wavelength and potential applications.2,3 Among those, the chiral ligands stabilized colloidal semiconductor nanocrystals (NCs) possess many remarkable characteristics, i.e., the easily adjusted circularly polarized luminescence (CPL) and the promise in gene editing. Chirality is a fantastic phenomenon in science related to different physics, chemistry, and biology fields. Recently, chiral nanomaterials progressed fast with the rapid growth of nanotechnology with widespread potential applications in chiral medicines, chiral catalysts, spin electronic devices, and so on. Optical activity is a curial property of the chiral materials to evaluate the chiral strength of the chiral materials. Hence, determining the crucial parameters of the flexible regulation of the optical activity on nanomaterials is critical to directing and improving the advanced chiral nanomaterials.

Here, the optical activity of chiral semiconductor nanocrystals and the self-assembled superlattice are deeply investigated.4,5 It was found that the same chiral ligand and the crystal structure of wurtzite (WZ), with the shape change from spheric NCs to one-dimensional quantum rods (1D QRs) and then to two-dimensional nanoplatelets (NPLs), the CD intensity increased exponentially. Furthermore, as for CdSe NRs, the CD peak red-shifted and reached a particular value with length increasing, while the CD intensity showed a similar tendency due to the continuous electron state along the length. Interestingly, the CD spectra obviously differed in CD intensity and the line shape between WZ and zincblende (ZB) CdSe NPLs. Moreover, the chiral deformation of the two-dimensional NPLs superlattice induced by chiral molecules would cause huge optical activity in the system. The above results demonstrate that symmetry of the shape and crystal structure is the key to affecting the optical activity of the chiral semiconductor nanosystem. Moreover, the array of the chiral ligands on the surface of nanoparticles also would help to increase the optical activity of the system.

Keyword： Chirality, Nanocrystals, Semiconductor, Circular Dichroism, Optical Activity

最终交流类型: Invited

Crystalline framework materials self-assembled by non-classical bonds

张章静

福建师范大学

The breaking and formation of chemical bonds is the essence of chemistry as well as the basis of creating new substances, new materials and new functions. Crystalline framework materials provide a wonderful platform for exploring the characteristics of chemical bonds, wherein it is essential to establish stable frameworks with permanent porosities. Beyond the limitation of current chemical bonds in the previous frameworks, we put forward two considerations from the view of chemical nature. Can other bonds be used to build stable framework materials besides the classical metal-organic coordination bonds, covalent bonds and hydrogen bonds? Can synergetic weak interaction (single bond energy<15 kJ/mol) be used to build stable framework materials?

Facing these challenges, three key issues need to be solved, including non-classical bond self-assembly law, functional exploration and dynamic change. We have carried out revolutionary research on framework materials assembled by non-classical bonds in three directions. Firstly, exploring new stable framework materials with permanent porosities based on BN coordination bond, -CN···H interaction, and -CHO···H interaction, respectively. Secondly, considering from the interactions between frameworks and guests, to develop the weak-interaction functionalization strategy for achieving high performance in gas separation and unique functionality in optical and electronic properties. At last, developing the in-situ detection technologies to explore the dynamic structural change as well as structures-properties relationship of the frameworks in the confined space.

In a word, our work can provide some new strategies for constucting stable frameworks to expand the new direction of Reticular Chemistry, but also can achieve materials with high performance and unique functionalization.

Keyword： nano porous materials, framework materials, structure-property relationship, coordination chemistry, reticular chemistry

最终交流类型: Invited

2D and 3D Metal Aerogels and their Applications

Alexander Eychmüller

TU Dresden

After a brief introduction on nanoparticle-based aerogels [1] and elemental distribution in bimetallic aerogels [2], I will report on two recent studies conducted in my group.

The physical properties of nanomaterials are determined by their structural features, making accurate structural control indispensable. As for metal aerogels, highly porous networks of aggregated metal nanoparticles, such precise tuning is largely pending we studied the capabilities of precise morphology design by deploying Au-Ni as a model system to combine common aerogel morphologies under one system [3]. Au-Ni aerogels were synthesized via modified one- and two-step gelation, partially combined with galvanic replacement, to obtain aerogels with alloyed, heterostructural (novel metal aerogel structure of interconnected nanoparticles and nanochains), and hollow spherical building blocks (cf. Fig. 1). Our work significantly improves the structural tailoring of metal aerogels and possible up-scaling. Preliminary ethanol oxidation tests demonstrate that morphology design extends to the catalytic performance.

Continuous advancements in science and technology in the field of flexible devices encourage researchers to dedicate themselves to seeking candidates for new flexible transparent conductive films (FTCFs). Our recently developed two-dimensional (2D) metal aerogels are considered as a new class of FTCFs. We describe a new large scale self assembly synthesis of bimetallic Pt-Ni 2D metal aerogels with controllable morphology during the synthesis [4] (Fig. 2). The obtained 2D aerogels require only a low quantity of precursors for the synthesis of percolating nanoscale networks with areas of up to 6 cm2 without the need of an additional drying step. Stacks of the obtained monolayer structures display low sheet resistances (down to 270 Ω/sq), while decreasing the optical transparency. In perspective, the 2D bimetallic Pt-Ni aerogels not only enrich the structural diversity of metal aerogels, but also bring forth new materials for further applications in flexible electronics and electrocatalysis with reduced costs of production.

Fig.1 SEM micrographs (1) and STEM EDX-based element mapping (2) of the alloy AuNi3 (A), heterostructure AuNi3 (B), and hollow shere (HS) AuNi6 (C) aerogels. All samples exhibit a sponge-like gel character regardless of their morphology. Moreover, the structural trends observed by TEM reappear. Alloy gels and HS gels show fairly homogeneous element distributions (with enhanced Ni signals at the surfaces), while in the heterostructure gels, the elements separate into Ni NPs and Ni-doped Au nanochains.

Fig.2 EDX based element distributions of the 2D Pt Ni aerogels transferred via the stamping (a-d) and the up-scaled (e-h) methods: Pt1.5Ni (a and e), Pt3Ni (b and f), Pt4.5Ni (c and g), Pt6Ni (d and h).

Acknowledgements

The author is grateful to all people participating in this research over the past years at TU Dresden. Financial support by the DFG, the EU, the AvH foundation, the CSC, the BMWi and the State of Saxony is gratefully acknowledged.

Keywords metal networks, 2D metal gel, 3D aerogels

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最终交流类型: Keynote

Chemical synthesis and magnetic regulation of two-dimensional nonlayered magnetic materials

侯仰龙

北京大学

2D nonlayered magnetic materials have attracted extensive attention due to their high magnetic transition temperature, rich structure, and novel physical properties. In recent years, we have focused on the controllable synthesis and spin modulation of 2D nonlayered magnetic nanomaterials. On the one hand, we have synthesized a series of ultrathin iron-based nanosheets using a liquid-phase method and studied the influence of surface chemistry on the nucleation and growth processes. On the other hand, we have obtained a series of 2D nonlayered magnetic nanomaterials using chemical vapor deposition (CVD) method: wedge-shaped EuS nanosheets were obtained induced by steps on substrate, and room-temperature magnetic Fe7Se8 nanoflakes were synthesized by confined space. Importantly, we have developed a thermodynamics-triggered competitive growth to provide a quantitative criterion for predicting and guiding the growth of 2D materials, based on which we have designed universal methods for growing 2D transition metal oxides and rare earth metal oxyhalide nanosheets. In addition, we have established a new paradigm for thin film epitaxy and grown Cr5Te8 crystals on single-layer WSe2. These studies provide powerful guidance for the controllable synthesis of two-dimensional magnetic materials and lay a foundation for the development of new spin devices.

Furthermore, we have explored the unique magnetic structures of 2D magnetic materials. It was found that ultrathin Fe nanosheets have thickness- and geometry-dependent magnetic vortex structures. Moreover, we have achieved direct and efficient control of magnetic flipping in the ferromagnetic semimetal Co3Sn2S2 via electric current and established a current-assisted domain-wall motion model. This model can further reduce the threshold current for changing coercivity and change the symmetry of currents. These findings combine magnetism, topological structure, and metallic properties, laying a material foundation for low-energy computing and storage spin devices.

In summary, we have designed a series of chemical methods for the controllable synthesis of 2D magnetic materials, studied and controlled their magnetic properties, and will further explore their applications in spintronics and magnetic devices.

Keyword：Two-dimensional nonlayered magnetic materials; chemical synthesis; magnetic regulation

最终交流类型: Oral

Balancing Multivariant Interactions for the Synthesis of Novel Mesoporous Nanodrug Formulations

赵天聪

复旦大学

Mesoporous nanomaterials, with high surface area, large pore volume and unique loading capacity, has been given much attention as nano-drug carriers for biomedical applications. Yet, the drug loading capacity remains rather low (< 10 wt%), and the mesoporous nanoparticles themselves cause toxicity issues. Drawing inspiration from pro-drug nanosystems, we seek if drug molecules themselves can be directly assembled into mesoporous nanoparticles, so as to become mesoporous nanodrug formulations that combines the advantages of both small molecules and nanomaterials.

During the assembly process of mesoporous nanomaterials, amphiphilic surfactant and precursor molecules form micelles, and micelles further crosslink into mesoporous nanomaterials. Multiple interactions are involved during assembly, including hydron-bonding, covalent-bonding, π-π interaction, charge interaction, hydrophobic/hydrophilic interaction, etc., making the system extremely complicate. In the case of drug formulations, it is also required that the therapeutic function of drug molecules is not hindered, further complicating the systems.

Herein, we propose a balancing multivariant interactions approach to generate mesoporous poly-catechin. In a microemulsion system, the hydrogen bonding between catechin/catechin, catechin-F127 and the π-π interaction between catechin-toluene are finely balanced through solution composition, generating delicate mesoporous poly-catechin nanoparticles with tunable morphology. The antimicrobial and antioxidant properties of the mesoporous nanodrug formulation are then evaluated. We demonstrate that while maintaining the antimicrobial abilities of catechin, the mesoporous structure further provides unique nano-bio interactions that enable strong bacterial adhesion and thus enhanced antibacterial abilities.

Keyword：Mesoporous, nanoparticle, antibacterial.

最终交流类型：Oral

Design of MOF-derived hierarchical nanoflowers for efficient electrocatalytic activity

高俊阔

浙江理工大学

Constructing an efficient alkaline hydrogen evolution reaction (HER) catalyst with low platinum (Pt) consumption is crucial for the cost reduction of energy devices, such as electrolyzers. Herein, nanoflower-like carbon-encapsulated CoNiPt alloy catalysts with composition segregation are designed by pyrolyzing morphology-controlled and Pt-proportion-tuned metal-organic frameworks (MOFs).[1,2] The optimized catalyst containing 15% CoNiPt NFs (15%: Pt mass percentage, NFs: nanoflowers) exhibits outstanding alkaline HER performance with a low overpotential of 25 mV at a current density of 10 mA cm-2, far outperforming those of commercial Pt/C (47 mV) and the most advanced catalysts. Such superior activity originates from an integration of segregation alloy and Co-O hybridization. The nanoflower-like hierarchical structure guarantees the full exposure of segregation alloy sites. DFT calculations suggested that the segregation alloy components not only promote water dissociation but also facilitate the hydrogen adsorption process, synergistically

accelerating the kinetics of alkaline HER. Additionally, the activity of alkaline HER is volcanically distributed with the surface oxygen content, mainly in the form of Co3d-O2p hybridization, which is another reason for enhanced activity. This work provides feasible insights into the design of cost-effective alkaline HER catalysts by coordinating kinetic reaction sites at segregation alloy and adjusting the appropriate oxygen content.

Keyword： Metal-organic frameworks, oxygen evolution reaction, hydrogen evolution reaction, nanoflower, hierarchical

最终交流类型: Invited

Functional Crystalline Porous Materials

陈志杰

浙江大学

Reticular chemistry has developed into a powerful tool for the design and synthesis of porous, crystalline framework materials such as metal–organic frameworks (MOFs). In this presentation, I will introduce how fundamental reticular chemistry can be applied to the precise synthesis of targeted stable porous MOFs for the onboard storage of clean-energy gases such as hydrogen and methane. A designed ultraporous MOF shows impressive balanced gravimetric and volumetric storage performances for these gases. Additionally, I will report a generalizable and scalable approach for integrating MOFs and non-volatile polymeric bases onto textile fibers for the practical destruction of nerve agents.

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Keyword： metal–organic frameworks, porous crystalline frameworks, hydrogen and methane storage

最终交流类型: Oral

Liposome-templated Green Synthesis of Mesoporous Metal Nanostructures with Universal Composition for Biomedical Application

王金平

Hebei University of Technology

Porous noble metal nanoparticles have received particular attention recently for their unique abilities to achieve those optical, thermal, and catalytic functions desirable for biomedical needs. However, limited progress has been made to synthesize such porous metallic nanostructures with large mesopores (≥ 30 nm) due to the lack of robust fabrication methods. Here, we report a green yet facile synthesis strategy using the biocompatible three-dimensional (3D) liposome aggregates as the templates to mediate the formation of mesoporous metallic nanostructures in a controllable and universal fashion. Various monodispersed nanostructures with well-defined mesopore shape and large mesopores (≈ 40 nm) are successfully synthesized from mono- (Au, Pd, and Pt), bi- (AuPd, AuPt, AuRh, PtRh, and PdPt), and tri-noble metals (AuPdRh, AuPtRh, and AuPdPt). Along with successful demonstration on its effectiveness in synthesis of various mesoporous nanostructures, we also reveal the possible mechanism of liposome-guided formation of such nanostructures via time sectioning of the synthesis process (monitoring time-resolved growth of mesoporous structures) and computational quantum molecular modeling (analyzing chemical interaction energy between metallic cations and liposomes at the enthalpy level). These mesoporous metallic nanostructures exhibit a strong photothermal effect in a broad near-infrared region, effective catalytic activities in the hydrogen peroxide decomposition reaction, and the high drug loading capacity. Thus, the liposome-templated method provides an inspiring and robust avenue to synthesize mesoporous noble metal-based nanostructures for versatile biomedical applications.

Keyword： Biomedical applications, Liposome-templated synthesis, Noble metal nanomaterials, Large pores, Outside-in mesoporous nanostructures

最终交流类型: Invited

Metal–Organic Framework Micro-Nanoreactors

张伟娜

南京工业大学

Enzyme and chemical catalysis have greatly improved the efficiency of manufacturing chemicals, drugs, and new materials, and have received widespread attention from the scientific and industrial communities. However, the incompatible reaction conditions of these two catalysts can easily cause catalyst deactivation. The traditional solution is to perform enzyme and chemical catalysis in multiple steps, which results in high energy and material consumption, complex processes, and low yields. Therefore, if enzyme and chemical catalysis can be achieved in the same reactor under the same conditions, it can not only save energy and reduce consumption, simplify the separation and purification process, but also improve the temporal and spatial yield. However, in this system, the problems of incompatible interface between the two catalysts and poor compatibility of the two reaction systems must be solved. To address these problems, we used a MOF micro/nano reactor with micro/nano channels to separate the enzyme and chemical catalysts in physical space, and used the MOF chemical microenvironment to regulate the activity of the chemical catalyst to match the enzyme activity under mild reaction conditions, thus realizing the interactive synthesis of enzyme catalysis-chemical catalysis. We used UiO-66-NH2 as the building unit, self-assembled and encapsulated alcohol dehydrogenase (AlcDH) at the oil-water interface to prepare AlcDH@MOF micro/nano reactor, and cooperated with the metal complex Pt[(C6H5)3P]4 to show high activity and good enantioselectivity, achieving one-pot enzyme-chemical cascade reaction. The construction strategy of functional MOF micro/nano reactors provides an important research platform for developing efficient chemo-bio cascade reactions.

Keyword： Micro-nano reactor; Metal-organic framework; Chemo-bio cascade reaction

最终交流类型: Invited

Design and Application of Framework Polymer Film Materials

霍峰蔚

南京工业大学

The construction of metal–organic framework (MOF) films is a crucial step for integrating them into technical applications. However, due to the crystallization nature, it is difficult to grow most MOFs spontaneously or process them into films. Here, a convenient strategy is demonstrated for constructing MOF films by using modulators to achieve homogeneous assembly of MOF clusters. Small clusters in the early growth steps of MOFs can be stabilized by modulators to form fluidic precursors with good processibility. Then, simple removal of modulators will trigger the crosslinking of MOF clusters and lead to the formation of continuous films. This strategy is universal for the fabrication of several types of MOF films with large scale and controllable thickness, which can be deposited on a variety of substrates as well as can be patterned in micro/nano resolution. Additionally, versatile composite MOF films can be easily synthesized by introducing functional materials during the crosslinking process, which brings them broader application prospects.

Keyword：Framework polymer；Covalent-organic frameworks；Metal-organic framework；Polymerization inhibition regulation；Functional film

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最终交流类型: Invited

Supramolecular engineering of photoluminescence metal-organic materials with multi-path photon conversion

潘梅

中山大学

Taking advantage of various photophysical mechanisms and, especially, by the combination of multiple chromophore centers/origins incorporated in the metal-organic materials (MOMs), UV-OPA (one-photon absorption) or NIR-TPA (two-photon absorption) excited emissions with WLE (white light emitting), PLCT (photoluminescence color-tuning),

or LPL (long persistent luminescence) attributes can be achieved. These PL properties are further coupled with structural transitions/deformations in coordination supramolecular matrices, resulting in controllable and multi-responsive thermo/solvato/rigido/piezo/ mechano-fluorochromism, etc. Assembly and fabrication of these opto-functional MOMs into specific material morphologies or device models, various kinds of applications are implemented, including ultrasensitive water sensing, optoelectronic memoring, pressure signal harvesting and magnifying, decorating, displaying, barcoding and anticounterfeiting, and so on.

Keyword： Supramolecular engineering, photoluminescence, metal-organic materials, multi-path photon conversion

最终交流类型: Keynote

Bioinspired Nanotrap for Nuclear Fuel Resource Mining from Ocean

Shengqian Ma

University of North Texas

The long-term use of nuclear power for energy applications relies on the secure and economical supply of nuclear fuel. Among various natural sources of uranium for use in nuclear reactors, sea water is highly appealing given that the oceans contain about 4.5 billion tons of dissolved uranium, almost 1000-fold that estimated for mineral reserves. Nonetheless, the concentration of uranium in seawater is extremely low (3–3.3 mg/L or 3–3.3 ppb); this, coupled with the presence of relatively high concentration of other metal ions, makes uranium mining from seawater a daunting challenge. Inspired by the features of metalloproteins for metal binding in nature, a series of highly robust and water/chemical stable porous organic polymer (POP)-based uranium “nanotraps” have been rationally designed and investigated for efficient and effective uranium extraction from seawater.

Keywords porous organic polymer, nanotrap, seawater uranium extraction

最终交流类型：Invited

CeO2-encapsulated noble metal nanocatalysts with enhanced activity and stability

Shuyan Song

Changchun Institute of Applied Chemistry, CAS, China

Encapsulation of small noble metal nanoparticles has received attention owing to the resulting highly increased stability and high catalytic activity and selectivity. Among the types of inert metal oxides, CeO2 is unique. It is inexpensive and highly stable, and, more importantly, the unique electronic configuration gives it a strong capability to provide active oxygen. The method of fabricating CeO2-encapsulated noble metal nanocatalysts is determined by the requirements of the application. It is believed that these interesting findings can indicate a direction for the design of novel functional core@shell nanocatalysts with low cost and high efficiency. Furthermore, such a synthesis combining the autoredox and seed growth strategies is expected to be of great significance in nanosynthesis for real-world applications.

Keyword：CeO2；Noble metal

最终交流类型：Invited

Precise Synthesis and Catalytic Application of Noble Metal-based Nanomaterials

张志成

天津大学

Centering on the key issue in achieving the precise synthesis of noble metal-based nanomaterials with high atom utilization efficiency, several effective strategies, such as crystal phase engineering, defect control, dimensional confinement and so on, have been developed. The general and robust wet-chemistry approaches have been developed to fabricate noble metal-based nanomaterials at atomic scale. The high atom utilization efficiency of noble metals could be realized via the underpotential deposition, selective electrochemical etching, site-selective growth and so on. Particularly, the effect of crystal phase, facet and defect on the catalytic performance of noble metal-based nanomaterials have

been systematically investigated. Moreover, the structure-performance relationship as well as the catalytic mechanism of noble metal-based nanomaterials have been clarified.

As known, metallic nanostructures are commonly densely packed into a few packing variants with slightly different atomic packing factors. The structural aspects and physicochemical properties related with the vacancies in such nanostructures are rarely explored because of lack of an effective way to control the introduction of vacancy sites. Highly voided metallic nanostructures with ordered vacancies are however energetically high lying and very difficult to synthesize. Here, we report a chemical method for synthesis of hierarchical Rh nanostructures (Rh NSs) composed of ultrathin nanosheets, composed of hexagonal close-packed structure embedded with nanodomains that adopt a vacated Barlow packing with ordered vacancies. The obtained Rh NSs exhibit remarkably enhanced electrocatalytic activity and stability toward the hydrogen evolution reaction (HER) in alkaline media. Theoretical calculations reveal that the exceptional electrocatalytic performance of Rh NSs originates from their unique vacancy structures, which facilitate the adsorption and dissociation of H2O in the HER.

Keyword：Synthesis, metal nanomaterials, catalysis, electrocatalysis

最终交流类型: Invited

Intrinsic Chirality of Colloidal Nanostructures with Tunable Chiroptical Properties

王鹏鹏

西安交通大学

Chirality is a fundamental geometric attribute found in nature that plays important roles in diverse fields such as the study of evolutionary of processes, enantioselective chemical reactions, and spin polarization in Spintronics. While intrinsic chirality is extensively observed in organic materials, research on inorganic materials has been limited. In this presentation, I will show our recent work on the solution-phase synthesis and assembly of chiral inorganic nanostructures with intrinsic chirality originating from different sources including chiral lattices, chiral morphologies and assembled structures. Various bottom-up synthetic approaches have been developed to achieve the control of handedness and materials parameters, enabling tuning of their chiroptical properties, including circular dichroism and circularly polarized luminescence. Our study has enabled an emerging class of inorganic nanostructures with tailored chirality that is important for advancing our fundamental understanding of inorganic chirality as well as a wide range of applications utilizing inorganic chiroptical building blocks.

Keyword： chiral nanostructures, colloidal nanoparticles, circular dichroism, circularly polarized luminescence, synthesis

最终交流类型: Invited

Pore chemistry and structure control in anion-functionalized microporous materials for gas separation

邢华斌

浙江大学

That society increasingly depending upon gases as commodities and fuels means that the “age of gas” has dawned, creating with it an urgent demand for designing energy-efficient porous materials to address challenges in gas separations. However, the generally existed trade-off between capacity and selectivity of porous materials creates a major barrier toward gas separation/purification through physisorption. We reveal that basic anions with suitable pore chemistry are sensitive to subtle properties difference of hydrogen atoms of hydrocarbon molecules in addressing the challenging separation of acetylene and ethylene, and the designed anion-pillared ultramicroporous materials set new benchmarks for selectivity. The mechanism behind the impressive separation performance revealed by the neutron diffraction and modeling studies, lies on the different way of molecular recognition towards hydrocarbon molecules, hydrogen recognition instead of the common carbon recognition. The deep understanding into the anion-based pore chemistry enables the wide exploitation of the anion-based hydrogen recognition in novel anion-pillared ultramicroporous materials, ionic ultramicroporous materials, as well as the extended application in other gases, olefin/paraffin,C4 olefins, C8 aromatics, carbon dioxide, sulfur dioxide and etc. Pore size, as the key metric, determines the access of the guest molecule according to their molecular size, and is an important tool to improve the matching between guest molecules and porous materials. The size of the aperture achieves the size control within 0.1 nm scale through quantitatively stuffed heteroatom cluster, and the developed novel ultramicroporous zeolite realize the rigid sieving of other molecules from carbon dioxide, as well as the benchmark carbon dioxide capacity. Our demonstrations unravel the practical solution to improve the

separation performance by exquisite control of pore structure and pore chemistry in porous materials, and reveal the great promise of physisorption as non-thermal driven alternatives associated with low energy footprints.

Keyword： Hydrocarbon separation; Adsorption; Carbon Dioxide Capture; Metal-Organic Frameworks; Zeolites

最终交流类型: Oral

Copper Chalcogenide Nanodisks: From Localized Surface Plasmon Resonance Tuning to Photoelectrocatalytic and Photocatalytic Applications

李运超

北京师范大学

Localized surface plasmon resonance (LSPR) is well known for its unique ability to tune the reactivity of plasmonic materials via photoexcitation. Among various plasmonic materials, copper chalcogenide (Cu2-xA，A=S、Se) nanomaterials have distinguished themselves as a special kind of plasmonic material with a remarkable LSPR feature in near infrared (NIR) region, owing to the rather high concentration of free holes in their valence bands. However, untill now, it remains a great challenge to tune their LSPR peaks to better match the solar spectrum and to enhance their LSPR photostability, which are particular important for their practical applications. Keeping such challenges in mind, our group has recently made some progress in tuning the LSPR spectra, improving LSPR photostability and performing photoelectrocatalytic or photocatalytic applications of Cu2-xA nanodisks (NDs) . To be specific, we are able to tune the LSPR peak positions of Cu2-xA NDs from NIR to middle infrared region, and to significantly enhance their LSPR photostability via core-shell modification. More importantly, we have identified that the as-prepared Cu2-xA NDs possess a fascinating illumination-enhanced oxygen evolution reaction (OER) performance upon using as electrocatalysts. In particular, we have observed an unprecedented illumination-induced decrease of OER overpotential on the Cu2-xA NDs-coated NiFe LDH electrodes under xenon lamp illumination. Furthermore, we have utilized transient absorption along with Mott-Schottky measurements to disclose that the NIR irradiation generate abundant hot holes from LSPR damping in the Cu2-xA NDs accounting for the remarkable OER performance

enhancement. Very recently, we have identified that Cu2-xSe NDs are ideal photocatalyst for hydron evolution reactions (HERs). More attractively, we have achieved a ultrahigh HER rate upon hybridizing them with regular HER photocatalysts. We believe our work on the direct utilization of plasmonic hot holes in Cu2-xA nanomaterials opens up a new route to designing NIR-active photocatalysts/ electrocatalysts by exploiting their unique LSPR properties.

Keyword： localized surface plasmon resonance, Cu2-xA nanodisks, Spectrum tunning, Photocatalysis/ photoelectrocatalysis

最终交流类型: Invited

Molecular Manipulation of Heterogeneous Electrocatalytic CO2 Reduction Using Metal-Organic Frameworks

Idan Hod

Ben-Gurion University of the Negev, Israel

Electrocatalytically driven CO2 reduction reaction (CO2RR) to produce alternative fuels and chemicals is a useful means to store renewable energy in the form of chemical bonds. in recent years there has been a significant increase in research efforts aiming to develop highly efficient CO2RR electrocatalysts. Yet, despite having made significant progress in this field, there is still a need for developing new materials that could function as active and selective CO2RR electrocatalysts.

In that respect, Metal–Organic Frameworks (MOFs), are an emerging class of hybrid materials with immense potential in electrochemical catalysis. Yet, to reach a further leap in our understanding of electrocatalytic MOF-based systems, one also needs to consider the well-defined structure and chemical modularity of MOFs as another important virtue for efficient electrocatalysis, as it can be used to fine-tune the immediate chemical environment of the active site, and thus affect its overall catalytic performance. Our group utilizes Metal-Organic Frameworks (MOFs) based materials as a platform for imposing molecular approaches to control and manipulate heterogenous electrocatalytic systems. In this talk, I will present our recent study on electrocatalytic CO2RR schemes involving MOFs, acting as: i) electroactive unit that incorporates molecular CO2RR electrocatalysts, or ii) non-electroactive MOF-based membranes coated on solid CO2RR catalysts.

Key Words Metal-Organic Frameworks (MOFs); Electrocatalysis; CO2 Reduction Reaction (CO2RR); Secondary-Sphere; Molecular Catalysts.

最终交流类型：Invited

Coordination-Assembly of Functional Supramolecular Rare-Earth Complexes

孙庆福

中科院福建物构所

Coordination supramolecular complexes hold great potential in sensing, biomimetic catalysis, stabilization of fleeting species, drug-delivery et al. By employing the coordination-driven self-assembly strategy, numerous of metallocycles/cages constructed with transition metals have been reported. While rare-earth ions have a lot of optical, electromagnetic and catalytic properties to offer to the aesthetically appealing 3D supramolecular edifices, coordination-assembly with rare-earth metals is difficult due to their unpredictable and labile coordination numbers/geometries. We are interested in the rare-earth supramolecular chemistry, in particular on their controlled assembly, fine-tuned photophysical properties and applications of functional supramolecular rare-earth complexes (SRECs). Recently, precise synthesis of SRECs with different molecular composition and geometry has been accomplished in our group. Their photophysical including chiroptical properties have been investigated, with proof-of-concept applications such as high selective and efficient sensing toward biological relevant molecules/ions, ion separation, luminescent thermometers, bio-imaging, MRI contrast agents and chiral catalysis et al. We envisage these SRECs will find great potential in both biomedical and material fields.

Keyword：Coordination-assembly; Rare-earth; Supramolecular; Luminescence; MRI

最终交流类型：Oral

Mesoporous silica nanoparticles mediate siRNA delivery for long-term multi-gene silencing in intact plants

蔡垚

国家纳米科学中心

RNA interference (RNAi) is a powerful tool for understanding and manipulating signaling pathways in plant science, potentially facilitating the accelerated development of novel plant traits and crop yield improvement. The common strategy for delivering siRNA into intact plants using agrobacterium or viruses is complicated and time-consuming, limiting the application of RNAi in plant research. Here, we reported a novel delivery method based on mesoporous silica nanoparticles (MSNs), which allows for the efficient delivery of siRNA into mature plant leaves via topical application without the aid of mechanical forces，achieving transient gene knockdown with up to 98% silencing efficiency at the molecular level. In addition, this method is non-toxic to plant leaves, enabling the repeated delivery of siRNA for long-term silencing. White spots and yellowing phenotypes were observed after spraying the MSN-siRNA complex targeted at phytoene desaturase and magnesium chelatase genes. After high light treatment, photobleaching phenotypes were also observed by spraying MSNs-siRNA targeted at genes into the Photosystem II repair cycle. Furthermore, we demonstrated that MSNs could simultaneously silence multiple genes. Our results suggest that MSN-mediated siRNA delivery is an effective tool for long-term multi-gene silencing, with great potential for application in plant functional genomic analyses and crop improvement.

Keyword：mesoporous silica nanoparticles, siRNA delivery, gene silencing, plant biotechnology

最终交流类型: Invited

Nanoporous Photonic Glass

何进

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Transparent nanoporous glass (NPG) is a promising optical material, which inherits the excellent physical and chemical stability of inorganic glass with a high specific surface area and pore structure. Due to its unique properties, the NPG has found wide applications in the manufacturing of nanofilters, substrates for biological preparations, photonic crystal fiber laser and the production of micro-optic components. The most typical NPG, which is well known as Vycor glass commercialized by Corning company, was fabricated using spinodal

decomposition in multi-component oxide glass and leaching out one of the decomposed phases with the acid solution. However, heat-treated phase separation technology is highly limited in expanding the chemical and nanoporous structure design of new NPG. Sol-gel process, which inherently creates nanopores via the hydrolysis and condensation reactions of metal salts, offers a distinct pathway to fabricate NPG. Recently, we and collaborators developed a template-free sol-gel route using metal chelates, which results in transparent nanoporous fully polymerized glasses in several compositional systems including AlPO4, AlPO4-SiO2, Al2O3-SiO2. In this sol-gel route, organic chelating ligand leads to a gel with 3D continuous structure of the preceramic metal-organic polymer, which is pyrolyzed to form a transparent NPG. Nanoporous glasses offer great advantages for designing functional devices via the nano-confined growth or loading of target functional molecules or nanoparticles. The rational design of NPG via this efficient sol-gel route results in a new optoelectronic device-relevant material platform.

Keyword：Sol-gel, Nanoporous, Photonic Glass

最终交流类型: Oral

Understanding the Electrochemical Sensing Interfaces: Charge Transport and Electronic Structure

蔡彬

山东大学

Electrochemical sensors have attracted great attention in various fields. The sensing performance depends heavily on the charge transfer process, binding of the analyte, and the electrochemical reactions. Thus, understanding of the charge transfer pathways, structure-performance relationship, and reaction mechanisms is of great significance for optimizing sensing performance and developing next-generation electrochemical sensors. The first part of this talk will focus on the charge transfer mechanism of electrochemiluminescence (ECL). The ECL generation upon quantum dots (QDs) has been studied over the past two decades. However, it is challenging to differentiate the two possible routes to generate excitons, namely an intraparticle charge-transfer route between radicals of a coreactant and a QD, or an interparticle charge-transfer route between two QD radicals. The main obstacle lies in the hardly controllable charge transfer between/within coreactants and QDs. We designed an aerogel structure to enhance the electronic coupling between QDs, and successfully obtained direct experimental evidence of the inter-particle charge transfer by matching the energy levels of different QDs and selecting appropriate coreactants. Next, this talk will explore how the electronic structure affects the sensing performance. Revealing the structure-performance relationship and reaction mechanism of the interface is crucial to developing electrochemical sensors. Generally, the modulation of the electronic structure is accompanied by changes in the geometric structure, causing complex and intertwined variation problems. We designed Hg-Pd alloy and Ni-based MOF materials with robust geometric structures to achieve a systematic study of the electronic structures and revealed the structure-performance relationships of Pd and Ni sites. By applying this knowledge in the design of novel sensors, a large increase in sensitivity has been achieved for detecting biochemical molecules and metal ions.

Keyword：Aerogel, Quantum Dots, Nanocrystals, Electrocatalysis, Sensors

最终交流类型: Oral

Fabricating and tunning liquid nanoparticles through controlling of liquid-liquid nucleation and growth

王若徐

西湖大学

A solvent-induced phase separation (SIPS) approach[1] has been developed to synthesize nanoscale droplets in a manner analogous to solid nanoparticle synthesis. By introducing kosmotropic solutes into infinitely miscible water-ethanol solutions, liquid-liquid phase separation can be triggered through nucleation and growth processes that closely resemble those of solid nanoparticles. The droplets thus produced are liquid nanoparticles that can be manipulated with the same methods used for solid nanoparticles to control their shapes and structures. We have developed ways to encapsulate these nanoscale droplets in various materials, resulting in hollow nanocapsules made of silica, polymers, metal oxides, magnetic materials, insoluble salts, and metal-organic frameworks (MOFs). These nanocapsules can serve as nanoreactors and drug delivery vehicles. The key feature of SIPS is its ability to adapt the synthetic methods of solid nanosynthesis to droplets, enabling many possibilities.

Based on SIPS, we have achieved heterogeneous nucleation of liquids in addition to homogeneous nucleation. The heterogeneous nucleation of liquids on liquid nanoscale droplets allows us to fabricate multilayer hollow nanoshells. We have also reproduced seeded growth, a classic method of solid nanoparticle synthesis, in liquids[2]. With carbohydrates as kosmotropic solutes, sugar solutions were heterogeneously nucleated on solid nanoparticle seeds to yield yolk-shell nanostructures. This approach is highly generalizable and robust, applicable to nanoparticles with various capping ligands.

We have captured early intermediates in the SIPS process and found that extraction occurs during nanoscale droplet growth.[3] Combined with silica encapsulation, rapidly growing droplets can burst the silica shells to form broken nanocapsules. By tuning the extraction rate and shell formation rate, eccentric hollow nanostructures can be obtained.[4] Overall, the SIPS approach allows the adaptation of solid nanosynthesis methods to droplets, opening up many possibilities.

Keyword： Droplet, Nucleation, Hofmeister series, Kosmotropicity, Hollow nanostructures.

最终交流类型: Oral

Surface Engineering of Nanoporous Metal-Organic Frameworks for Chemical Sensing

涂敏

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Chemical sensors play significant roles in myriad areas, such as medicine, industrial processes, and air quality monitoring systems. Although they have been used in various areas, the improvements in their performances would open up a range of new opportunities. As a novel class of crystalline porous materials, metal-organic frameworks (MOFs) have been considered potential candidates as sensory materials for chemical sensing.[1] The applications of MOFs in chemical sensors require developing microfabrication techniques to integrate them into signal transduction devices.

We developed a robust deposition technique that enables high-quality MOF thin film deposition with a controllable thickness.[2] In addition, we pioneered direct, resist-free patterning of MOFs by X-ray and e-beam lithography, which allows high-quality patterning with record sub-50-nm resolution.[3] Several MOFs-based chemical sensors have been implemented into signal-transduction schemes, including quartz crystal microbalances, surface acoustic waves, and diffraction gratings.[4-5] These sensors have shown sensitive and selective sensing performances towards various volatile organic compounds. The effects of MOF pore size, pore opening, surface functionality, and structural flexibility on sensing performances are systematically investigated. The promising results would benefit the integration of MOF-based sensors in the application of array-sensing technology.

Keyword： nanoporous materials, nano-scale patterning, metal-organic frameworks, thin films, chemical sensing,

最终交流类型: Oral

Ligand-Mediated Surface Structure Regulation of Noble Metal Nanomaterials and Their Catalytic Properties

刘墨宣

西安科技大学

Noble metal nanomaterials are widely used in catalytic reactions due to their unique physicochemical properties. Noble metal nanomaterials play an irreplaceable role in many important catalytic reactions. For example, Pt-based nanomaterials are the optimal catalyst for the cathode oxygen reduction reaction (ORR) in proton exchange membrane fuel cells and Ru (Ir)-based nanomaterials are the excellent catalysts for the anodic oxygen evolution reaction (OER) in the electrolysis of water to produce hydrogen. However, low abundance and high cost limit the practical application of noble metals. Facing the increasing demand for noble metal nanomaterials, researchers urgently need to design efficient catalysts to solve this problem. Since the catalytic reaction occurs on the surface of the catalyst, the surface structure of the noble metal nanomaterial is the key to its catalytic activity and selectivity. Based on this, we developed a series of ligand-assisted synthesis methods, starting from the "bottom-up" and "top-down" approaches to achieve the controllable construction of the surface structure of noble metal nanomaterials. The controllable construction significantly improved the selectivity and activity of the fuel cell electrode reaction. For example, through the coordination of small molecular ligands, we effectively reduce the reduction potential of Pd precursors, thus constructing unconventional core-shell structures, and finally effectively regulating the surface strain of Pd-based catalysts[1]. In addition, we also use the large difference of adsorption energy of small molecular ligands on different metal surfaces to

achieve the self-terminated growth of Pt, and obtain Pt-based catalysts with single atomic structure[2].

Keyword：Noble metal, surface structure, ligand, strain, ensemble size

最终交流类型: Invited

‘MOLECULAR COMPARTMENTS’ CREATED IN METAL-ORGANIC FRAMEWORKS FOR PHOTOCATALYTIC CO2 OVERALL CONVERSION

邓鹤翔

武汉大学

‘Compartmentalization’ is an effective strategy to enable efficient collaboration between various functional units in biological system. However, creating such ‘molecular compartments’ in artificial solid-state materials still faces many challenges. Metal-organic frameworks (MOFs), with a plethora of choice of topologies, offer modifiable and periodic pore structures ideally suited for the spatial arrangement of substances utilizing their pores. Therefore, we propose a strategy of constructing ‘molecular compartments’ by filling nanoparticles into MOF pores. In our research, we found that when semiconductor nanoparticles are filled in MOF pores non-destructively, the resulting composites allow for synergy between the nanoparticles and the MOF backbones, and achieve high photocatalytic CO_2 overall conversion efficiency. The modifiability of MOFs and the diversity of guest nanoparticles are two main aspects of ‘molecular compartments’. On the one hand, different pore sizes and chemical environments lead to different catalytic performance. On the other hand, by selecting guest semiconductors with different bandgap widths, ‘molecular compartments’ responding to different light regions can be synthesized. Specifically, the composite, 42%-TiO_2-in-MIL-101-Cr-NO_2, where 42 weight percent of TiO_2 nanoparticles are filled in nitro modified MIL-101-Cr, achieves a CO_2 conversion rate of 12 $mmol\cdot g^{-1}\cdot h^{-1}$ under UV light and an apparent quantum efficiency (AQE) of 11.3% at 350 nm. Another ‘molecular compartments’, constructed by narrow band semiconductor, namely, 24%-$WO_3\cdot H_2O$-in-MIL-100-Fe, is capable of reducing CO_2 under visible light and its AQE at 420 nm reaches 1.5%. This ‘molecular compartment’ strategy not only represents a new way to explore customized catalysts, but also provides some guidance for the design and application of MOFs.

Keyword：Metal-Organic Framework; Photocatalytic CO2 conversion; Molecular Compartment

最终交流类型: Invited

Directional Bonding of Inorganic Nanoparticles Like Atoms

聂志鸿

复旦大学

Molecules are the most important building blocks of matter. They exhibit astonishing precision in the arrangement of atoms and are capable of assembling into functional structures with high complexity and diverse functions. The ability to organize organic or inorganic nanoparticles into molecular-like nanostructures holds great promises to manipulate matter at nanoscale scale and to exploit the emergent optical, electronic, or magnetic properties of nanoparticle ensembles. In this talk, I will present our efforts to the design of functional nanoscale colloidal molecules and polymers through directional assembly of nanoparticles, as well as the development of new materials (e.g., metasurfaces and metamaterials) from these nano-molecules.

Keyword：Inorganic nanoparticles, Self-assembly, Colloidal molecles, plasmonic, metamaterials

最终交流类型: Oral

Electrostatic Self-assembly of Inorganic Nanoparticles

卞僮

东南大学

Nanostructured materials assembled from inorganic nanoparticles (NPs) exhibit a wide range of beneficial electronic, optical, and catalytic properties. Coulombic interactions represent an attractive means to assemble NPs into higher-order structures, and ultimately materials; however, they often lead to kinetic traps in the form of amorphous aggregates. Here we report a new strategy to assemble charged NPs functionalized with dense layers of charged ligands (superionic NPs) into crystalline assemblies of unprecedented quality. By employing Coulombic interactions, it is possible to mediate the assembly of superionic NPs with oppositely charged partners like structure simple small molecules, polymers, and also NPs. With that, a variety of well-ordered nanostructures are obtained, which we believe would greatly facilitate the fabrication of nanostructured materials and harnessing their applications in catalysis, sensing, and photonics.

Keyword：Self-assembly, Coulombic interaction, Superionic nanoparticles, Small molecule, Polymer

最终交流类型: Invited

Synthetic Chemistry of Multicomponent Metal-Organic Frameworks

李巧伟

复旦大学

Metal-organic frameworks (MOFs) are usually constructed by one kind of metal and one kind of organic link. It remains a challenge to increase the number of components in one single framework, since the installation of multiple components in a well-ordered framework requires careful design of the lattice topology, judicious selection of building blocks, and precise control of the crystallization parameters. In this talk, I will present several strategies to introduce multiple metals and linkers, in an ordered way, into one framework. We created ordered metal vacancies and linker vacancies in a cubic MOF by symmetry-guided removal of the metal ions and the linkers. By filling the vacancies with new metals and new linkers, new single-crystalline MOFs with four components (two metals and two linkers) are introduced. Furthermore, multinary MOF structures were prepared by consolidating two metal ions with distinct coordination preferences and geometries, and two or three different linkers, achieving quaternary and quinary MOFs. We have further shown that the valence of the Cu ions can be switched between Cu(I) and Cu(II) without destroying the framework in these multinary MOFs. The redox chemistry of these open metal sites was further evidenced by H_2O_2 decomposition, CO oxidation, and demonstrated for photodynamic therapy.

Keyword： Metal-Organic Frameworks, Crystal Engineering, Multicomponent, Water Harvesting, Photodynamic Therapy

最终交流类型: Oral

Rational Synthesis and Application of Semiconductor-Based Nanoheterostructures

吴雪军

南京大学

Heterostructures, integrating distinct components with different functionalities into one system, have attracted tremendous attention due to their fascinating synergistic properties. However, it is still a great challenge to delicate control of the spatial composition, morphology, interconnection, and integration of the components into well-defined nanoheterostructures. In this talk, I will summarize our recent research on the design and synthesis of nanoheterostructures from simple to complex with controlled architectures. The main content including three parts: 1) Seed-mediated heat-up approach has been developed for large-scale synthesis of high-quality II-IV core/shell QDs with intriguing optical properties, i.e., a narrow photoluminescence emission peak, near-unity PL quantum yield, and suppressed blinking. 2) A variety of dimensional heterostructures with complex hierarchical architectures were successfully obtained by epitaxial growth through delicate tuning the crystal structures and exposed facets of the 1D(2D) nanostructures as seeds. 3) A noble metal-seeded epitaxial growth strategy is used to prepare highly symmetrical noble metal-semiconductor branched heterostructures with desired spatial configurations, albeit a large lattice mismatch (more than 40%). These heterostructures exhibit an enhanced properties or/and better performance as phototransistor and water splitting catalyst compared with that of a single-component counterpart. The enhancement results from the formation of internal field in heterojunction which can improve the electron-hole separation under light excitation. Our research works provide an effective strategy for the rational design of nanoheterostructures and enriches the varieties of hierarchical nanostructures, which are fundamentally important in material science and chemistry and might have various promising applications.

Keyword： heterostructure; semiconductor; controlled synthesis; interface; optoelectronic device

最终交流类型: Invited

Synthesis and Reactivity of Polynuclear Organometallic Clusters

Liang Zhao

Tsinghua University, China

Polynuclear organometallic clusters, featured by the aggregation of several interactive metal atoms through the linkage of metal-metal interactions and metal-carbon bonds, have been deemed as an elusive intermediate in the catalytic process of metal cluster-based catalysts or heterogeneous metal catalysts. We have endeavored to establish a general synthetic strategy to achieve controllable synthesis of multinuclear organometallic clusters. Inspired by the template synthesis in supramolecular chemistry, we tried to utilize macrocyclic ligands, polyanionic species and coordinative ligands as a template to guide multimetallic assembly and achieve structurally well-defined polynuclear organometallic clusters. Our investigation revealed that a kind of flexible macrocycle showed a significant cooperative coordination effect in the metal ion binding process, which facilitated the easy formation of a polymetallic assembled structure. Taking advantage of the cooperative coordination effect and the tunable and highly fluxional conformation of macrocyclic ligands, we laid our focus on the nuclearity number control by tuning the size of macrocycles and their adaption with different organic anionic centers in metal cluster synthesis. Furthermore, a cluster-to-cluster transformation inside the cavity of macrocyclic ligands has been presented to showcase the use of the acquired metal cluster-macrocycle complexes to achieve unconventional metal cluster entities. In addition, the encapsulation of organometallic species within an organic macrocycle followed by a further steerable transformation provides a viable pathway to achieve organometallic nanocluster intermediates. In this talk, I will present the synthesis of several hexakis aromatic vicinal dicarbanion-protected Ag13/Ag15 silver nanoclusters by the reductive elimination and assembly of protonated aryl dicarbanion-Ag4 clusters, which are generated from the acidification of polymetalated aromatic complexes protected by a macrocyclic ligand. The successful determination of the bipyridine coupling product validates the intermediate characteristic of Ag13/Ag15 silver nanoclusters by further

acidification, which provides inspiration for the potential advantage for further organometallic transformation. The acquired key organometallic cluster intermediates facilitate our understanding of the transformation details for various organic or small molecule substrates when multimetallic complexes are utilized as catalysts.

Keywords Polynuclear Organometallic Clusters

最终交流类型: Invited

Inorganic chiral nanoparticles to disclose origin of homochirality

黄陟峰

香港中文大学

as attached

Keyword： inorganic chiral nanoparticles; optical activity; enantiospecific interactions; homochirality; glancing angle deposition.

最终交流类型: Invited

Chiral inorganic nanoparticles for disease therapy

匡华

江南大学

Chiral inorganic nanomaterials were found similarities with biological molecules in size, shape and geometric conformation. We have found that truncated CdTe nanoparticles could cut DNA specifically, similar to natural enzymes . Unique chiral CuS nanoparticles recognized tobacco mosaic virus(TMV) and cut the coating protein selectively. Recently, we found the chiral inorganic nanomaterials can resist the digestive system and cross talk with gut microbiota. The mirror nanomaterials showed differentially effects in bacteria metabolism, which lead to neurodegenerative Disease improvement. We believe that the chirality design of nanomaterials is very crucial in bioapplication and shape nano research.

Keyword： chiral nanomaterials , differential biological effects

最终交流类型: Invited

Molecular and Polymeric Porous Nanostructures Enabled by Dynamic Covalent Chemistry

Wei Zhang

University of Colorado Boulder

Dynamic covalent chemistry (DCvC) has proven to be highly effective toward the construction of well-defined molecular architectures and structurally ordered polymers. The error-correction mechanism enabled by the reversible formation of dynamic covalent bonds leads to the formation of structurally ordered, thermodynamically favored species. One such example is the solvothermal synthesis of covalent organic frameworks (COFs) with periodic structural order and low defect density. The chemical compositions of such frameworks are usually well-defined and inter-monomer connectivity (covalent bonding) is very robust. Bottom-up synthesis of covalently linked polymers through DCvC has many critical advantages, such as easy tunability of functional and structural properties in a controlled fashion through rational design of the precursors, formation of highly stable linkages, minimized structural defect, and possible access to sophisticated architectures that are hard to obtain otherwise. This talk will focus on our recent progress in the development of two types of DCvC, namely spiroborate exchange and dynamic nucleophilic aromatic substitution (DySNAr). These powerful synthetic tools enabled the bottom-up design and synthesis of a variety of molecular and polymeric porous nanostructures, including organic molecular cages (OMCs), ionic covalent organic frameworks (ICOFs) and an unprecedented single-crystal DNA-like helical covalent polymer (HCP).

Keywords Covalent organic framework, dynamic covalent chemistry, organic molecular cage

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最终交流类型: Invited

Nanoionics-based Emerging Room Temperature Conductance Quantization Effects

李润伟

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Moore's law has been long-term driving the scaling down of electronic devices which promotes innovations in information science and underpins the development of big data, the Internet of Things, and artificial intelligence technologies. So far, further device minimization toward atom size is constrained by the challenges in semiconductor manufacturing and the current leakage and heat dissipation problems incurred by quantum effects. Atomic point contact is a one-dimensional atom chain that shows quantized conductance states, holding the potential for ultrahigh-density information storage, in-memory computing, and multiple information functionalities integration. Atomic point contacts can be achieved by nanoionics approaches, where the electric field drives the redistribution of ions at the atom scale. However, utilization of such technologies for application is difficult, as it demands the precise manipulation of ions at the atomic scale and tuning the room temperature quantized conductance states.

In this talk, we report on our latest progress in the engineering of room-temperature quantum conductance effects in nanoionic devices through materials and multi-field control methods. On the one hand, using two-dimensional material with atomic layered structures, we controlled ion transport and tune the configuration of the atom-scale point contact. We discovered the fractional quantum conductivity effect at room temperature, which increases the storage density by an order of magnitude. On the other hand, we combined the light illumination and electrical approaches to concurrently control the transport of ions in photosensitive halides, leading to new photo-quantum conductance effects. This observation allows for the high-precision regulation of quantum conductance states, and enables the integration of computing and storage of optoelectronic information. Finally, we prospected the application prospects of nanoionc devices based on quantum conductance effects for next-generation high-performance electronics.

Keyword： Nanoionics, Conductance quantization effects, High-density information storage, Multifunctional integration

最终交流类型: Oral

Heteropolyacids Induced Synthesis of Titania Nanostructures

Bilal Akram

Women University of Azad Jammu & Kashmir

To exploit the unprecedented features of the nano building blocks at macroscale, the bottom-up fabrication of precisely tunable assembled structures has been extensively investigated. Instead of alike individual building blocks, the rationally designed assembly structures are anticipated to have combinatorial properties. Among different nanobuilding blocks, heteropolyacids (HPAs) are a promising class of structurally well-defined nanoclusters having unprecedented physical properties. Owing to discrete nanometric size, multiple coordination sites, and dynamic ability to form extended structures, HPAs offer numerous opportunities to develop new functional materials.[1] Despite owing all these merits, the progress in the co-assembly of HPAs cluster and other unrelated (like inorganic) materials is still very limited. To design HPAs based advanced functional nanoarchitectures through controlled harnessing of various interactions between HPAs nanoclusters and other inorganic nuclei, will be the theme of my talk.

A new one-step solution-based assembly system of POMs nanoclusters and other inorganic materials has been developed which provides an enormous control on size, shape, and stability of the resulting hybrid structures.[2] By effective exploitation of various non-covalent interactions between the POMs and other inorganic nanobuilding blocks, we have achieved several unprecedented co-assembly structures.[3-5] All co-assemblies form through the precisely ordered organization of two distinct nanobuilding blocks.

Several HPAs based titania co-assembled nanostructures have been constructed, which not only exhibit enhanced catalytic efficiencies towards various organic reactions but also provide easy and fast catalyst recovery from the reaction system. A library of co-assembled multidimensional superstructures has been obtained by varying various experimental conditions.

Keywords Polyoxometalates, co-assembly, superstructures, inorganic material, oxidation catalyst.

最终交流类型: Invited

Toward Total Synthesis of Molecular Metal Nanomaterials

姚桥峰

天津大学

Atom-by-atom customization of nanomaterials represents the most ambitious dream of materials scientists. Such dream should be rooted in total synthesis of nanoparticles (NPs), where NPs could be produced at atomic precision with known step-by-step reactions.

Here, we present such precise synthesis and functionalization chemistry could be revealed by employing thiolate-protected metal nanoclusters (NCs) as paradigm NPs (Fig. 1). Based on advanced mass spectrometry (and tandem mass spectrometry) analyses, we are able to trace the size-growth (including reduction growth and seeded growth), alloying reaction and ligand exchange of Au and Ag NCs with isotope resolution, unraveling their constituting step-by-step reaction maps at molecular and atomic levels. Specifically, we identify the driving force (e.g., 2 e- reduction), initiation step (e.g., selective adsorption of reductive species on the growing metal core) and detailed size growth patterns for the size growth reaction of metal NCs. We also find that the alloying and ligand exchange reactions could be uniformly driven by a surface motif exchange (SME) mechanism. Such synthesis and mechanism exploration also facilitates further development (e.g. crystallization and sustainable applications) based on high quality NCs.

Keyword: Metal Nanoclusters, Atomic Precision, Precise Synthesis, Controlled Assembly, Growth Mechanism

最终交流类型: Invited

Porous Organic Materials for Metal-Free CO2 Capture and Electrocatalytic Conversion

Charles Frederick James Faul,Charl F. J. Faul

University of Bristol

In the quest for new materials to help to solve global challenges, we have focused our efforts in recent years on the production of functional porous polymeric materials.[1a, b] The focus in this presentation will be on various strategies we are employing to tune both structure and function in these materials, and how we exploit this control to address the significant challenge posed by the high levels of CO_2.

The field of microporous conjugated polymers (CMPs), especially nitrogen-rich 3D CMP analogues of the well-known conducting polymer, poly(aniline), will be introduced.[2] Various simple design rules will be explored, showing the successful use of simple inorganic salts to carefully tune porosity, pore size distributions, as well as CO_2 uptake with high

selectivity.[3a, b] The versatility of these materials will be shown in their application for gas capture, and routes to the electrocatalytic conversion and fixation of CO_2 as useful feedstock into high value chemicals will be explored.[4a, b] Future focus areas of research will also be highlighted.

Keywords porous organic materials, CO2 capture, CO2 conversion, energy storage

最终交流类型:

Bioresponsive MOF-based nano-antibacterials against refractory implant-related infections

苏政

中国科学技术大附属第一医院

There is an increasingly growing demand for nonantibiotic strategies to overcome drug resistance in bacterial biofilm infections. Here, a novel “gas-sensitized hyperthermia” strategy is proposed for appreciable bacteria killing by the smart design of a metal-organic framework (MOF)-sealed Prussian blue–based nanocarrier (MSDG). Once the biofilm microenvironment (BME) is reached, the acidity-activated MOF degradation allows the release of diallyl trisulfide and subsequent glutathione-responsive generation of hydrogen sulfide (H2S) gas. Upon near-infrared irradiation, H2S-sensitized hyperthermia arising from MSDG can efficiently eliminate biofilms through H2S-induced extracellular DNA damage and heat-induced bacterial death. The generated H2S in the biofilm can stimulate the polarization of macrophages toward M2 phenotype for reshaping immune microenvironment. Subsequently, the secretion of abundant regeneration-related cytokines from M2 macrophages accelerates tissue regeneration by reversing the infection-induced pro-inflammatory environment in an implant-related infection model. Collectively, such BME-responsive nano-antibacterials can achieve biofilm-specific H2S-sensitized thermal eradiation and immunomodulatory tissue remodeling, thus realizing the renaissance of precision treatment of refractory implant-related infections.

Keyword：metal-organic framework, hydrogen sulfide, implant-related biofilm infections, immunomodulation

最终交流类型：

Sub-nanomaterials for Photo/Electro-catalytic CO2 Reduction: Achievements, Challenges, and Opportunities.

Kiran Zahra

Tianjin University

With the increasing dilemma of energy crisis and climate change caused by excessive greenhouse gas emissions, it is an effective way to design low-cost and efficient catalysts to recycle CO_2 into value-added chemicals and fuels to solve these problems. Downsizing catalysts close to a single crystal cell, sub-nanomaterials(SNMs) show unique size-dependent properties and great potential applications in CO_2 reduction reaction (CO_2RR) compared with conventional nanomaterials. In this review, basic principles of CO_2RR and brief classification of SNMs are elucidated. Then, recent advances of SNMs in photo/electrocatalytic CO_2RR are comprehensively summarized. Finally, the current challenges and future outlooks are emphasized to pave the development of CO_2RR on SNMs.

Keyword：Sub-nanomaterial; CO2 reduction; Electrocatalysis; Photocatalysis; Photoelectrocatalysis

最终交流类型: Invited

Microfabrication and devices for optoelectronic functional materials

吴雨辰
中国科学院理化技术研究所

The advanced manufacturing and information technology industry represented by integrated circuits is an important strategic development direction for the country. With the development of nanotechnology in the past decades, a variety of nanomaterials with excellent properties have been produced, but these materials are incompatible with traditional inorganic semiconductor micromachining technology and are difficult to be integrated into optoelectronic devices. Solution-processing technology with mild conditions is a key pathway to introduce nanomaterials into optoelectronic functional devices. To control the macroscopic patterning construction and microscopic orderly assembly of materials during solution processes has become a key technological bottleneck for the industrial development of high-performance optoelectronic functional devices. To this end, the reporter has developed a liquid-bridge-confined lithography from the key medium of solution processing, the interface, by combining the synergy of interface microstructure and chemical modification. In the macroscopic liquid film, the reporter has found that the Laplace pressure, which is inversely proportional to the radius of the liquid meniscus, can balance the adhesion force at the solid-liquid interface, yielding a continuous and uniform dewetting process. Therefore, modulating the local capillary force gradient distribution through designing the distance between micropillars induces controlled contraction of the liquid film to form patterned micro-liquid bridges for the accurate regulation of the structure size. In the micro-liquid bridge, modulating the dynamic balance of evaporative capillary flow and Marangoni flow through regulating the wettability of substrate, the length of liquid bridge and the evaporation rate of solvent can generate a low-speed flow zone to extend the relaxation time of structural units. Long relaxation time ensures the orderly assembly of structural units at the near thermodynamic equilibrium state, which enables the preparation of large-area, high-precision patterned micro-single crystals and the construction of high-performance optoelectronic devices and functional coupling devices. This liquid-bridge-confined lithography can achieve the long-range-ordered patterning of various functional materials, including organic small molecules, polymers, inorganic materials, complex materials, and micro/nanoparticles.

Keyword:functional materials, optoelectronic devices, pattern, interface confinement, liquid transportation

最终交流类型: Invited

Two-dimensional field-effect transistor sensors

魏大程
Fudan University

Two-dimensional field-effect transistor (2D-FET) sensors are one of the frontier research fields of advanced sensing technologies. These materials have large surface area and ultra-thin thickness approaching the physical limit, which give rise to remarkably enhanced sensitivities. On the other hand, all of the electron processes take place at the material surface or interfaces. The interfaces will largely influence the performances. Thus, the interfacial modulation is an important scientific question. This research is focused on the interfacial modulation of the 2D-FET sensors. Main results include: new methods are developed to controllably produce high quality 2D sensing materials and the interfaces of the 2D-FET sensors[1]; a new approach is demonstrated to improve the interface between the semiconductor and the dielectric substrate by using conformal h-BN[2]; new mechanisms such as giant photoelectrical-gating effect, photoelectrical enhancement effect of molecular crystals at 2D limit, controllable charge doping at the sensing interface, etc. are developed to modulate the electron processes at the sensing interface, which improves photoelectrical or chemical sensing performances of 2D-FET sensors[3-5]. As an application, we fabricate 2D-FET sensors for nucleic acid detection of SARS-CoV-2, showing ultra-high sensitivity.

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Keyword:two-dimensional sensing materials; field-effect transistors; photoelectrical sensors; chemical sensors; interfacial modulation; sensing interface

最终交流类型: Invited

Tuning the exciton dynamics of organic semiconductors: singlet fission vs charge separation

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Singlet fission (SF), a multiple exciton generation process that generates two triplet excitons after the absorption of one photon, can potentially enable more efficient solar cell designs by harvesting energy normally lost as heat. While the growing field of intramolecular SF has established important structure-function relationships that can be used to optimize exciton dynamics for isolated molecules in solution, it has not been shown that these characteristics can be consistently maintained in films. This is a major outstanding issue for the field, as it is essential to establish the molecular control of SF dynamics in the solid-state due to the inherent necessity of the condensed phase for devices. Recently, great efforts have been focused on deeply understanding the SF mechanism, particularly with regard of the role of the charge transfer (CT) state. The acknowledged theoretical model of SF assigns an essential mediating role to CT states which exhibit strong coupling to singlet and triplet pair states and drive ultrafast SF process. It has been shown that contribution from high-lying CT state could lower the energy of multiexciton state and promote the mixing of 1(S1S0) and 1(TT) state to enable singlet fission, while the low-lying CT state in polar solvent would collapse to the charge separation state and thus inhibited SF process. Varying the energy of CT by side-group engineering strategy, CT states could mediate SF via a virtual or distinct form in pentacene dimers.

Our group is interested in the design and synthesis of novel SF-capable conjugated small molecules and polymers, as well as the underlying SF mechanism of new materials. Very recently, we have achieved independent control of the singlet and triplet decay in the condensed phase by using “molecular engineering” approach, and developed a new design principle for intramolecular SF, I would like to show the latest results from our lab with the audiences.

Keyword: Organic semiconductor, exciton dynamics, singlet fission, ultrafast spectroscopy

最终交流类型: Invited

Multi-scale interfacial modulating organic optoelectronic devices

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The development of organic optoelectronic devices is highly desirable for applications in electronic skins, foldable displays, energy storage, medical diagnosis, and bioelectronics. Interfaces are widely present in organic optoelectronic devices and are crucial for their performance and applications. Therefore, the research on device interfaces is of great significance. In organic field-effect transistor, the interface between insulating layer and semiconductor is one of the most important interfaces. Herein, how to obtain high-quality insulating layer interfaces directly determines device performance and integrated applications. As we all know, an appropriate gate dielectric is one of the most critical components determining the performance of a device, since the conducting channel locates at the dielectric-semiconductor interface, which affects the growth, morphology, crystallinity, and traps of organic semiconductor. In order to further study the structure-activity relationship between device interface and performance, the functional groups, chain structures, and aggregated state structures of the insulating layer are investigated. On this basis, we further study the transport mechanism of charge carriers and the multifunctional applications of devices, such as the preparation of integrated devices for artificial vision systems such as "sensing, memory and computing".

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Keyword:interface modulation, organic semiconductors, artificial vision systems

最终交流类型: Invited

The preparation of high-resolution and planar asymmetric heterogenous junction

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One of the unique advantages of molecule-based semiconductors lies that the easy construction of nanoscale device by self-assembly technique. Thanks to the powerful tool of synthesis chemistry and the rich supramolecular chemistry, organic molecules could form nanomaterials with adjustable structures and controllable dimensionalities. The device applications of such organic nanomaterials will fuel the development of organic optoelectronics and phontonics.[1,2] Recently, we have made breakthrough in the self-assembly of polymeric semicondcuting nanofibers of P3HT, and have figured out the challenge of re-distributing these nanofibers in orthogonal solvent. In detail, we succefully obtained P3HT nanofibers being well-dispersed in hexane/ethonal mixture solvent and showed uniform nanofibers film assembling at water surface made of P3HT nanofibers. This nanofibers film could be transferred onto arbitary substrates. Most importantly, such a P3HT nanofiers colloidal film could be patterned highly-precisely through a standard photolithography and lift-off procedure. On this basis, we fabricated a planar asymmetrical heterojunction with interelectrodic distance ranging from 100 nm to 1.5 µm. The photovoltaic characterization illustrated that the photoelectrical conversion efficacy is a function of channel length. When the interelectrodic distance is in the range of 200 nm and 300 nm, the photoelectric conversion efficiency peaks. Such a phenomenon suggests that the edge of gold electrode could scatter the photons and boost the light absorption close to the electrodes. This observation implies a possible way to maximize the performance of nanoscale optoelectronic devices by harnessing the light scattering at the edge of metal electrode. The other kinds of polymeric semiconductors are also expected to exhibit similar orthogonal solvent dispersion property and would be patterned by photolithography technique to realize high-resolution structures. More recently, a nano-fabrication technology has been devised featuring double self-alignment that is applied to construct zebra-like asymmetric heterojunction arrays. Such nanostructured composite, which covers a surface area of 5 x 4 mm(2) and contains 500 periodic repeating units, is capable of photo generating voltages as high as 140 V on a flexible substrate.[3]

Keyword:nano-structured organic photovoltaics, nano-fabrication

最终交流类型: Invited

Control over Solution Phase Structure and Thin Film Morphology for High Performance Conjugated Polymers

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Polymer semiconductors (PSCs) are important materials for the preparation of flexible and stretchable electronic devices such as field-effect transistors (OFET), organic light-emitting diodes (OLEDs), and organic solar cells (OPVs) with excellent ophotoelectric conversion behavior, low-cost solution, large-area processing, and light weight. The solid-state properties of conjugated polymers depend sensitively on their morphologies across all length scales. This multiscale morphology in the solid state is largely affected by solution-state aggregates and their assembly pathways from solution to thin films. Solution processing is a characteristic of conjugated polymers, and the initial solution memory effect and non-equilibrium aggregation kinetic processes of conjugated polymers are the key to affecting the microstructure of polymers. The molecular chain conformation in solution directly affects the microstructure of the film. However, due to the polydispersity of conjugated polymers and the existence of strong intramolecular, intermolecular and π-π interactions, serious entanglements within and between molecular chains are serious, which limits the movement and rearrangement of molecular chains. How to effectively regulate the solution state and film formation process of conjugated polymer is one of the bottlenecks in optimizing the microstructure of thin films. In this talk, I will address two issues, 1) how to control the precise solution-aggregate structures by changing the strength of attractive interactions between segments and 2) how the solid-state morphology and electronic and mechanical properties can be determined by solution-phase structure and assembly pathways in a

controllable fashion. The method of to regulate solution aggregation structure and film-forming path through polymer main and side chain selective solvents, side-chain dispersion differences and hydrogen bond interactions, nucleation-crystallization matching, specific conformational growth strategies and crystallization-phase separation equilibrium was established. The optimization of thin film microstructures was realized by the influence of solution memory effect and non-equilibrium aggregation kinetics on nucleation, growth. The mechanism of microstructure change during stretching of conjugated polymer films was revealed. Two fracture modes were found along the side chain stacking surface and perpendicular to the molecular backbone fracture, and the mechanism of synergistic deformation of semicrystalline conjugated polymer films and amorphous regions could effectively dissipate strain energy, which provided a theoretical basis for the construction of fatigue-resistant electronic device conjugated polymer films. A stretchable film with an percolation network structure was constructed, and the correlation between the microstructure of the film and the mechanical/electrical properties was established, which solved the contradiction between the mechanical and electrical properties of the conjugated polymer.

Keyword: Conjugated polymers, Solution Phase Structure, solid-state morphology, electronic and mechanical properties

最终交流类型: Invited

Spin-related phenomena in molecular materials

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The notion of spin conservation was introduced into chemical reactions nearly 100 years ago. A process is called “spin-allowed” when the spin angular momentum space spanned by the reactants intersects the spin angular momentum space spanned by the product; otherwise, it is “spin-forbidden”. We are working on the spin-dependent transitions of excited states in molecular systems, including the spin conversion between singlets and triplets in optoelectronic molecular devices, as well as the spin-related formation/breakage of chemical bonds in molecular reactions. The steady-state and transient magnetic field effects on electric conductivity, luminescence and other physical parameters are measured with our home-built setups with an accuracy of ~0.01%. It is essential for us to explore the spin-related phenomena in molecular materials and devices. For example, we investigate the spin

conversion of reverse intersystem crossing in thermally-activated fluorescent materials, which helps us to improve the electroluminescence efficiency of OLEDs with spin sensitizer or dopant. The spin conversion is found to be critical for the excited state process of singlet fission and triplet fusion, which could lead to anomalously large magnetic field effect on the photoluminescence of fluorescent molecules. These experimental results are of importance to the future development of organic spin-optoelectronics, and may lead to the device applications including new types of magneto-optical modulators and magnetic field sensors. We further explore the idea of spin conversion in electrochemical reactions, in which the spin-parallel and antiparallel spin alignments of spin 1/2 pairs in reaction intermediates may undergo reaction pathways leading to the formation of different products.

Keyword:magnetic field effect, spintronics, excited state chemistry, spin manipulation, spin catalysis

最终交流类型: Invited

Heteroaryl Azoswitches for Molecular Electronic and Solar Thermal Devices

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Photoisomerization of photoswitches is currently investigated as a potential solution for solar energy storage and conversion. However, its development remains to be severely limited by low energy density, short storage lifetime, and low temperature level of the released heat. Here we show that photon energy and ambient heat can be co-harvested by photoswitches using photochemical crystal↔liquid transitions (PCLTs) and demonstrate energetic, stable solar thermal batteries. Rationally designed small-molecule azo-switches achieved high energy densities of 0.3-0.4 MJ/kg and allowed long-term energy storage (half-life of about 3 months). Rechargeable, flexible solar thermal battery devices are fabricated, which, upon triggered by light, offer a high power density of 2.7 kW/kg and produce a temperature increase of more than 20 oC. They can be readily recharged and show robust performance during multiple charging/discharging cycles. Deicing functionality of the solar thermal battery film has been demonstrated. Thermodynamics analysis reveals that PCLTs-based energy storage is not a simple combination of photoisomerization-based photo energy storage and phase-transition-based thermal energy storage. The two streams of energy collaborate with each other to go beyond the energetics of conventional solar energy storage

and enables the upgrading of thermal energy that cannot be achieved by phase-change materials. Our work demonstrates a new concept of energy utilization—combining solar energy and low-grade heat into higher-grade heat, which unlocks the possibility of developing sustainable energy systems powered by a combination of solar energy and ambient heat. On this basis we further explore the great potential of Het-N=N-Het architecture in developing new molecular systems with excellent photoswitch properties. In specific, we have developed a family of six azobispyrazoles, all of which show (near-)quantitative bidirectional photoconversions, and their Z-isomer half-life can be broadly tuned from hours to years. Two important discoveries are made:1) two five-membered rings remarkably weaken the intramolecular steric hindrance, providing new possibilities for engineering the geometrical and electronic structure of azo photoswitches; 2) Het-N=N-Het architecture substantially reforms the structure-property relationships relative to Ph-N=N-Het, thereby overcoming the conflict existing in the latter between effective photoconversion and Z-isomer stability.

Keyword:heteroaryl azoswitches, molecular electronics, photochemical phase transitions, energy storage, flexible solar thermal devices

最终交流类型: Invited

Bioinspired Structural Color Materials

李明珠
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Bioinspired Structural Color Materials

Controlling the interaction between light and matter through optical structures has laid the foundations for a broad spectrum of applications, ranging from colors, lasers, and optoelectronics, to quantum information processing. To design and fabricate optimum optical structures towards highly efficient light management has been of growing interest.

Inspired by the natural hierarchical optical structures, we developed a series of composite optical structure materials with a low spatial footprint and enhanced light-matter interaction. Deep-strong coupling of different optical structures, such as Fabry-Pérot interferometers, distributed Bragg reflectors, photonic crystals and grating structures, unlocks a large variety of novel phenomena spanning traditionally distant research areas. Moreover, we emerge composite optical structure materials with surface-functionalization, chemical regulation, and optoelectronic device which open prospects for diverse applications, including anti-counterfeiting, encryption, sensing, displays, photovoltaics and imaging.

Keywords: structural color, colloidal assembly, light trapping, composite optics, polarization

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Keyword:structural color, colloidal assembly, light trapping, composite optics, polarization

最终交流类型: Invited

Tetraphenylbenzene-based AIEgens and their non-doped OLEDs

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Aggregation-induced emitting (AIE), a scientific concept coined by Professor Ben Zhong Tang in 2001, refers to a unique phenomenon that molecules that emit weakly or non-luminously in solutions are induced to emit intensely in the aggregate and solid states. The restriction of intramolecular motion (RIM), which includes restriction of intramolecular rotation (RIR) and restriction of intramolecular vibration (RIM), has been rationalized as the cause of the AIE phenomenon. Under the guidance of RIM, tremendous AIE luminogens (AIEgens) based on tetraphenylethene, silole, and 9,10-distyrylanthrance etc. have been designed and prepared. They also have been widely applied in optoelectronics, sensing and biolologic areas, and advantages over traditaional fluorophores have been well demonstrated. To further expand the research fields of AIE, more AIE cores need to be designed and synthesized.

In this talk, I will report our recent efforts on development of tetraphenylbenzene-based AIEgens under the guidance of restrictiction of intramolecular rotation. At the same time, the applications of these AIEgens as emitign layers in non-doped OLEDs will be discussed. The reason why the external quantum yields of the non-doped devices are higher than the theoretical limit of 5% was elaborated.

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Keyword: Aggregation-induced emission, tetraphenylbenzene, non-doped OLEDs, blue emssion.

最终交流类型: Invited

Printable Multifunctional Nanocomposites for Tactile Sensing Applications

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Skin is the main tactile sensing and protective layer of human body. As a sensing layer, human skin has unique sensing properties, e.g., response to multiple tactile signals (pressure, stress, temperature, humidity, etc.) independently with high sensitivity, fast response, and high resolution. In addition, as a protective layer, human skin has multiple functions, including excellent stretchability, healing or self-healing features after injury. In recent years, focusing on new sensing materials, sensing mechanism, and sensing device, the development of bionic tactile sensing system (electronic skin) to imitating the versatility of human skin has become one of the most important research areas.

At present, the key challenges for the development of electronic skin include a) Lack of high-performance multifunctional sensing materials; b) Lack of effective integration technology compatible with flexible form factor; c) Limited by the traditional sensing mechanism. Our research focuses on resolving the above interdisciplinary problems by 1) designing and developing printable multifunctional nanocomposite systems; 2) developing stretchable and high-performing tactile sensing nanocomposites; 3) integrating stretchable electronic skin with unique sensing and protective properties.

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Keyword: Printed electronics, Multifunctional Nanocomposites, Tactile sensors, Wearable electronic, Electronic skin

最终交流类型: Invited

Fabrication and mechanism study on high-performance OFET Sensors

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Organic field-effect transistor (OFET) sensors have been arousing great interests o scientists due to advantage of multi-parameters such as charge carrier mobility, threshold voltage, current on/off ratio and, etc. Hence, the sensing behavior can be characterized more accurately like the fingerprint recognition. Many gas analytes have been detected with organic field-effect transistor (OFET) sensors. However, most of the analytes are detected with known concentrations and few OFET sensors have been used to quantify analytes. Here, we proposed the novel strategy to integrate the multiple independent parameters of OFETs with artificial neural network (ANN) to quantify toxic H2S as a model. The precise concentration recognition was confirmed as the difference between real and predicted values was less than 5%. The H2S sensors also showed high responsivity over 6500% at 150 ppm, and quick response in ten seconds. Moreover, the multiple parameters provided the possibility to differentiate eight different analytes. Thus, the artificial intelligence combined with OFET sensors realized precise quantification and fingerprint recognition of gas analytes for real applications. The sensing mechanism is investigated, which is helpful to make high-performance gas sensors in the future. In another work, we found an interesting phenomenon that the electrical current of p-type OFET sensors decrease while that of n-type OFET sensors increase with H2S gas passing through the surfaces of the two sensors. It is found that H2S gas is an electron donor, so H2S doping reduces the concentration of hole carriers in the conductive channel of the p-type sensors, and increases the concentration of electron carriers in the conductive channel of the n-type sensors, thus improving the electrical performance of the sensors. The above mechanism study provides an important theoretical basis for the preparation of high-performance gas sensors.

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Keyword:organic semiconductors, transistors, sensors, mechanism

最终交流类型: Invited

Investigating Unstable Spinterface in Organic Spin Valves: Advancements through Electrode Transfer and Enhanced Spin Injection

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Organic spin valves hold great promise for the development of efficient spintronic devices, enabling advancements in information processing and storage technologies. The spinterface, the interface between an organic semiconductor and a ferromagnetic electrode, plays a critical role in the performance of organic spin valves. In this seminar, we will emphasize the importance of studying the unstable spinterface in organic spin valves and present novel approaches to address the associated challenges, including electrode transfer technology, precise spin signal detection, enhanced spin injection via doping, and the development of controllable bottom spinterfaces.

Firstly, unraveling the unstable spinterface in organic spin valves is crucial for improving device stability and performance. The spinterface is prone to degradation due to phenomena such as top electrode penetration during thermal evaporation, leading to reduced spin injection efficiency and compromised device functionality. By thoroughly investigating and understanding the underlying mechanisms causing instability, we can develop strategies to mitigate these effects and enhance the long-term stability of organic spin valves. To address the challenges posed by an unstable spinterface, electrode transfer technology is proposed as a solution. This technique allows high-quality ferromagnetic electrodes to be transferred onto the organic semiconductor layer, ensuring improved and controllable interfacial properties. This approach provides a means to stabilize the spinterface and optimize the device performance, paving the way for the development of reliable and efficient organic spin valves. Accurate evaluation of true spin signal detection is another critical aspect in organic spin valve research. Precise characterization techniques are necessary to distinguish the genuine spin signal from potential noise and artifacts. By employing temperature-dependent and angular-dependent measurements, we can understand the spinterface properties and device performance. Doping, the intentional introduction of impurities into the organic semiconductor, offers a promising avenue for enhancing spin injection efficiency. By a simple F4-TCNQ doping approach, we can modify the electronic and magnetic properties at the spinterface, leading to improved spin polarization and enhanced spin injection. Additionally, the development of controllable bottom spinterfaces presents an exciting opportunity to tailor the interface properties and improve device performance. Precise control over spin injection was achieved by carefully engineering the interfacial characteristics at the bottom of the organic spin valve. This advancement allows for the realization of highly tunable and customizable organic spintronic devices.

In conclusion, we unravel the significance of studying the unstable spinterface in organic spin valves and propose innovative approaches to address associated challenges. These advancements pave the way for the realization of reliable, efficient, and tunable spintronic technologies with diverse applications in information processing and storage.

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Keyword:spinterface, organic spin valve, organic spintronics, magnetoresistance.

最终交流类型: Invited

Regulating Aggregation Structures of Organic/Polymeric Materials for Optoelectronics

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Aggregation structures is a bridge connecting molecular structures and optoelectronic properties. However, it is highly challenging to tailor aggregation structures to improve the optoelectronic properties of molecular materials due to the weak nondirectional intermolecular interactions in organic solids.1

Herein, we discuss the rational control of packing structures of organic semiconductors by the three main approaches i.e. molecular structures modification, crystal polymorph control and coassembling. Firstly, by the introduction of imide or naphthyl group into the molecular backbone, face-to-face columnar or slipped packing structure was achieved with excellent electron transport or integrated optoelectronic properties. Secondly, we rationally controlled crystal polymorphs of organic semiconductors through the induction of surface nanogrooves, solution supersaturation and vapor transport temperature gradient.Thirdly, we have demonstrated that non-equal ratio cocrystal engineering can be employed as an effective strategy to tailor packing structures of organic semiconductors toward significantly improved charge transport characteristics relative to the single component material. Last but not the least, we employ thermal conversion method to in-situ achieve hydrogen bonding sites in the backbone of DPP polymers, which neither break the conjugation of polymer backbone nor introduce bulky softer side chains, thus benefiting the intrachain and interchain charge transport while maintaining excellent stretchability and self-healability.

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Keyword:crystal engineering, organic/polyer semiconductors, charge transport, optoelectronic properties

最终交流类型: Invited

Ultrasensitive e-skins for robotic and bioelectronic applications

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An electronic skin (e-skin) or a flexible pressure sensor can respond to applied pressure. However, existing e-skins often exhibit limited sensitivity at elevated pressures. Another challenge is that few sensors can well balance high sensitivity and high mechanical stability. In this work, I will discuss a type of flexible pressure sensors based on iontronic sensing mechanism—by using an ionic active material to form electric double layers with the electrode. We introduce a strategy to engineer microstructures that can significantly boost sensitivity, while simultaneously broadening the pressure responding range. We further design an embedded device configuration, which shows high robustness and negligible crosstalk under complicated mechanical modes, while without scarifying sensing properties. Robots using such iontronic skins can precisely detect pressure distribution during manipulation tasks without any interfacial failure.

Keyword: Flexible electronics; iontronic sensor; working range; microstructures

最终交流类型: Invited

Photodeformable Linear Liquid Crystal Polymers and All-Optical Microfluidic Chips

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复旦大学材料科学系

Photodeformable liquid crystal polymers can magnify the change of molecular conformation into macro-deformation of materials by combining the photoisomerization of molecules and the synergistic effect of liquid crystals, and show broad application prospects in many fields such as micro-mechanical systems, artificial muscles, and micro-robots. Recently, we have developed a series of linear liquid crystal polymers (LLCPs), which have excellent photodeformation properties, and can be used to fabricate three-dimensional microtubes [1-3]. Laplace pressure was generated when the microtubes deformed from cylinder-like to cone-like geometry due to the photoinduced reorientation of the liquid crystals, leading to the motion of the liquids toward the narrower side. In this work, a new type of optofluidic chip was fabricated by combining photodeformable LLCP film and general plastic chip substrates [4]. We further combined the Laplace pressure and the capillary condensation to integrate liquid transportation, fusion, separation, and mixing into a single chip, constructing the first all-optical microfluidic chip (AOMC) for micro reactions and detections. Laplace pressure, attributed to the photodeformation of the LLCP film, was generated to pump the liquid. Capillary condensation was introduced by the delicate design of the fluid channels, allowing the liquid fusion and separation without any connected microvalves. Catalytic oxidation reaction and protein detection processes were realized in the AOMC, which were amenable to a variety of miniaturized bio-medical applications, such as portable analysis and point of care testing.

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Keyword:liquid crystal polymers, photodeformation, microfluidics, optofluidics, protein analysis

最终交流类型: Oral

3D Lithography Enable Ultrathin Flat Compound Eye for Moving Object Imaging.

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With a hemispherical surface, the compound eye cameras inspired by arthropod eyes provide a large field of view (FOV), low aberration, and a large depth of field. However, to match the hemisphere-imaging plane, the cameras require a hemisphere-photoelectric sensor instead of a standard planar complementary metal oxide semiconductor (CMOS) sensor. Additionally, the hemispheric shape of the imaging system restricts the miniaturization of high-performance compound eye cameras at the millimeter scale. Here, inspired by the working principle of the Fresnel lens, an ultrathin flat compound eye (UFCE) composed of an off-axis microlens array (OMLA) was developed. 3D lithography enabled the fabrication of the UFCE with a complex morphology. Compared to the traditional artificial compound eye (ACE), the thickness of the UFCE was greatly reduced. Meanwhile, a flat substrate and ultrathin structure allowed for direct integration of the UFCE into the surface of a CMOS. The resultant UFCE had a FOV of up to 110° and a resolution close to the diffraction limit and low dispersion. Furthermore, the UFCE allowed for fast imaging of mobile objects in any plane within the depth of field, which is the unique function of the UFCE. In brief, the fabricated UFCE based on OMLA reduces the complexity of constructing compound eye cameras while significantly optimizing the volume, suggesting an alternative method for creating high-performing optical elements with the possibility of simple integration and miniaturization.

Keyword: Ultrathin flat compound eye, Off-axis microlens array, Moving object imaging, 3D lithography, Simple integration, Miniaturization.

最终交流类型: Invited

Interfacial Crystallization for Large-Area 2D Molecular Crystals

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天津大学

2D molecular crystals (2DMCs) are monolayer or few-layer organic single crystals. Compared with 2D atomic crystals, one distinct advantage of 2DMCs is that they are composed of soluble building blocks (i.e., organic molecules), enabling low-temperature solution processes on plastics for large-area flexible electronics. Due to their molecular scale thickness, unique optoelectronic properties that cannot be found in bulk organic materials were discovered and thus they are attracting more and more attention in recent years.

However, it is challenging to produce large-area 2DMCs due to the lack of control over dimensionality in conventical crystallization method. Here, we developed an **Interfacial Crystallization** method based on thermodynamic and kinetic considerations of crystallization. Wafer-scale monolayer 2DMCs were successfully produced by Interfacial Crystallization and their unique charge, exciton, and spin transport properties are explored.

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Keyword: Organic single crystal, 2D molecular crystal, Interfacial crystallization, Charge transport, Organic field-effect transistor

最终交流类型: Invited

Device physics and material chemistry of quantum-dot light-emitting didoes

金一政

浙江大学

Quantum dots (QDs) are a unique class of emitters with size-tunable emission wavelengths, saturated emission colors, near-unity luminance efficiency, inherent photo- and thermal- stability and excellent solution processability. In the past few years, the efficiency and lifetime of quantum-dot light-emitting diodes (QLEDs) achieved tremendous progress. These encouraging facts foreshadow the commercialization of QLEDs, which promises an unprecedented generation of cost-effective, large-area, energy-saving, wide-color-gamut, ultra-thin and flexible displays1. Here we review our activities associated with QLEDs, including exciton-generation mechanisms, material chemistry of charge-transporting layers and device engineering2-9.

Keyword: Quantum dot　Light-emitting diode　Solution process

最终交流类型: Invited

3D Network Acceptors Driven by Non-covalent Interactions for Efficient Solar Conversions

何凤
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The morphology and organic photovoltaic materials are mainly decided by the secondary intramolecular/intermolecular interactions from their constructing components, which includes the types of backbones and substitution units. Over past five years, we have focused on the precise regulation of non-covalent intermolecular interactions, such as Cl-S and Cl-π, to achieve series of three-dimensional (3D) structures for elevated solar conversions. And more significant, we have explored the relationship between different morphologies and performance from a single crystal view.

We have successfully realized the transformation of the molecular structures from the linear stacking to 3D network arrangement by precise positioning of chlorine atoms, which provided a promising pathway to design highly efficient non-fullerene acceptors with more isotropic electron transmission identity. The single-crystal X-ray diffraction shows that the 3D interpenetrating isomer has a better molecular planarity and a closer π-π interaction distance than the linear one. Recently, the trifluoromethylation has been proved to be an effective strategy to achieve an ultra-narrow bandgap acceptors (named BTIC-CF3-γ) with a 3D structure, a PCE of 15.59% has been achieved which is the highest value in reported ultra-narrow bandgap acceptors. The single crystal structure of BTIC-CF3-γ has also been successfully presented, which helps us to understand the charge transportation in blend films and provide a facile method for efficient solar conversion.

Keyword:3D network, acceptor, organic solar cell, chlorination, halogenation

最终交流类型: Invited

Nano Green Printing Smart Devices

苏萌
中国科学院化学研究所

The development of micro and nano manufacturing technology is the core topic from nanomaterials to device manufacturing and application. We use the microscale templates to precisely control the droplet manipulation and the assembly and patterning of functional materials, which achieves the printing and manufacturing of ultra-high precision 3D micro and nano structures and devices with an accuracy of 100 nm. [1] The droplet self-shaping strategy driven by the minimization of surface energy is introduced into the of micro and nano printing manufacturing, and the structure-function integrated strategy is developed to achieve printing flexible solar cells, wearable electronics and intelligent photoelectric sensors. [2-3] We have printed and fabricated photonic resonance structures with single nanoparticle accuracy, verifying for the existing critical size of the scattering-diffraction transition in nanostructured photonic interactions. When biological particles such as viruses are adsorbed on the surface of the resonant structure, the scattering resonance via the near-field enhancement effect will be generated, significantly changing the color of the scattered light. The detection of targeted viruses directly from serum or sputum is achieved within 15 minutes, and real-time response can be made to the viral load in the range of 0 to 1.0 x 10^5 PFU/mL. It is very suitable for rapid screening of viruses and bacteria in areas lacking of professional laboratory equipment. [4-5]

Keyword:printing, self-assembly, nanomaterials, bio-detection, wearable devices

最终交流类型: Invited

Preparation and Photoelectric Properties of Organic Co-Crystal Materials

张小涛
Tianjin University, China

Organic cocrystals, use two or more material molecular assembly methods to achieve new material properties, are connected through weak noncovalent bonds among different constituent compounds, which can be altered much easier than that of strong covalent in inorganic crystalline materials, offering an opportunity to tune their bulky physicochemical properties when respond to various external stimuli, and they have great advantages for constructing new optoelectronic devices, such as bipolar field effect transistors. We designed and prepared a series of organic cocrystal materials by simple methods. For example, the cocrystal (DTC) of DBTTF and TCNB under the irradiation of near-infrared laser, the temperature of DTC rises rapidly in a short time, which has high efficiency of photothermal conversion. (18.8%), the femtosecond transient absorption spectroscopy reveals that its mechanism is due to the active non-radiative pathway and the suppression of the radiative

transition process. Recently, we prepared a multi-stimuli responsive cocrystal system that the luminescent properties can be dynamically controlled and the responsive mechanism of cocrystal under multiple stimuli (acid/alkali vapor, force and heat) is elaborately demonstrated. Detailed spectroscopic, computational and structural studies exhibit that obvious charge transfer interactions in loosely mixed-stacking cocrystal are displayed, which can be weakened by acid vapor fuming due to the strong electron-withdrawing of acid cation; while they can be strengthened under mechanical grinding. Furthermore, the response time of cocrystal is in the order of seconds, which is much superior to the majority of previously reported stimuli-responsive cocrystals. Accordingly, high-sensitive fluorescence switching in a charge transfer cocrystal is demonstrated under multiple stimuli, which provide an effective strategy to develop smart materials.

Keyword: Organic cocrystals, semiconductor

最终交流类型: Keynote

Flexible high performance organic solar cell materials and devices with ADA type of materials

陈永胜
Nankai University, China

绿色能源技术是未来社会和经济发展的重要基础。其中利用功能有机高分子材料的有机太阳能电池和利用碳纳米材料的储能器件方面的研究具有重要的科学意义和应用前景。针对目前有机光伏领域最重要问题之一，即 Eloss 偏大问题，本报告将介绍我们通过 ADA 型分子中间和末端共轭单元的扩展和修饰发展的新的 CH 系列高效 ADA 型光伏分子。这类新型 CH 系列分子，具有多维多点修饰和优化等优势，可以更好地对光伏分子进行能级和堆积方式调控。据此我们获得了更低的 Eloss 和更高的效率及稳定性的有机光伏器件。

Keyword:有机光伏，柔性器件，Eloss

最终交流类型: Invited

Organic thin-film fluorescent sensor and its application

付艳艳

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Organic thin-film fluorescent sensors for vapor with high sensitivity, rapid response, and no pollution to analytes have received widespread attention in public safety, environmental protection, and public health. However, the development of fluorescent vapor sensors is very slow. The challenges lie in: 1) Many organic semiconductor materials have aggregation induced quenching effect, which makes it difficult for fluorescent materials applying in gas phase detection due to their weak luminescence in solid state; 2) Conventional film forming methods, such as spin coating and evaporation, usually lead to densely stacked surface morphology, which brings long response time and low sensitivity. 3）The existing devices based on geometrical optics are large, suffering from weak light output in solid-state, incompatibility with CMOS process.

To meet the need of low-power hazardous gas detectors in the national public security field, our study focusses on the preparation and application of organic fluorescent sensitive materials and devices. Representative work include: 1) A design strategy for improving the performance of fluorescent sensitive materials through the synergistic effect of the skeleton and the side chain is proposed for highly sensitive detection; 2) Various methods are used to control the surface aggregation state and microscopic morphology of the fluorescent sensitive material such as oxygen plasma treatments and breath figure method in order to improve the sensing performance; 3) The first chemical vapor detector based on fluorescence sensing by the evanescent field of the waveguide on silicon nitride platform is reported.

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Keyword: Organic thin-film fluorescent sensor；breath figure method；silicon nitride waveguide

最终交流类型: Invited

Solution-Grown Organic Single-Crystalline Heterojunctions

李寒莹
Zhejiang University, China

Organic heterojunctions are widely used in electronics and well ordering in the molecular packing inside the heterojunctions is highly desired. However, it is still challenging to interface organic single crystals to form single-crystalline heterojunctions. In this work, two novel methods will be introduced to describe how to prepare, from solutions, single-crystalline heterojunctions. On one hand, organic single-crystalline planar heterojunctions are grown in a single step from a mixed solution of p-type and n-type molecules. Based on crystallization of six organic semiconductors from a droplet on a substrate, two distinct crystallization mechanisms have been recognized in the sense that crystals form at either the top interface between the air and solution or the bottom interface between the substrate and solution. The preference for one interface rather than the other depends on the semiconductor-substrate pair and, for a given semiconductor, it can be switched by changing the substrate, suggesting that the preference is associated with the semiconductor-substrate molecular interaction. Furthermore, simultaneous crystallization of two semiconductors at two different interfaces to reduce their mutual disturbance results in the formation of bilayer single crystals interfaced together for organic heterojunctions. On the other hand, single crystals are prepared in organogels of a typical conjugated polymer. Instead of pure crystals, crystals containing the gel nanofibers are obtained. Essentially, nanofiber networks are incorporated into growing crystals and penetrate through the crystals, resulting in a crystal/gel-network interpenetrating composites. Based the two types of single-crystalline heterojunctions, charge transport and charge transfer process are studied. Hence, by demonstrating these two solution methods for the preparation of single-crystalline heterojunctions, this work should greatly harvest the highly ordered organic crystalline materials for high performance electronics.

Keyword:organic electronics

最终交流类型: Invited

Efficient perovskite solar cells and light-emitting diodes

游经碧
Institute of Semiconductors, CAS, China

Halide perovskite materials own excellent semiconductor properties, which showed great potential in photovoltaic and emission display. In this talk, I will summarize our recent work in perovskite solar cells (PSCs) and light-emitting didoes (PeLEDs). 1). By charge transport layer and perovskite composition engineering, for the bandgap around 1.5 electron volt, we have achieved close to 25 percent efficiency with the FF around 85 percent of organic-inorganic PSCs; 2). By surface re-construction, we have pushed the PCE of inorganic perovskite CsPbI3 based solar cells to 20 percent efficiency; 3). According to several strategies, such as non-radiative recombination suppression, band structure modulation and charge injection balance, we have achieved over than 25 and 16 percent external quantum efficiency electroluminescence in red and blue region, respectively.

Reference

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Keyword: Perovskite, Solar Cells, Light-emitting diodes

最终交流类型: Invited

High-Throughput patterning of all inorganic perovskite micro-nano structures by droplet evaporative assembly and their optical /optoelectronic applications

巫金波
上海大学

Based on the lyophilic surface patterning and discontinuous dewetting technology, we can generate droplet array by liquid strip sliding in high throughput manner. Combining droplet evaporative self-assembling, we can fabricate the micro/nanoscale all-inorganic perovskite single-crystal or thin-film arrays in one-step. Our method can adjust the pattern size and dewetting process and can be used to easily tune the perovskite crystal size position,

with versatility in fabricating perovskite arrays in wafer scale. We studied systematically the split-ring topography from wettability, evaporative assembly to optoelectronics. We simultaneously fabricated the split-ring lyophilic patterns and electrode arrays using a dual-function laser etching technique. Compared to the fully lyophilic and square ring patterns, our split-ring pattern can capture 82% of precursor solution while the deposition area was reduced to 38%. This scheme not only assisted the highly efficient directional transportation of liquid, high-throughput fabrication of perovskite arrays and high compactness of perovskite film, but also simplified the preparation process and reduced the cost of the devices. Due to the high compactness and excellent optoelectronic properties of the split-ring structured, the photodetector we developed has the maximum responsivity reached 1.44×105 mA/W, the maximum on/off ratio reached 8.2×10^3, and the response time reached 150 μs in 1.5 kHz.

Keyword:droplet array, optoelectronic, split-ring, all-inorganic perovskite, evaporative assembly

最终交流类型: Invited

Bubble-Template Molecular Printing for Precise Patterning at Molecular Scale

乔雅丽
Institute of Chemistry, CAS, China

The development of micro/nano pattern manufacturing technology for ultra-high precision organic functional materials is of great significance for the development of organic electronics. Inspired by the evolution of bubbles in nature, we proposed a new idea of bubble-template printing method for molecular scale patterns and devices [1-5]. The Newton Black Film with a bubble film thickness limit of up to two molecular layers provides a unique solution for ultra-high precision patterning of organic functional materials.

The research achievements: (1) proposing a dual component molecular design strategy to realize the use of bubble templates for organic functional molecular patterning with an accuracy of about 80 nm; (2) proposing a "dual fragment" single component molecular design strategy to obtain molecular patterns with an accuracy of up to 12 nm, verifying the broad prospects of bubble printing molecular scale ultra-high precision patterns; (3) proposing a bubble-assisted quasi one-dimensional interface strategy to achieve precise orientation control of asymmetric system. These studies fully demonstrate that bubble template printing methods can accurately regulate molecular scale assembly and patterning, providing a new theoretical and technical basis for the preparation and application of molecular devices.

Keyword: Bubble template; Amphiphilic molecules; Confined assembly; High precision pattern; Optoelectronic device

最终交流类型: Invited

Flexible Molecular Crystals with Optical Waveguides

张红雨
Jilin University, China

Organic crystalline materials, possessing many advantages such as long-range ordered structures, anisotropic photophysical properties, intense luminescence, and high carrier mobility, are considered to be one of the core materials in future flexible organic optoelectronics. However, the application of organic functional crystals in advanced optoelectronic devices is severely restricted by two major drawbacks—high brittleness and difficulties with implementation in devices. Generally, cracking or even fractures occur when external stress is applied onto organic crystals, and this proneness to damage increases the difficulties with fabricating all-organic crystal-based devices. In this sense, improving the mechanical compliance of the organic crystals is one of the key issues to be addressed in view of the projected applications of organic crystalline materials. This report will focus mainly on our research achievements on designing flexible molecular crystals based on structural optimization at both molecular and supramolecular levels as well as the exploration of molecular crystals as soft light transducing media including optical waveguides, amplified spontaneous emission, and light polarization rotation.[1-3] In addition, soft robots and sensitive actuators based on flexible hybrid molecular crystals will be presented. [4-8]

Keyword: Molecular Crystals, Elasticity, Plasticity, Optical Waveguides

最终交流类型: Invited

Device Analysis and Large ZnSe Nanocrystals for Blue QLED

钟海政
Beijing Institute of Technology, China

With the rapid improvements in both of the external quantum efficiency and operating lifetimes of QLEDs, it approaches to the gate of industrialization for flat display applications. Since blue QLED is known to be one of the most important remaining difficult, it has been of great interests to develop the materials and device for OLEDs. In the past three years, we have tried to remove the bastion of blue QLEDs. In this talk, I will introduce our recent progress in the colloidal synthesis large sized ZnSe nanocrystals with pure blue emission as well the introduction of machine learning methodology in device analysis. Large-sized ZnSe nanocrystals with an emission peak of 455-475 nm are synthesized with a general strategy of reactivity-controlled epitaxial growth (RCEG) was developed through sequential injection of high-reactivity and low-reactivity Zn and Se precursors. We further fabricated stable, large-sized ZnSe/ZnS core-shell nanocrystals with photoluminescence quantum yields up to ~60%. Very recently, we build up a machine learning assisted methodology to predict the operational stability of blue QLEDs by analyzing the measurements of over 800 devices. By developing a convolutional neural network (CNN) model, the methodology is able to predict the operation lifetime of QLED.

Keyword:QLED

最终交流类型: Invited

Conjugated coordination polymers for batteries

王成亮
华中科技大学

Conjugated coordination polymers (CCPs) have attracted extensive attention for various applications due to their high conductivity. Owing to the possible redox activity of both conjugated ligands and transition metals, CCPs are also promising for high-performance batteries. However, the chemical states, the relationship between structure and electrochemical performance and the charge storage mechanism of CCPs are still blurry. This talk will discuss our findings on CCPs and their applicaitons for batteries.

Keyword:conjugated coordination polymers; conductive MOFs; organic batteries; chemical states; charge storage mechanism

最终交流类型: Invited

ZnO Nanowire Field Emitter Arrays for Flat-Panel X-ray Source Application

Jun Chen
Sun Yat-sen University

X-ray sources have broad applications in medical diagnosis, industrial inspection, security screening and scientific instruments etc. Cold cathode flat-panel X-ray source consists of arrays of micro-X-ray source pixels, which can realize localized X-ray emission. Nest generation low-dose stationary CT imaging system without mechanical scanning can be developed using flat-panel X-ray source. Large-area field emitter arrays (FEAs) with excellent performance are key to realize the flat-panel X-ray source.

In this talk, the progresses about large area ZnO nanowire field emitter arrays and their applications in flat-panel X-ray source will be introduced. Large area ZnO nanowire FEAs were prepared using thermal oxidation method. Optimal field emission characteristics were obtained by adjusting the spacing between the emitters and tuning the electrical property of nanowires to diminish screening effect and enhance the conductivity. ZnO nanowire FEAs with uniform emission and high emission current were obtained. Fully vacuum-sealed diode-structured flat-panel X-ray source devices with diagonal size up to 8 inches was fabricated. For dynamic imaging applications, imaging characteristics of the flat-panel X-ray source driven by pulse voltage are studied. Enhanced emission under pulsed driving was found, which was attributed to a plasma-induced emission mechanism. For the addressable flat-panel X-ray source, we designed and fabricated gated ZnO nanowire FEAs with addressing and focusing capability. The controllable growth of ZnO nanowires in the gated microstructure was achieved. Fully vacuum-sealed addressable flat-panel X-ray source device based on ZnO nanowires FEAs was fabricated. The device realized addressable X-ray emission and imaging. Furthermore, a novel transparent flat panel X-ray source using ITO transmission anode and ZnO nanowire FEAs was also fabricated, showing application prospects in intraoperative radiotherapy (IORT) and industrial inspection.

Keyword: ZnO nanowire, field emitter arrays, flat panel, X-ray source, X-ray imaging

最终交流类型: Invited

Excimer-Mediated Ultrafast Intermolecular Nonradiative Decay Enables Superior Photothermal Effects for Phototheranostic

范曲立
Nanjing University of Posts and Telecommunications

High-performance organic photothermal materials (OPMs) have aroused broad attention in both fundamental research and industry applications. The current strategy to develop OPMs mainly relies on the manipulation of intramolecular nonradiative (*intra*NR) decay that always requires quite complicated and time-consuming molecular engineering processes. Moreover, most of the available photothermal conversion efficiency (PCE) remains below 60%, unsatisfactory the practical applications. In addition to *intra*NR decay, intermolecular nonradiative (*inter*NR) decay is equally important and more convenient in governing photothermal performance. However, the origin and dynamics of *inter*NR decay remain unclear, making the practical utilization of *inter*NR decay greatly challenging.

Here, systemic investigation of *intra*NR and *inter*NR decay directs the first demonstration of simple manipulation of interNR decay to produce a giant photothermal performance for optimized phototheranostic. Three conjugated polymers with variable fluorine-substitutions reveal that dimer formed by intermolecular C-F···H hydrogen bond could initiate *inter*NR decay to improve photothermal performance. This finding inspires a simple aggregation control strategy to form an excited dimer, namely excimer, which initiates an approximately 100-fold enhancement in *inter*NR decay rate over conventional *intra*NR decay. This unique interNR decay results in an ultrahigh PCE of 81% and intense near-infrared absorption around 808, enabling highly efficient in vivo photoacoustic imaging-guided photothermal therapy. This work provides keen insights into *inter*NR decay for the first time to develop high-performance OPMs, which presents substantial interest to a broad readership in biomedical science, chemical science, materials science, photonics etc.

Keyword:organic electronics, ultrafast spectra, biophotonics, phototheranostic

最终交流类型: Invited

Flexible organic semiconductors and optoelectronics

郭云龙
Institute of Chemistry, CAS, China

organic semiconductors own unique properties of molecular structure designing, easy solution process and low cost. These properties attracted eyes from scientific and industry field to use these materials in organic field-effect transistor, organic light-emitting diode, organic solar cells and so on. Recently, we focus on intrinsically flexible materials and its application in skin electronics, such as photodetectors, photoelectronic synapse and touch sensors.

Keyword:organic semiconductor, flexible, photodetector

最终交流类型: Keynote

Atomic/Molecular Scale Fabrication

刘云圻
Institute of Chemistry, CAS, China

The manufacturing industry is the main body of the national economy, the foundation of establishing a country, the tool of revitalizing the country, and the foundation of a strong country. The current manufacture industry is developing with two obvious trends: one is that the products are becoming bigger and bigger, such as large aircraft, aircraft carriers, and shield tunneling machines, etc. The other is to make smaller and smaller, such as millimeters, micrometers to nanometers in size. For the latter, if further developed, it enters the molecular and atomic levels. Atomic/molecular fabrication is constructed, built, regulated material forms at the atomic/molecular scale, and directly fabricate functional devices. Atomic/molecular fabrication might adopt a “top-down” transformative technology roadmap in order to break the bottleneck of the technical barriers encountered in “bottom-up” processing technology. Atomic/molecular fabrication has been studied for many years, and a series of technologies have been developed, for example, scanning tunneling microscope (STM)/atomic force microscope (AFM) chemical vapor deposition (CVD), molecular beam epitaxial growth (MBE), controllable chemical reactions, and controllable preparation of two-dimensional metal framework compounds/covalent framework compounds, etc.

This presentation will include two aspects: 1) controllable preparation of graphene; 2) controllable preparation of two-dimensional framework compounds. The applications of these materials in optoelectronic devices will also include.

Keyword: atomic/molecular fabrication, graphene, two-dimensional framework materials, optoelectronic devices

最终交流类型: Invited

Printable Functional Materials: Unlocking Potential for Flexible Electronics

吴卫平
中科院上海光机所

Printing has emerged as a highly promising techniques for the large-area fabrication of flexible electronic devices. Various optoelectronic devices can be printed, including field-effect transistors (FETs), photovoltaic devices, organic light-emitting diodes (OLEDs) and photodetectors. Materials including organic semiconductors, nano conductive inks have been studied as printable materials for optoelectronic devices. However, there are still numerous challenges concerning printable materials, processes and devices. In this talk, I will present several solution processed or printable functional materials, for device applications such as field-effect transistors and photodetectors. One of our notable achievements involves fabricateding photodetectors using solution processed organic-inorganic hybrid thin films comprising two different WS_2 nanomaterials, one-dimensional (1D) WS_2 nanotubes (WS_2-NTs) and zero-dimensional (0D) WS_2 nanofullerenes (WS_2-FLs) in conjunction with poly (n-vinyl carbazole) (PVK). We also fabricated low cost, self-powered near-infrared (NIR) photodetectors with solution processed heavy metal-free AgAuSe quantum dots (QDs). The QD photodetector devices exhibit a high specific detectivity of 1.55×10^{10} Jones ($>10^9$ Jones) under weak (0.05 mW/cm^2) 808 nm illumination at 0 V bias and room temperature. These printed functional materials and devices are promising in a wide range of applications, such as smart sensors, the Internet of Things (IoT), imaging devices and wearable devices.

Keyword:printed electronics, inkjet printing, field-effect transistors, photodetectors

最终交流类型: Invited

Printable photovoltaic materials and devices

李耀文
Soochow University, China

The preparation of solution-printable photovoltaic devices is highly influenced by the solvent effect. Precise control of their electronic and aggregation states is one of the highlighted questions due to the lack of fundamental theory. In the past five years, the applicant has devoted his research on establishing ordering theory in printable thin film, and accomplished comprehensive research on charge carrier dynamic. The main academic achievements are as follows: 1) proposed a molecular template strategy using organic/polymer materials for active layer growth to overcome the stress/scale confinement effect, and developed controllable growth methods across the length scales to promote charge carrier separation and diffusion[1-2]; 2) developed a new molecular targeting method for repairing "associated defects" at the interface of the solar cells, and achieving perfect interfacial electrical contact[3]; 3) proposed a novel idea of constructing nanostructures of functional layers by employing supramolecular force, and significantly increased the charge carrier transport and collection abilities[4-5]. Finally, the efficiency of a 10×10 cm^2 flexible organic solar module reached 14.26%, promoting the industrialization of printable photovoltaic devices.

Keyword:photovoltaic device, organic/polymer solar cells, electrode material, perovskite solar cell, printable solar cell

最终交流类型: Invited

Printed Organic Thin-Film Transistors

刘旭影
郑州大学

We have developed a wide variety of printed electronic materials, including conductive inks, dielectric inks, and organic semiconductor inks, for realizing fully-printed electronics. Recently, we developed a general, scaling-up strategy to fabricate large-scale, high-performance FLP-free organic TFT (OTFT) arrays by using printed vdW contacts. Room-temperature processes allow for a physically stacked junction without any structural or chemical damages. The OTFT arrays can be printed on a large-area silicon wafer or plastic film with 100% yield, exhibit ultrahigh field-effect mobility over 17.0 square centimetres per volt per second, high on/off ratio exceeding 10^8, relatively low contact resistance of 3k ohm micrometres. The work function of the printed electrodes can be tuned at a wide range of 4.8-5.6 eV, thus significantly lowering the charge-injection barrier at the contact interfaces with ideal FLP-free character (the interfacial factor reaches 0.99).

Keyword: Printed OTFTs; organic semiconductor; Work function; Van der Waals contact; Fermi level;

最终交流类型: Invited

Flexible and Printed Electronics: Organic Thin-Film Transistors and Synaptic Devices

阳军亮
中南大学

Flexible organic thin film transistors (f-OTFTs) exhibit great potential applications in flexible electronic devices such as flexible displays, sensors, logic circuits and wearable electronic devices. Neuromorphic synaptic devices have significant advantages such as parallel computing, high fault tolerance and low power consumption, thus they can realize the integration of sensing, memory and computing of efficient information, and provide a new idea for building low-power and efficient information processing intelligent systems. Our group has conducted relevant research in the construction of f-OTFTs, organic transistor synaptic devices, biomimetic vision, and intelligent sensing applications. (1) High-performance f-OTFTs were constructed on PET flexible substrate based on organic semiconductor 2,7-dioctyl [1] benzothiophene [3,2-b] [1] benzothiophene (C8-BTBT) active layer and PVP-HDA gate dielectric layer. It should be mentioned that roll-to-roll slot-die coated ultra-flexible silver nanowires (AgNWs) and AgNWs-PEDOT:PSS composite conductive thin films instead of conventional ITO were used as gate electrodes. The corrected mobility of C8-BTBT f-OTFTs exceeded 13 cm2 /(Vs) and 18 cm2/ (Vs), respectively[1-2]. (2) Analogous to biological synapses, based on electrolyte regulation, an organic three terminal synaptic transistor with biological synaptic function has been constructed, and a new multi gate ion regulated organic synaptic transistor has been further constructed, achieving angle recognition function similar to visual neurons. Self-supporting ion regulated organic flexible synaptic transistors with highly interconnected neuromorphic architecture were innovatively developed, and they are expected to be further applied in complex signal processing neural neuromorphic systems [3-6].

Keyword:organic thin film transistor; electrochemical doping; artificial synapse; flexible

最终交流类型: Keynote

2D,3D and 4D printing of electronics and optoelectronic devices

Shlomo Magdassi
The Hebrew University of Jerusalem, Israel

Functional printing brings additional performance of printed patterns beyond graphic output, and enable digital fabrication of electronic and opto-electronic devices. Our research is focused on synthesis and formulations of dielectric and conductive inks, and their utilization in various devices. These inks address major challenges in fabrication of 2D and 3D flexible and stretchable devices, in which the printing should be performed at sufficiently low temperatures that will not damage the polymeric substrates. The conductive inks are mainly composed of dispersions of nanomaterials, including silver, copper and CNT, and the dielectric materials are polymers and ceramics. The formulations are tailored to various printing technologies, such as inkjet printing and Digital Light Processing. The printing of the functional materials will be demonstrated for fabrication of 2D films and 3D objects , with optical, electrical and electro-optical performance. Thes include fabrication of flexible solar cells, harvesting of wind energy, shape-morphing objects, sensors for soft robotics, E-textile and antennas for the growing field of Internet of Things.

Keyword: Printing, electronics, inks, conductive, soft robotics

最终交流类型: Invited

Azulene-Based π-Functional Materials

高希珂
Shanghai Institute of Organic Chemistry, CAS, China

Azulene, an isomer of naphthalene, is a nonbenzenoid aromatic hydrocarbon with beautiful blue color and a large dipole moment [1]. The unique chemical structure and

physicochemical properties of azulene make it one of the ideal building blocks for constructing novel organic π-functional materials. A class of azulene-based conjugated diimides, 2,2'-biazulene-1,1',3,3'-tetracarboxylic diimides (BAzDIs), have been created and used for constructing high performance n-type organic/polymeric optoelectronic materials with mobility of up to 0.52 cm2 V^{-1} s^{-1} [2]. Later on, our lab developed a series of 2,6-azulene-based conjugated polymers, where the dipole arrangements of 2,6-azulene units in the polymeric backbone were finely regulated by monomer design and reasonable selection of synthetic methods, and it was found that the dipole orientation of azulene units affects the aggregation structure and optoelectronic properties of the polymers [3,4]. Some 2,6-azulene-based conjugated polymers exhibit dynamically reversible proton response properties, high acid-doped conductivity, and the ability to accelerate proton conduction [4]. Recently, we have constructed a series of azulene-fused (hetero)aromatics, which exhibit unique physicochemical properties and molecular functions [5]. Our study demonstrates that the properties and functions of azulene-based π-functional materials even can be predicted in terms of their molecular structures. Therefore, azulene-based π-functional materials would play their unique advantages in proton conductive materials, organic ferroelectric materials, single molecule device materials as well as carbon nanomaterials.

Keyword: Azulene, conjugated polymer, optoelectronic property, molecular design and synthesis, Functions.

最终交流类型: Invited

From Single Molecule to Molecular Aggregate

李振
武汉大学

To construct pi-molecules with different structures is one of the key points in the research field of opto-electronic materials. In many cases, the molecular structure not only affects the intramolecular-conjugation, but also the intermolecular p-p stacking, to result in the different functionalities. In this talk, some typical examples will be presented to partially demonstrate the interesting different properties with minor or even ignorable structural difference.

Keyword: Single molecule, Aggregates

最终交流类型: Invited

Heterogeneous wettability for liquid manipulation and advanced manufacturing

李会增
Institute of Chemistry Chinese Academy of Sciences

Liquid manipulation plays a central role in solution-based materials patterning and manufacturing technology. Among the numerous liquid manipulation strategies, the surface wettability-based method possesses the advantages of non-energy consumption, simplicity, and high efficiency, thus arousing significant research interests. Inspired by smart insects including desert beetle and mesovelia, heterogeneous wettable surfaces combine the characteristics of hydrophilic and hydrophobic domains, and can be specifically designed on demand. Our research focuses on the design and fabrication of heterogeneous wettability surfaces for liquid manipulation and solution-based manufacturing technologies. Diverse interesting and novel liquid behaviors, such as self-splitting and gyrating, are realized on symmetry-designed heterogeneous surfaces. Meanwhile, area-selective electrochemical deposition, spatially-controllable self-assembly, and highly-precise patterning, are achieved taking advantage of the heterogeneous wettability systems. Our research has been highlighted by Science, Nature Asia, New York Times, NHK, CGTN, etc.

Keyword:advanced manufacturing, patterning, wettability, liquid manipulation

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最终交流类型: Invited

Imide-Functionalized n-Type Polymers and Their Applications in Organic Electronic Devices

郭旭岗
Southern University of Science and Technology (SUSTech)

Imide-functionalized conjugated polymers are highly promising n-type semiconductors in the field of organic electronics. Semiconducting polymers based on naphthalene diimide (NDI) and perylene diimide (PDI) are the benchmark n-type materials for organic thin-film transistors (OTFTs) and all-polymer solar cells (all-PSCs). We report here a series of new imide-functionalized ladder-type bithiophene imide derivatives (BTIn, n = 1-5) with up to 5 imide groups and 15 rings in a row. In addition, novel imide-functionalized thiazoles are also developed. The invention of these new imides enables the access of acceptor-acceptor type homopolymers, which exhibit unipolar n-type transport in OTFTs with the highest electron

mobilities (μes) > 3 cm2 V−1 s−1. Notably, these polymers do not show undesirable kink in transistor curves, thus avoiding mobility overestimation. The deep-lying polymer energy levels of both highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) result in suppressed Ioffs of 10−10-10−11 A, thus remarkable Ion/Ioffs of 107-108 achieved in OTFTs. Besides acceptor-acceptor homopolymers, these novel imide-functionalized arenes are incorporated into donor-acceptor and donor-acceptor-acceptor copolymers, which also show unipolar n-type transport with substantial μes approaching 3 cm2 V−1 s−1. When applied as acceptor materials, the all-PSCs yield power conversion efficiencies (PCEs) of >18%. The substantial electron mobilities and deep-lying LUMO energy levels of these n-type polymers indicate their great potentials for organic thermoelectrics (OTEs). Finally, we will also report our breakthrough in developing new n-type doping method. When doped with molecular dopants, the n-type polymers deliver electrical conductivity of > 150 S cm-1 and power factor of > 110 mW m-1 K-2.

Keyword:n-type polymer semiconductors; imide-functionalized polymers; organic transistors; organic thermoelectrics; n-doping

最终交流类型: Invited

Topological synthesized micro/nano material patterned sensor device

李立宏
中国科学院化学研究所

The rapid development of wearable and implantable intelligent sensors puts forward high requirements for flexibility, accurate sensing and miniaturization of controllable and energy-saving devices. Currently, there is a significant gap between the piezoelectric properties of flexible organic polymer piezoelectric materials and those of inorganic piezoelectric ceramic materials, such as the widely used perovskite type lead zirconate titanate (PZT) based materials, which contain lead and are environmentally unfriendly. Using the idea of graph theory, we maintain the similarity of the lattice of the conversion intermediate, achieve a number of controllable one-dimensional quasi-homomorphic phase boundary lead-free piezoelectric materials and two-dimensional atomic thick functional materials, and achieve performance enhancement based on optimized structures. The high-precision patterned control mechanisms for the surface and interface of nanomaterials - "printing interface capture" and magnetic field assisted printing strategies were innovatively proposed. The enhance device performance was due to interface band adjustment effects and anisotropic magnetic induction array effects, achieving high-performance micro/nano functional devices. Moreover, inspired by the morphology and function of outer ear hair cells in the mammalian cochlea, an artificial cochlear device simulating cochlear hair cells has been developed. This piezoelectric sensing cochlear implant device meets the waterproof requirements of natural humid environments, has high sensitivity, broadband, and biocompatibility, and is expected to become a strong competitor for cochlear implant implantation in the future.

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Keyword: Piezoelectric materials; Intelligent sensing; Structural function; Inorganic synthesis

最终交流类型: Invited

N-type Mixed Organic Ionic-electronic Conductors

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中山大学

Organic materials that can act as mixed ionic-electronic conductors of both ionic and electronic charges, which can be applied in orgnanic thermoelectricity and organic electrochemical transistor （OECTs）. OECT has mainly been approached through polymeric mixed conductors albeit some small-molecules is starting to appear as an alternative approach. However, a limited number of n-type materials with adequate performance metrics was reported. We will approach the design strategy of n-type OECTs materials in both conjugated polymers and small molecules. Their opto-electrical characteristics, microstructure, stability with ions doping/dedoping, the origin of the excellent performance metrics will also be given.

Keyword:n-type, OECT, organic mixed ionic-electronic conductors

最终交流类型: Invited

High-performance organic thermoelectric materials: From precise doping to device functionalization

狄重安
Institute of Chemistry, CAS, China

Organic semiconductor possesses the heat-electricity ability, excellent flexibility, and easy-to-take solution processability, enabling their flexible application in direct thermoelectric conversion for energy harvesting and cooling [1-3]. In recent years, research on organic semiconductor thermoelectrics (OTE) has gained widespread attention, becoming an emerging frontier in organic electronics. Over the past two decades, significant progress has been made in terms of high-mobility semiconductors, ordered molecular doping and device geometry evolution. However, there is still a long way to go for realizing their true benefits due to the issues in the efficient doping and precise control of charge carrier concentration.

Herein, high-TE performance organic semiconductors are investigated through the design of the microstructure of organic semiconductors. The study aims to reveal the constraints between key thermoelectric parameters, providing support for simultaneous improvement in the Seebeck coefficient and electrical conductivity of organic thermoelectric materials. By combining molecular stacking orientation control and layered heterojunction structure design, organic semiconductor thin films with a thermoelectric figure of merit of 0.4 have been achieved [4-6]. Furthermore, applications in self-powered sensing, photodetection, and wearable electronic devices have been expanded through the optimization of solution deposition processes and device integration technologies [6-8].

Reference

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Keyword:organic semiconductor, molecular stacking, flexible thermoelectronics

最终交流类型: Keynote

Ultralow Low Power Flexible Electronics

Arokia Nathan
Darwin College, Cambridge, UK

This presentation will review the TFT design and materials selection strategies for ultralow power operation. We examine the main issues underlying the TFT that lead to a high operating voltage, and discuss processing conditions for suppressing the interface trap density. Recent advances in low-voltage thin-film transistors show it is possible for the subthreshold slope to approach the thermionic limit, q/kT. Based on this technology, an all-inkjet-printed ultra-low-power high-gain amplifier, applied to eye movement tracking by detecting human electrooculogram signals, is presented.

Keyword:thin film transistors, deep sub-threshold operation, ultralow power

最终交流类型: Invited

Controllable-doping Ambipolar Conjugated Polymeric Semiconductors towards Simplified-constructed Organic Logic Circuits with Excellent Comprehensive Performance

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Institute of Chemistry, CAS, China

OFETs which function as electrical switches and signal amplifiers, are well known as the foundation of organic circuits, with promising application in printable flexible and wearable electronics. The ultimate goal of OFETs is to simplify the construction of organic integrated circuits with the unique advantages of the low-cost and large-area process. Compared to the use of a separate P-channel or N-channel transistor, the fabrication of organic circuits based on ambipolar semiconductors can significantly simplify the device process; for example, ambipolar NOR and NOT gates have two fewer transistors than those comprising unipolar transistors. However, the narrow bandgaps of intrinsic ambipolar polymers result in the low current on/off ratio (generally 102~103), impeding the generation of output signals with high accuracy and immunity, which are critical requirements for potential logic circuit applications. The quasi-unipolar transport properties for pristine well-balanced ambipolar polymers are obtained using a controllable-doping process, which results in a significant increase in current on/off ratios (105~107) for both P-channel and N-channel thin-film transistors. Furthermore, large-area organic logic circuits such as NOT, NOR, and NAND gates are constructed using a direct writing technique based on the same ambipolar conjugated polymer films with superior P- and N- conducting channels by controllable-doping process, demonstrating excellent overall performance with a high gain value of ~150, signal noise margins of 68% and fast response to input voltages. This study provides valuable guidelines for improving the on/off ratio of ambipolar materials by implementing the doping strategy and further promoting the possibility of practical applications in solution-printed integrated organic circuits.

Keyword: Ambipolar conjugated polymer, controllable doping, significantly enhanced on/off ratio, organic logic circuits, excellent comprehensive performance

最终交流类型: Keynote

Advanced Micro/Nano Manufacturing of Architectured Metamaterials

方绚莱
University of Hong Kong

Recent advances in data-driven and interconnected manufacturing have the potential to revolutionize the design and processing of multifunctional elements with unprecedented precision and heterogeneity. These elements include architectured metamaterials with integrated functions that are highly desirable for a broad range of applications in confined spaces, such as impact absorption, thermal management and chemical processing, optical transparency, structural morphing, and real-time monitoring and repair. To fully realize the potential of these multifunctional elements, an integrated knowledge base is crucial for setting up, steering, and analyzing their functionality. This requires combining different geometries and choices of digital voxels with domain-specific design constraints, as well as a library of accurate designer voxels with predictive analytics that capture essential mechanical and physical properties based on the microstructure.

In this keynote talk, we will explore the three-dimensional microfabrication techniques and expertise required to design and fabricate these architectured metamaterials for combined functions, including energy absorption, actuation/morphing, and micro-scale reactors for sustainable energy and environment. I will also discuss our effort on selective ion doping of oxide electrolytes with electronegative metals, which shows promise for reproducible resistive switching that is critical for reliable hardware neuromorphic circuits.

Keyword:advanced manufacturing, micro/nanofabrication, design for sustainability

最终交流类型: Invited

Conjugated Polymer Semiconductors and their Properties

于贵
Institute of Chemistry, CAS, China

Polymer semiconductors have attracted extensive attention of researchers and have been used to prepare organic photoelectric devices and organic spin devices. Developing new conjugated polymers with high mobility and expanding the types of conjugated polymers become the primary task of research in this field. Therefore, we developed a series of aromatic fused ring compounds containing sulfur or nitrogen atoms, fabricated field-effect transistor based on their micro-nano single crystal and thin film, and studied effects of molecular conjugation, heteroatom introduction and intermolecular interaction on carrier transporting properties. Based on these works, we fabricated new donor units of diarylethylenes and acceptor units of azaisoindigo derivatives, synthesized and designed DPP-, naphthalimide- isoindigo-based conjugated polymers, Controlled the coplanarity of their main chains, the energy level structures and the aggregation state structures in the films by introducing heteroatoms, fluorine atoms, cyano and trifluoromethyl groups into the main chain of the polymers, improving the carrier transmission types and transporting performances. Moreover, we proposed concept of finite conjugated polymer, and developed develflexible and stretchable polymers. Their highest mobility reached 7.25 cm^2 V^{-1} s^{-1}.

Keyword:conjugated polymer; semiconducting material; field-effect transistors; mobility

最终交流类型: Invited

General Spatial Confinement Recrystallization Method for Rapid Preparation of Thickness-controllable and Uniform Organic Semiconductor Single Crystals

陈小松
Tianjin University

Organic semiconductor single crystals (OSSCs) are ideal materials for studying the intrinsic properties of organic semiconductors (OSCs) and constructing high-performance organic field-effect transistors (OFETs). However, there is no general method to rapidly prepare thickness-controllable and uniform single crystals for various OSCs. Here, inspired by the recrystallization (a spontaneous morphological instability phenomenon) of polycrystalline films, we developed a spatial confinement recrystallization (SCR) method to rapidly (even at several second timescales) grow thickness-controllable and uniform OSSCs in a well-controlled way by applying longitudinal pressure to tailor the growth direction of grains in OSCs polycrystalline films. The relationship between growth parameters including the growth time, temperature, longitudinal pressure and thickness is comprehensively investigated. Remarkably, this method is applicable for various OSCs including insoluble and soluble small molecules and polymers, and can realize the high-quality crystal array growth. The corresponding 50 dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) single crystals coplanar OFETs prepared by the same batch have the mobility of 4.1 ± 0.4 cm2 V−1 s−1, showing excellent uniformity. The overall performance of the method is superior to the reported methods in term of growth rate, generality, thickness controllability, and uniformity, indicating its broad application prospects in organic electronic and optoelectronic devices.

Keyword:organic semiconductor, single crystals, recrystallization, spatial confinement, organic transistors

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最终交流类型: Invited

Organic/polymer Infrared Optoelectronic Materials

刘俊
Changchun Institute of Applied Chemistry, CAS, China

Conjugated polymers as semiconductors are widely used in organic opto-electronic devices, such as organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs), and organic solar cells (OSCs). Compared with inorganic semiconductors and organic small molecular semiconductors, conjugated polymer semiconductors have the great advantage of solution processing with low cost and flexibility. There are much less n-type conjugated polymers than p-type conjugated polymers. Moreover, most of n-type conjugated polymers are based on imide-containing unit, such as naphthalene diimide unit or perylene diimide unit. We propose to design n-type conjugated polymer semiconductors using boron-nitrogen coordination bond (B←N) and develop a new family of n-type conjugated polymers containing B←N unit. In this talk, I will show you the principle of B←N unit, the molecular design of n-type conjugated polymers containing B←N unit, the functions of B←N in these polymers, and the unique electronic structures of these polymers. I will also show you how to use molecular design to tune the absorption spectra, energy levels and electron mobilities of these polymers, and the application of these polymers as p-type polymer electron donor in all polymer solar cells (all-PSCs).

Keyword:infrared optoelectronic, organic/polymer semiconductor, anti-counterfeiting, NIR photodetector, transparent thermal-shielding

最终交流类型: Keynote

Printed organic field-effect transistors and circuits

胡文平
Tianjin University, China

The fundamental advantages of organic semiconductors have attracted the world's attention at recent decades and resulted in the rapid development and progress of organic electronics (or called molecular electronics). However, there remain some key challenges in this field such as the low mobility, the not fully understanding structure-properties relationship, the absence of techniques for the fabrication of high performance devices and circuits etc. It is prospective that high-quality single crystals of organic semiconductors could answer these questions and further advance the development of this field. However, the growth, characterization, and application of organic semiconductor crystals are full of challenges. Here we will focus on organic micro- and nanocrystals, two dimensional crystals and cocrystals for a brief introduction.

Keyword:organic field-effect transistors, organic circuits, printing

最终交流类型: Invited

Phase Alignment Management in Quasi Two-Dimensional Perovskite Solar Cells

张渊
北京航空航天大学

Two-dimensional (2D) perovskites with excellent stability and optoelectronic properties have aroused great interest for use in perovskite solar cells (PSCs). To date, the power conversion efficiencies (PCEs) of state-of-the art 2D-PSCs are non-satisfactory because of higher recombination losses in 2D quantum wells. Here, based on a series of alkylic ammonium spacers (ethylamine to hexylamine) with different chain lengths, we present a strategy via the molecular van der Waals interaction to realize modified crystallization, phase distribution, and quantum-confined behaviors in Ruddlesden-Popper 2D perovskites ($n = 4$). With the optimal amylamine (AA) spacer, high-quality 2D perovskites featuring well-aligned phase alignments with fewer unfavorable n-value species and a reduced exciton binding energy have been realized, leading to sufficient charge transfers through different n-value components. The devices based on (AA)2MA3Pb4I13 yield a champion PCE of 18.42%, showing an impressive open-circuit voltage of 1.25 V and a fill factor exceeding 0.80.

Keyword: Quasi-2D perovskite; Photovoltaic efficiency; Phase alignment; Charge transport; Stability

最终交流类型:

The Development of Printable Materials for Flexible Electronics

赖文勇
Nanjing University of Posts and Telecommunications

Flexible electronics have attracted particular interest from the diverse fields including materials, chemistry, electronics, engineering and so on. With significant advances, various flexible electronic products, such as flexible displays, wearable devices, and smart electronic skins, are bringing profound impact on human life. After years of development, organic light-emitting diodes based on organic small molecules is becoming more and more mature and

now become real in the market, which are widely used in cell phones and TV sets. While the flexible electronic technology based on optoelectronic functional polymers still remains largely to be explored. The development of novel materials and new technologies makes this field rather attractive. Our work focuses on the design and development of high-performance printable organic polymer optoelectronic materials, organic interfacial materials, flexible electrodes, the regulation and optimization of their functionality, with the aim to develop high-performance large-area printed flexible electronics.

Keyword: Optoelectronic functional polymers, organic optoelectronics, flexible electronics, printing electronics

最终交流类型:

Design and Optimization of Polymer Electrolyte Membrane for lithium batteries with High Energy Density

李忠涛
中国石油大学（华东）

In recent years, the demand for extending the driving range of electric vehicles has become increasingly urgent, necessitating a breakthrough in the energy density of power batteries. In special fields such as aerospace, the requirements for energy storage sources go beyond specific energy indicators and also include wide temperature adaptability and long-term safety over the entire lifecycle. The performance improvement space for traditional lithium-ion batteries in these aspects is limited, thus there is an urgent need to develop a new generation of battery systems to meet the significantly improved performance requirements for energy storage sources. After many years of development, solid-state batteries (SSEs) currently show the most promising potential to fundamentally address these issues.

Flexible polymer electrolytes represented by PEO have good interfacial compatibility and processability. They adopt a chain transport mechanism for lithium ion migration, resulting in higher ionic conductivity at temperatures above 60°C. However, at room temperature or lower, the crystallization of polymer chains hinders the chain transport mechanism, leading to a rapid decrease in lithium ion conductivity, limiting its widespread application. To enhance the performance of polymer electrolytes, our research team has taken a molecular design approach to synthesize various polymer electrolytes with different functional groups and apply them to specialty power sources. The designed polymer electrolytes achieve multi-functional applications such as low-temperature quasi-solid-state

batteries (charge/discharge at -30°C), high-temperature batteries (charge/discharge at 100°C), high-safety flexible batteries, and all-solid-state batteries. These findings have the potential to be widely applied in specialty power sources. Experimental results demonstrate that the performance improvement of these power sources can be attributed to the optimization of the internal ion solvation structure and enhancement of the stability of the interface electrochemical deposition layer. The research results can be used to develop new polymer-based solid-state electrolyte systems and overcome limitations of existing electrolyte systems.

Keyword:lithium batteries Polymer Electrolyte

最终交流类型:

Two-dimensional organic-inorganic van der Waals heterojunctions Title

耿德超

Tianjin University, China

Two-dimensional (2D) materials have gained significant attention in recent decades ascribed to their exceptional optoelectronic properties. To meet the growing demand for multifunctional applications, 2D organic-inorganic van der Waals (vdW) heterojunctions have become increasingly popular in the development of optoelectronic devices. These heterojunctions demonstrate an impressive capability to synergistically combine the favourable characteristics of organic and inorganic materials, thereby offering a wide range of advantages. Herein, an ultralow-power vertical transistor is demonstrated based on transition-metal carbides/nitrides (MXene) and organic single crystal. The transistor exhibits a high JON of 16.6 mA cm−2 and a high JON/JOFF ratio of 9.12 × 105 under an ultralow working voltage of −1 mV. Furthermore, it can successfully simulate the functions of biological synapse under electrical modulation along with consuming only 8.7 aJ of power per spike. It also permits multilevel information decoding modes with a significant gap between the readable time of professionals and nonprofessionals, producing a high signal-to-noise ratio up to 114.15 dB. This work encourages the use of vertical transistors and organic single crystal in decoding information and advances the development of low-power neuromorphic systems.

Keyword:two-dimensional, van der Waals heterojunctions, organic-inorganic

最终交流类型:

Bubble Assisted Printing Approach

闵凡一
中国科学院化学研究所

In foams, bubbles are stacked with each other and possess a huge area of air water interfaces. Naturally, Ostwald ripening can lead to the merging and collapse of the bubbles. In our study, utilizing the silicon pillar arrays, the Ostwald ripening can be suppressed. Between two neighbouring and contacting bubbles, thin liquid film in the confined space can reach the thickness from the scale of micrometre to several nanometres, which provides a platform for the assembly of the solutes in the solution. Utilizing the bubble assisted printing approach, we have patterned various materials including organic molecules, nanoparticles and polymers. And benefiting from the thin liquid film between bubbles, the resolution of patterns thickness can be reduced to tens of nanometres.

Keyword: Self-assembly; Bubble; Patterning;

最终交流类型:

Flexible substrates enabled highly integrated patterns with submicron precision toward intrinsically stretchable circuits

吕文坤
中国科学院化学研究所

Fabricating high integration density, high resolution, and intrinsically stretchable patterns by patterned technologies remain challenging. Template printing enabled high-precision patterned fabrication at a facile operation. However, the pattern spacing constraint is the major limitation to high integration density. In this study, we develop an elastomer-assisted strategy to improve the template printing process, which involves patterning on the prestrain elastic substrate. This strategy overcomes the spacing limitation and enables the realization of a centimeter-scale pattern with submicron precision. Particularly, the integration density of fabricated intrinsically stretchable patterns can reach 1932 lines on a substrate of 0.5 cm2; the assembly lines with a feature size of 880 nm and an interval of 955 nm. Furthermore, we demonstrate a facile approach for constructing silver nanoparticle/liquid metal alloy composite conductive patterns. The as-prepared flexible electrodes can withstand up to 150% strain and a 2-mm bend radius. This method provides new insights into template printing technology. Additionally, it opens a route for the simultaneous construction of functional patterned arrays with large scale, high integration density, and intrinsic stretchability, which will be useful for the integrated fabrication of various flexible electronic devices.

Keyword:flexible devices, highly integrated patterns, liquid metal alloys, printed electronics, stretchable electronics

最终交流类型: Keynote

Phase Engineering of Nanomaterials (PEN): 2D Nanomaterials

Hua Zhang
City University of Hong Kong, China

In this talk, I will summarize the recent research on phase engineering of nanomaterials (PEN) in my group, which in particular focuses on the rational design and synthesis of novel 2D nanomaterials with unconventional phases for various promising applications. For example, by using gas-solid reactions [1], we report a general synthetic method for the large-scale preparation of metastable 1T′-phase group VIB TMDs, including WS2, WSe2, MoS2, MoSe2, WS2xSe2(1-x) and MoS2xSe2(1-x), We solve the crystal structures of 1T′-WS2, -WSe2, -MoS2 and -MoSe2, with single-crystal X-ray diffraction. The as-prepared 1T′-WS2 exhibits thickness-dependent intrinsic superconductivity, showing critical transition temperatures of 8.6 K for the thickness of 90.1 nm and 5.7 K for the single layer, which we attribute to the high intrinsic carrier concentration and the semi-metallic nature of 1T′-WS2. Moreover, a facile, one-step salt-assisted general strategy is reported for the controlled phase transformation of commercially available TMDs with conventional 2H phase, yielding a large amount of metastable 1T′-phase TMDs, including WS2, WSe2, MoS2, MoSe2 and WS2xSe2(1-x). It is found that the easily accessible metal salts, such as K2C2O4·H2O, K2CO3, Na2CO3, Rb2CO3, Cs2CO3, KHCO3, NaHCO3, and NaC2O4, can be used to assist the 2H-to-1T′ phase transformation, greatly simplifying the synthetic process for producing metastable 1T′-TMDs [2]. The phase transformation of TMDs during our developed electrochemical Li-intercalation process has also been observed [3]. Impressively, we show that the lithiation-induced amorphization of layered crystalline Pd3P2S8 activates this otherwise electrochemically inert material as a highly efficient hydrogen evolution catalyst. Electrochemical lithiation of the layered Pd3P2S8 crystal results in the formation of amorphous lithium-incorporated palladium phosphosulfide nanodots with abundant vacancies. The structure change during the lithiation-induced amorphization process is investigated in detail. The amorphous lithium-incorporated palladium phosphosulfide nanodots exhibit excellent electrocatalytic activity towards the hydrogen evolution reaction with an onset potential of -52 mV, a Tafel slope of 29 mV dec-1 and outstanding long-term stability.

Experimental and theoretical investigations reveal that the tuning of morphology and structure of Pd3P2S8 (for example, dimension decrease, crystallinity loss, vacancy formation and lithium incorporation) contribute to the activation of its intrinsically inert electrocatalytic property [4]. Currently, my group focuses on phase engineering of nanomaterials (PEN) [5], including the investigation of phase-dependent physicochemical properties of novel nanomaterials and their applications in catalysis, (opto-)electronic devices, clean energy, chemical and biosensing, surface enhanced Raman scattering, photothermal therapy, etc.

Keyword： Phase engineering of nanomaterials (PEN), Transition metal dichalcogenides, Unconventional phases, Amorphous phase, Heterophase nanomaterials

最终交流类型: Oral

Heat transfer and electrochemical synergistic effects of proton exchange membrane fuel cells based on N, P co-doped graphene substrate electrodes

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Proton exchange membrane (PEM) fuel cell system is considered to be the most promising power generation technology owing to zero noise pollution and minimal harmful gas emissions [1-3]. Platinum and carbon composite (Pt/C) is the most widely used electrode catalyst material in in fuel cells due to its optimum catalytic activity.In addition to efficient catalysts, the thermal management of the PEM fuel cell[4], especially the uniform temperature distribution on the electrode surface, also plays an important role in changing the performance of the PEM fuel cell[5]. Graphene, as a two-dimensional carbon material, with its large specific surface area and excellent thermal and electrical properties[6], has also demonstrated outstanding performance as a catalyst and thermal conductive materials for PEMFC. In this article, the synergism of thermal transport and electrochemical characteristic of carbon nanoparticles with nitrogen phosphorus co doping (AC@N, P) graphene substrate electrode was studied. The objective was to develop a kind of electrode substrate material with excellent thermal conductivity and catalytic properties for PEM fuel cell, which can decrease the amount of precious metal catalysts used and reduce the cost of PEM fuel cell. Herein, the N and P co-doped graphene (N, P -G) with different content of the spacer by AC is prepared by a simplicity one-step synthesis route.

To understand the enhancement mechanism of thermal diffusion, scanning electron microscopy (SEM) along with a simplified model of the heat transfer path with 10%Pt/C and 10%Pt/C@ (10%AC@N, P-G) substrate electrodes are proposed in Fig.1. Irregularly-shaped carbon nanoparticles are evident on the 10%Pt/C electrode, and using point contact mode between the different carbon nanoparticles, the heat transfer process between particles is hindered. The electrode surface of the 10%AC@ N, P -G substrate was covered with a cross-linked graphene layer using surface contact mode, which is beneficial to forming a highly effective thermal network. Therefore, compared with the traditional 10%Pt/C electrode surface, the 10%Pt/C@ (10%AC@N, P-G) based electrode catalyst had more continuous thermally conductive pathways, which was more conducive to the heat transfer process of the electrode surface.the average surface temperature and temperature change rate (TCR) change over time is applied in the gas diffusion electrode under horizontal and vertical heating conditions, as shown in Fig.2, respectively. Firstly, it can be seen from Fig.2(a) that the thermal diffusion process of the horizontal surface by 10%Pt/C@ (10%AC@N, P-G) needs 17 s to be stable, while the 10%Pt/C surface needs more than 27 s. In addition, both the TCR decreases rapidly and approaches the steady point within 5 s, but the electrode surface of 10%Pt/C@ (10%AC@N, P-G) is 6.4 oCS-1 higher than the 10%Pt/C at the second second time of the heat transfer process. Therefore, the thermal response time is longer and the average surface temperature at the stable time is lower for the origin 10%Pt/C electrode surface. The same trend can be found in vertical heating condition, as shown in Fig.2(b) that the stable point of heat transfer time by 10%Pt/C@ (10%AC@N, P-G) is much shorter than that of 10%Pt/C surface, and the stable temperature is 36.5 and 34 oC for the substrate of 10%Pt/C@ (10%AC@N, P-G) and 10%Pt/C, respectively.

The experimental results with different cathode mass ratios of 10%Pt/C and 10% AC @ N, P-G under the condition of 100% humidification rate and 60oC are presented in Fig. 3. It can be concluded from the figure that the output power density (0.551 Wcm-2) is the highest when the mass ratio is 2:1. Nevertheless, when the mass ratio change to 1:1 (0.491 Wcm-2) and 3:1 (0.453Wcm-2), the maximum value was decreased by 12.45% and 22.44%, respectively. It should be noted that too much graphene covered for the Pt/C substrate would prevent the infiltrated by the reactant gas from contacting the catalyst surface, thus the reaction efficiency is reduced remarkably. However, the deficient amount of substrate material is no guarantee enough heat transfer path on the electrode surface from the thermal transport between the catalyst and substrate, so it is also not conducive to improving the performance of the fuel cell. Regarding the PEM fuel cell, AC @ N, P-G as the electrode

substrate material can not only improve the ORR efficiency by its ability to catalyst the reactant gas, but also provide intact surface heat transport path and increase the heat dissipation capacity of the electrode surface. Also importantly, the effect of temperature and humidity on the performance of the battery can be reduced by the microporous structure of the AC @ N, P-G for the substrate with proper mass ratio.

Keyword： P/N co-doped graphene; Unequal amount; Activated carbon spacer; Oxygen reduction reaction; Heat transport; PEM fuel cell.

最终交流类型: Invited

Precise p-type and n-type doping of two-dimensional semiconductors for monolithic integrated circuits

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Doping, the addition of small, controlled amounts of specific impurity atoms to a semiconductor to favorably alter the electrical properties, is the real power we can fabricate all kinds of semiconductor devices. By adding dopants such as phosphorus or boron before silicon is melted, single-crystal silicon wafers with different conductivity types and various conductivity can be grown through the Czochralski method. Meanwhile, it is the core technology of silicon-based integrated circuits to further dope semiconductors in selected regions by ion implantation to generate hole-conducting p-type regions and electron-conducting n-type regions. Precise p-, n-doping can be used to adjust the threshold voltage of the complementary metal-oxide-semiconductor field-effect transistor (CMOSFET). Due to their atomic thickness and stackability, two-dimensional (2D) semiconductors are considered one of the best candidates for extending Moore's Law, especially in terms of transistor scaling and interlayer interconnection. A prerequisite for the realization of large-scale integrated circuits made of 2D semiconductors is the controllable preparation of patterned p-type and n-type channels with precisely controlled doping. However, ion implantation doping is not applicable to 2D semiconductors. Most of the large-area 2D semiconductor wafers reported so far are n-type MoS_2 layers (non-intentionally doped) prepared by lattice-matched epitaxy on specially treated sapphire wafers. If integrated circuits are produced, they must be transferred to the device substrate by a wet method. So far, there is still a lack of a general

method for controllable p-type and n-type doping of 2D semiconductors, let alone the patterned preparation of p-type and n-type channels.

This work demonstrates a synthesis method of large-scale, spatially patternable, precisely controlled carrier types and concentrations of 2D semiconductor 2H-$MoTe_2$ via substitutional doping. By precisely incorporating the amount of Nb or Re dopants in the initial Mo film, the carrier concentration of the as-grown p-type and n-type few-layer 2H-$MoTe_2$ thin films can be well controlled with a doping resolution of 10^{10} cm^{-2}. Patterned p-type and n-type 2H-$MoTe_2$ semiconductor channels can be further realized by one-step tellurization of Mo films selectively incorporated with Nb or Re dopants prepared in advance by conventional lithography and etching techniques. Thus, a large-scale 2D CMOS inverter array is fabricated, showing excellent device yield. A typical 2D CMOS inverter exhibits a voltage gain of 22.3 and a corresponding peak static power consumption of 107 nW at V_{dd}=4 V.

Keyword： 2D semiconductor, substitutional doping, CMOS, monolithic integrated circuits, MoTe2

最终交流类型: Invited

Designed growth of stacked graphene

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Graphene has attracted extensive attention in both fundamental research and practical applications due to its exceptional mechanical, electronic, and optical properties. However, the commercialization of graphene-based technologies is hindered by two main challenges, i.e., (i) the production of large-scale high-quality single-crystal graphene film and (ii) the precision control over its thickness and twist angles. In this talk, I will discuss our recent research on the designed growth of graphene single crystals, including meter-scale monolayer graphene [1], centimeter-scale twisted bilayer graphene [2], and 100,000-layer graphite films [3]. The developed growth technique is applicable for the designed growth of other 2D materials and will open up new opportunities for cutting-edge applications.

Keyword： stacked graphene

最终交流类型: Invited

Polarization-Sensitive Photodetector and Image Sensor based on 2D Materials

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As a typical representative of two dimensional (2D) semiconductors, group-IV chalcogenides have sparked considerable interest on account of its lattice structure, high compatibility with key semiconductor technology, and remarkable electrical and optical performance. Using group-IV chalcogenides with in-plane anisotropy as the photodetector's light absorption layer can effectively simplify the existing complex lens system, which can further promote device volume development toward miniaturization. Here, we demonstrate the application of polarizer-free polarization-sensitive photodetector/imagers made of 2D in-plane anisotropic layered semiconductors such as GeSe, SnSe, and GeAs, which are extremely sensitive to polarized light due to their reduced in-plane structural symmetry. Such 2D materials have been attracting high interest in recent years due to their low structural symmetry, excellent photoresponse, and high air stability. However, most 2D materials can only respond to specific light, which limits the development of wide-spectrum photodetectors. Proper bandgap and the regulation of Fermi level are the foundations for realizing electronic multichannel transition, which is an effective method to achieve a wide spectral response. SnSe crystals exhibit superior polarization detection performance with a high anisotropic photocurrent ratio (2.31 at 1064 nm) due to the structure formed by the Van der Waals superposition of covalently bonded atomic layers. Furthermore, SnSe-based photodetectors have high responsivity (9.27 A/W), high detectivity (4.08 ×10^10 Jones), and fast response (in the order of nanoseconds). We have successfully incorporated the 2D GeSe device into an imaging system for the polarization imaging and captured the polarization information of the radiant target with a high contrast ratio of 3.45 at 808 nm (NIR band). This proposed imager reveals the ability to sense dual-band polarization signals in the scene without polarizers and paves the way for polarimetric imaging sensor arrays for advanced applications.

These results suggest a new method for fabricating 2D fast-response polarization-sensitive photodetectors and image sensors in the future.

Keyword：Keyword: Polarization-Sensitive, Photodetector, Image Sensor, 2D Material

最终交流类型: Keynote

Epitaxial substitution of metal iodides: a low-temperature growth method of 2D metal chalcogenides

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The integration of various two-dimensional (2D) materials on wafers enables a more-than-Moore approach for enriching the functionalities of devices. On the other hand, the additive growth of 2D materials to form heterostructures allows to construct materials with unconventional properties. Both may be achieved by materials transfer but often suffer from mechanical damage or chemical contaminations during the transfer. The direct growth of 2D materials generally requires a temperature at least 600~1000 °C to achieve high-quality crystals, retarding the additive growth or monolithic incorporation of different 2D materials owing to the high thermal budget. Here, we report a general approach of growing crystalline 2D layers and their heterostructures at a largely suppressed temperature (lower than 400 °C). The metal iodide (MI; M= In, Cd, Cu, Co, Fe, Pb, Sn, Bi) layers are epitaxially grown on mica, MoS2 or WS2 at a low temperature, and the subsequent low-barrier-energy substitution of iodine with chalcogens enables the conversion to at least 17 different 2D crystalline metal chalcogenides (MCs). Interestingly, the MCs obtained after the substitution reaction still maintain the epitaxial feature on TMD, provided the lattice of MCs is commensurate with the TMD template. The well-defined Moiré superlattices appeared in commensurate MC/TMD heterostructures, not easily achieved by mechanical stacking, provide an excellent platform for exploring the unique physical phenomena.

The 1st step, growth of metal iodides, is the temperature-determining step because the subsequent iodine-chalcogen exchange reaction to form desired MCs can proceed at a lower temperature. The MI layers can be epitaxially grown on TMDs templates with a low-temperature vapor deposition process. Without breaking the vacuum, the subsequent thermal substitution of iodine by chalcogen (S or Se or Te) enables the conversion of MIs to MCs. As an example, the 2D In2S3 grown on MoS2 at 280 oC delivers a high photoresponsivity comparable to those grown by conventional high temperature vapor deposition (700~1000 °C). Multiple 2D materials have also been grown sequentially on the same wafer, promising a feasible pathway to monolithically integrate different high-quality 2D MCs.

Keyword： 2D materials

最终交流类型: Oral

Large-Scale, Controllable Synthesis of Ultrathin Platinum Diselenide Ribbons for Efficient Electrocatalytic Hydrogen Evolution

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2D platinum diselenide ($PtSe_2$) shows outstanding layer-dependent electrical properties and high hydrogen evolution reaction (HER) catalytic activity, representing an ideal 2D material system for structure-activity correlation studies. Controllable synthesis of high-quality atomically thin $PtSe_2$ materials is essential for following research and application. However, the synthesis of high-quality atomically thin $PtSe_2$ materials remains challenging. Here, through the long-term annealing of Au substrate and the design of precursor and reaction device, a simple chemical vapor deposition (CVD) method was designed to synthesize high-quality ultrathin 1T-$PtSe_2$ ribbons with adjustable thickness and superstability. The $PtSe_2$ ribbons attached to the steps on the Au substrate grew in a regular arrangement. Based on the experimental results and theoretical analysis, the growth mechanism of the $PtSe_2$ ribbons was given. Theoretical and experimental results showed that the atomically thin $PtSe_2$ ribbons had rich catalytic sites and could be used as ideal electrocatalysts. The differences in the activity of the edges, base planes and defects of $PtSe_2$ ribbons in the HER were analyzed and confirmed, and the best HER performance was provided at the monolayer level. This study successfully achieved large-scale, controllable growth of 1T-$PtSe_2$ ribbons on Au foil using the CVD method, with adjustable thickness and superior stability. The $PtSe_2$ ribbons grew in a regular arrangement attached to the steps on the Au substrate, providing an ideal platform for exploring the electrocatalytic performance of 2D layered transition metal disulfides. This work provides a clear understanding of the morphology and structure of $PtSe_2$ ribbons, opening up new possibilities for the preparation of functional 2D $PtSe_2$ and for the rational design and modulation of high-performance 2D catalysts for HER. Our work contributes to the large-scale synthesis and potential application development of ultrathin transition metal disulfides and provides a novel method for the design and synthesis of highly active ultrathin catalysts.

Keyword: 2D ultrathin ribbons, chemical vapor deposition, electrocatalytic hydrogen evolutions reaction, platinum diselenide

最终交流类型: Invited

Signature of magnetism in zigzag graphene ribbon embedded in h-BN in the ballistic transport regime

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Zigzag graphene nanoribbons (zGNRs) are known as quasi one-dimensional strips of graphene associated by parallel zigzag edges. The zigzag edges possess a unique magnetic state that is near Fermi level and localized at the edge carbon atoms.[i],[ii] Recent progresses in GNRs synthesis enabled the fabrication of atomically precise GNRs, and then symmetry protected topological phases,[iii],[iv],[v] zero-mode metallicity[vi] and spin-polarized edge states[vii] are revealed via advanced scanning probe spectroscopy in GNRs with zigzag edge structures. However, experimental probing this magnetism by electronic transport remains elusive, mainly due to three reasons. Firstly, reliable formation of devices requires the technologically relevant length of GNR. Limited by surface diffusivity and kinetic factors on catalytic substrates, GNRs[viii],[ix] made from bottom- up assembly have length typically in a range of just tens of nanometers, which are too short to be technologically practical for device fabrication. Secondly, the open edges of zGNRs7,[x],[xi],[xii],[xiii],[xiv] are of relatively high chemical reactivity and thus cause instability or inhomogeneous doping in electronic properties.[xv],[xvi],[xvii] Thirdly, the edge states could become antiferromagnetically coupled across nanoribbon’s width if it is narrow enough, and the edges states become electrically undetectable.8 All the above reasons hurdle the direct transport measurement on the magnetism in GNR electronic device.

Here, we probe the signature of magnetism in embedded in h-BN in the ballistic regime by performing magneto-transport measurements. A ~9 nm wide zGNR was fabricated into field effect transistor with sub-50 nm channel length, and Fabry-Perot interference patterns were observed in the transistor at 4 Kelvin. It indicates a coherent transport through the channel. The variation in the device resistance on the application of a ~20 mT magnetic field is as high as ~175 Ω with a magnetoresistance of ~1.3 % at 4 K. The magnetoresistance exists even at room temperature. The result indicates the existence of ferromagnetic ordering in the zGNR even at room temperature. Our findings directly reveal the transport signature of the predicted magnetic order in zGNR and provide an effective platform for the exploration on graphene based spintronic devices.

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Keyword： zigzag GNR, hBN , ferromagnetism, edge state, ballistic transport. room temperature

最终交流类型: Invited

Synthesis of 2D materials and their properties tuning

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2D materials with atomic thickness are very promising to work as next-generation electronic devices and highly efficient electrochemical devices including electrocatalyst and energy storage. In this report, the reporter mainly focused on the synthesis of 2D material and methods to tune the properties of 2D materials. Firstly, we proposed, for the first time, an unprecedented and robust flux-assisted growth (FAG) approach to synthesize a wide range of atomically thin flakes of layered or non-layered materials, which was insensitive to the growth conditions and dynamically controllable. FAG has been employed to prepare more than 100 atomically thin compound flakes successfully. Secondly, intercalation method to tune the properties of 2D materials will be introduced, which could tune the electrical, magnetic and electrochemical properties effectively. By this, a new kind of single atoms catalysis was realized and ferromagnetic properties could be induced.

Research on the growth and mechanism of different kinds of two-dimensional materials by flux assisted growth (FAG). Aiming at the difficulty of two-dimensional synthesis of various functional two-dimensional materials and non-layered materials with rich potential applications, a new FAG method for bottom-up synthesis of ultra-thin nanosheets by liquid melt was developed by combining traditional single crystal melting growth with limited domain growth. The growth mechanism of FAG method was explored, including helpless flux crystallization, flux-assisted precipitation and melting reaction precipitation. Based on this method, more than 80 two-dimensional materials were grown, including a variety of non-layered materials and multiple two-dimensional materials, which solved the problems of large condition fluctuation and phase separation in CVD growth.

In order to solve the problems of easy phase separation and large component fluctuation in the growth of multi-component two-dimensional materials, the stoichiometric ratio of the precursor and the target product of multi-component compound FexGeTe2 was synthesized one-to-one by using FAG method. The controllable growth of Fe3GeTe2, Fe4GeTe2, Fe5GeTe2 with different Fe components and the adjustable Co and Ni-doped Fe5GeTe2 two-dimensional single crystal was realized. The thickness controllable and substrate universal growth research was realized, and the magnetic changes of the grown samples were explored. The Curie temperature or anisotropy which varies with the composition was determined.

Using FAG method to grow multi-component materials provides a new platform for the exploration and application of functional two-dimensional materials.

Keyword： 2D Materials； FAG； Synthesis

最终交流类型: Invited

Inorganic 2D material liquid crystals

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Liquid crystal (LC) is one of fundamental optical materials with their birefringence controllable by external magnetic/electric stimulus. Modulators based on organic LCs have shown desired modulation capability with an annual global market of >100 billion US$, but with challenges of weak sensitivity, material stability, toxicity, and limited light modulation range mainly in the visible to infrared regime. In this talk, I will show our recent results of using inorganic 2D materials as LCs. Such inorganic 2D material LCs possess extremely sensitive response to external magnetic or electric field, good stability, and capability to tune deep UV light down to 260 nm which is not possible previously. [1-4] In addition, such inorganic 2D material LCs can be produced in large quantities, suggesting their application potential. [5-7]

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Keyword： 2D materials, liquid crystals, mass production, optics

最终交流类型: Invited

Construction of Electronic Devices and Transport Properties of Two-dimensional Atomic Crystals

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While the scaling of devices continues, to meet the increasing demands for high performance, silicon-based technology will soon reach a critical limit. One of the key challenges is related to the unavoidable interfacial dangling bonds in ultrathin-body silicon, which causes substantial degradation in device performance. It is thus an urgent need to seek atomically sharp interfaces and seamlessly integrate them into the device architecture. Among all candidates, emerging two-dimensional (2D) materials and their heterostructures represent ideal atomically flat in-plane surfaces potentially free from surface dangling bonds and are immune to short-channel effects that can allow effective electrostatic control and mechanical flexibility.

In this talk, I will demonstrate that by mechanical exfoliation and dry-transfer method, InSe/hBN/graphite van der Waals heterostructure with atomically sharp interface have been successfully achieved. Using this heterostructure as the unit of 2D field-effect transistor (FET), with InSe as channel material, hBN as dielectric, and graphite as gate, respectively, we obtained high-performance heterostructured InSe FETs with high electron mobility up to 1146 $cm^2V^{-1}s^{-1}$ at room temperature and on/off ratio up to 10^{10}. Digital inverters are constructed by integrating two such FETs with local gate modulation and an ultrahigh voltage gain up to 93.4 is achieved. Furthermore, the heterostructured InSe FET stacked on a flexible substrate shows little change in performance at high strain level of ~ 2%.

The InSe/hBN van der Waals heterostructure can also work as the core component of the photodetector due to the superior optoelectronic properties of InSe. We will show that using ferroelectric organic P(VDF-TrFE) thin film as the top gate dielectric, the dark current in the photodetector can be successfully suppressed to 10^{-14} A. At the same time, hexagonal boron nitride (hBN) is used as substrate to improve the interface between the dielectric layer and the InSe channel. As a result, the ferroelectric-copolymer-gated InSe photodetectors not only show a high on/off ratio of over 10^8, but also exhibit high photoresponsivity up to 14250

AW^{-1} and detectivity as high as 1.63×10^{13} Jones even at zero gate voltage in the polarization-up state.

When we placed the InSe/hBN/graphite van der Waals heterostructure onto SiO2/Si substrate, this heterostructure can work as a floating-gated FET, an elementary device of flash memory, with InSe, hBN, graphite, SiO_2 and p^{++} Si serving as the channel, tunnel barrier, floating gate, control-gate dielectric and control gate, respectively. Due to the improved interfacial coupling and atomically sharp interface, ultrahigh-speed operation with nanoscecond write and read times that is limited by instrumentation response, extremely high extinction ratio of 10^{10} and a retention time of 10 year have been achieved in the floating-gate memory devices based on this van der Waals heterostructure.

All the above results highlight that van der Waals heterostructures offer a unique platform for next-generation high-performance electronic devices.

Keyword： two-dimensional atomic crystals, van der Waals heterostructures, field-effect transistors, floating-gate memories, photodetectors

最终交流类型: Invited

2D NbSe2 with Star-of-David CDW Superstructures --- A Versatile Platform for Exploring Quantum Phenomena

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北京理工大学

The charge density wave (CDW) is a superstructure due to lattice distortion and results in the modulation of electronic states. In recent years, the study of Star-of-David CDW in two-dimensional systems has been attracting more and more research attention. We dive into this exciting area by starting with the Mottness, spin, and CDW properties of single-layer 1T-$NbSe_2$, then we continue to build a variety of CDW superstructures (including bilayer homojunction/heterojunction, one-dimensional CDW reconstruction, chiral domains). We have used scanning tunneling microscopy /spectroscopy to measure these superstructures with high spatial, temporal, and energy resolution, and observed a variety of novel effects such as spin states in a triangular lattice, metal-insulator transition, CDW lateral size effect, one-dimensional band bending, and reversible switching of chiral domains [1-6]. These works provide novel insights for the understanding and potential application of low-dimensional CDW-based quantum materials in nanoelectronics.

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Keyword： 2D materials，CDW，NbSe2，STM，Heterojunctions

最终交流类型: Invited

Emergent Non-linear Phenomena via Symmetry Engineering at van der Waals Heterointerfaces

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Symmetry breaking in low-dimensional heterostructures can provide unprecedented possibilities to generate emergent quantum phenomena in condensed matter physics. Lattice symmetry breaking at van der Waals heterointerfaces can produce the geometric deformation of energy dispersion due to interfacial hybridization of the atomic orbital, serving as an excellent platform for realizing emergent non-linear phenomena. For example, at the WSe2/BP heterointerface, since the symmetry group is the common sub-symmetry group of the crystalline symmetries in monolayer WSe2 (C3v rotational symmetry around the z-axis) while black phosphrous (C2v rotational symmetry around the z-axis), the heterointerface will have no rotational symmetry (C1 symmetry). Theoretical rationale indicates that symmetry breaking at atomically-sharp interfaces will exhibit remarkable capabilities to control electronic states and further realize exotic quantum phenomena by forming moiré patterns

with a specific lattice mismatch. However, an experimental confirmation of such a strategy remains elusive.

Here, we demonstrate, with a universal strategy to intentionally break the lattice symmetry of heterointerface, an experimental observation of a spontaneous quantum mechanical shift current and a circular photogalvanic effect. Importantly, although the rotational symmetry of each material prohibits the generation of such a shift current and spin photocurrent under normal incidence of light, we observe a direction-selective photocurrent response, in which the shift current is found parallel to the mirror direction therein while the spin photocurrent is found perpendicular to the mirror. Since such direction-selective nature corresponds to the direction of in-plane polarization and the Berry curvature dipole therein, we reveal that the spontaneous quantum shift current is associated with the topological electronic nature with in-plane polarization at the WSe2/BP interface, while the circular photogalvanic effect originates from the interband Berry curvature dipole mechanism therein. In short, we provide a new strategy for generating exotic functionalities and geometric features at twisted dielectric/semiconductor interfaces via symmetry engineering.

Keyword： Symmetry breaking, nonlinear optical phenomena, quantum shift current, heterostructure.

最终交流类型: Oral

Multiple Quantum States Induced in 1T-TaSe2 by Controlling the Stacking Order of Charge Density Waves

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Van der Waals materials afford unprecedented opportunities for control of electronic properties by utilizing the stacking degree of freedom. It has been found that by controlling the number of layers and crystallographic stacking order of graphene, various exciting quantum phases, including unconventional superconductivity, correlated insulating state and quantum Hall effect can emerge. However, an intriguing frontier, largely unexplored, is the stacking of charge density wave phases that is a broken-symmetry state with periodically modulated charge density and the atomic lattice. Layered 1T-TaSe2 is archetypal charge density wave materials. At high temperature, each 1T-TaSe2 layer is composed by a triangular Ta lattice sandwiched between two triangular Se lattices. At low temperature, the triangular lattice of Ta atoms is unstable and forms a commensurate charge density wave superstructure. Employing density functional theory, it is uncovered that the stacking order can play a significant role in the quantum phase transitions of layered 1T-TaSe2. By controlling the vertical stacking order of commensurate charge density waves, bulk 1T-TaSe2 can host various electronic phases including quasi-1D and 3D metals and band insulators. Particularly, the ground-state stacking configuration shows 3D metallicity due to the enhanced intralayer and interlayer electron hopping, and the second lowest energy configuration shows band insulating behavior via interlayer dimerization, implying potential metal-insulator transition. In ultrathin-layer 1T-TaSe2, not only the stacking order but also the thickness dictate the electronic properties. While the monolayer is a Mott insulator, the bilayer (trilayer) is a band insulator (metal). More interestingly, the four-layer stacking configuration, which can be treated as two stacked semiconducting bilayer 1T-TaSe2 units, emerges as a semiconductor with a smaller gap or a semimetal dependent on its stacking order. Our results suggest that controlling the stacking order and thickness can manipulate effectively the band gap value and the metal-insulator transition of the 1T-TaSe2 CDW compound, providing new possibilities for future electronic devices.

Keyword:layered materials; stack order; electronic properties; first-principles calculations

最终交流类型: Oral

Reversible Semimetal-semiconductor Transition of Unconventional-phase WS2 Nanosheets

翟伟
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As a group of materials with polymorphs, the phase transition of TMDs provides opportunities to prepare new phases of TMDs for exploring their phase-dependent property, function, and application. However, different from the transition metal tellurides, due to the large energy difference between the thermodynamically stable phase (e.g., 2H) and unconventional phase (e.g., 1T and 1T′) in other TMDs, the phase transition in them can only be realized in either monolayers or localized domains. In addition, the previously reported phase transition of TMDs is mainly irreversible owing to the introduced structure damage, such as vacancies, amorphization, and composition alteration, during the phase transition

process. Here, we report a reversible phase transition in the semimetallic 1T′-WS2 driven by proton intercalation and deintercalation, resulting in a newly discovered semiconducting WS2 with a novel unconventional phase, denoted as 1T′d phase. Impressively, an on/off ratio of >106 has been achieved during the phase transition of WS2 from the semimetallic 1T′ phase to the semiconducting 1T′d phase. Our work not only provides a unique insight into the phase transition of TMDs via the proton intercalation, but also opens possibilities to tune their physicochemical properties for various applications. Compared to the commonly used guest ions for intercalation, lithium ions, the protons are much less aggressive, which can avoid the structural damage of TMDs during the intercalation process, leading to enhanced reversibility of the phase transition.

Keyword： Reversible, Phase transition, Unconventional phase; Transition metal dichalcogenide.

最终交流类型: Oral

Study on Nanoscroll Preparation and Organic Hybridization of Two-dimensional Transition Metal Dichalcogenides

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Transition metal dichalcogenides (TMDs) with atomic thickness can theoretically self-assemble into more complex topological structures, such as nanoscrolls, by scrolling and folding, arising from their excellent flexibility. These self-assembled structures can produce new and unique physical properties whilst inheriting the intrinsic properties of TMDs. However, limitations in mechanical strength and chemical stability present difficulties in producing high-quality TMD nanoscrolls. We have developed a tension-driven self-assembly scrolling strategy at nano scale. Using an inherent tension in the monolayer TMDs grown by chemical vapor deposition as the driving force, we scrolled chemical vapour deposition (CVD)-grown monolayer TMDs flakes into high-quality nanoscrolls in 5 s with a nearly 100% yield by only one droplet of ethanol solution. The mobility of field effect transistors of the MoS_2 nanoscroll obtained was about 30 times that of a single layer MoS_2 field effect transistor. We proposed a unique topology of such nanoscrolls that is externally self-encapsulated and internally semi open, and based on the internal open topological structure, TMDs nanoscrolls accommodating external substance of different sizes in their tunable van der Waals gaps were managed to be produced, which is expected to confer TMD nanoscrolls with novel properties and functions attractive for new applications.

On the other hand, semiconductor TMDs with excellent electrical conductivity are very promising as thermoelectric materials, but their thermoelectric performance has always been limited due the "trade-off" that high electrical conductivity is often accompanied with high thermal conductivity resulting in low thermoelectric merit (ZT). We demonstrated a simple and efficient covalent modification strategy that did not depend on boundaries or defects, in which organic/inorganic hybrid structures of TaS_2 were prepared by introducing organic side chains into the interlayer of TaS_2 via a non-destructive, facile electrochemical reaction. It was confirmed that the thermal conductivity of TaS_2 have been successfully suppressed without affecting its conductivity owing to the side chains effect by enhancing phonon scattering, which finally caused an improved ZT value of their thermoelectric devices. Thermal conductivity of TaS_2 after covalent modification was demonstrated 7 times smaller than that of the pristine TaS_2 crystal, with an improvement of about 10 times in the ZT value. This strategy enabling organic covalent modification of layered bulk single crystals deep into the crystal lattices while maintains their single crystal structure provides a new insight into the reduction of thermal conductivity of crystals, and can be extended to other layered materials, such as Bi_2Se_3, TiS_2 and $SnSe_2$.

Keyword： transition metal dichalcogenides, nanoscrolls, thermoelectric, thermoelectric merit, side chain covalent modification

最终交流类型: Oral

Mechanical and Phononic Anisotropy in Black Phosphorus Blisters

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Two-dimensional (2D) materials with atomic thickness possess excellent mechanical, optical, and electronic properties. Among them, anisotropic 2D materials with low-symmetry structures and anisotropic properties are promising building blocks for polarization-dependent optical and optoelectronic devices.[1] Limited by the biaxial stretching mode,

however, the orientation-dependent mechanical properties of anisotropic 2D materials cannot be measured by conventional testing methods, such as nanoindentation and blister test. Therefore, a uniaxial deformation method is imminent to reveal the orientation-dependent mechanical and other physical properties. Here, we develop a novel rectangular-shaped blister to uniaxially stretch atomic thickness membrane and further provide a promising platform to detect the orientation-dependent mechanical and physical properties. A typical anisotropic 2D material, black phosphorus (BP), was employed as a reference to measure its anisotropic Young's modulus and reveal both its orientation-dependent and strain-dependent phononic properties. Impressively, different from experimental results in the literature, the derived anisotropic factor of Young's modulus of BP sheets shows better agreement with the theoretical values based on first principles calculation. Further, we systematically investigated the strain-dependent Raman responses of specific Raman modes.[2] The anisotropic strain-dependent Raman shift rates were quantitatively evaluated and a calibrated relationship between Raman shift rates and crystal orientation was determined. Our results reveal the extra-high strain-dependent anisotropy of BP in both mechanical and phononic properties. The designed rectangular blister is expected to explore not only mechanical properties but also strain-orientation-dependent physical properties of various anisotropic 2D materials.

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Keyword： anisotropy, 2D material, mechanical properties, Raman spectra, strain engineering

最终交流类型: Oral

Valleytronic devices based on layered van der Waals heterostructures

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Utilizing the spin or valley degree of freedom is a promising approach for realizing more energy-efficient information processing devices. Circularly polarized light can be used to manipulate the spin and valley polarization in monolayer two-dimensional transition metal dichalcogenides and their heterostructures due to the chirality of the system, by pump spin/valley polarized photoluminescence or generate spin/valley current. In MoTe2 bilayers, we observed Zeeman splitting in magnetic field; In WSe2/MoSe2 heterostructures, we found long valley lifetime of the interlayer excitons of microsecond timescale, and observed pseudo magnetic field induced by optical spin pumping; In MoS2/WSe2 heterostructures, we demonstrated the geometrically dependent photocurrents and room temperature valley Hall effect. We proposed some microscopic models for interpreting the phenomena. These findings may facilitate the use of two-dimensional heterostructures as a platform for opto-valleytronics and opto-spintronics devices.

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Keyword： Valleytronics, van der Waals heterostructure, valley polarization, transition metal dichalcogenides

最终交流类型: Oral

Enabling Device Fabrication With 2D Materials Using NanoFrazor Technology

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Enabling Device Fabrication With 2D Materials Using NanoFrazor Technology

Combining thermal scanning probe lithography (tSPL) and direct laser sublimation (DLS), the NanoFrazor allows fabrication of devices with nano- and microstructures on arbitrary substrates. tSPL is carried out using a heated, ultrasharp probe tip to remove a thermal resist, in order to create patterns at the nanoscale. The integrated DLS module allows sublimation of the same thermal resists to conveniently write micron-scale patterns within the same lithography session. Device work, materials science, and rapid prototyping using the NanoFrazor technology has led to advances in nanoelectronics [1][2], among many different applications. The use areas span quantum electronics, bio-nano-devices, photonics, spintronics, and nanofluidics.

As tSPL becomes more and more mature as a nanofabrication technique, its use has widened significantly [3]. The technology is particularly suitable for research and development, as well as device fabrication on 2-dimensional materials, due to its damage-free lithography possibilities. Since this method is free of charged particles and high-energy beams, the sensitive surfaces of 2D materials are preserved during the writing. Furthermore, accurate overlay capabilities using the integrated topography sensor of the NanoFrazor allow for streamlined workflows and facile processing for device fabrication. The overlay features of the tool make it possible to detect buried flakes of 2D materials, selected nanowires, or pre-existing structures immediately before patterning. Figure 1 provides an example of single-layer molybdenum disulfide (MoS2) flakes with electrodes patterned by t-SPL[4], Figure 2 depicts an indium arsenide (InAs) nanowire device where the top-gate electrodes were fabricated with t-SPL [5]. Another challenging nanopattern, a nanodot array, is often applied directly to the surface of 2D materials, in order to manipulate electrical and optical properties of single layer materials. An example of such structures on hexagonal boron nitride (h-BN) is shown in Figure 3 [6]. NanoFrazor has also been used for its capability of direct manipulation of materials, such as cutting or strain nanopatterning on a thermosensitive polymer in ambient environments [7]. It has been shown to locally modulate the bandgap of strained 2D materials at nanoscale with patterning resolution down to 20 nm. The versatility and repeatability of the NanoFrazor enables it as a tool to investigate strain engineering in 2D materials, and thus shreds lights on fundamental mechanical and electronic properties of the materials.

The background and principles of tSPL will be briefly introduced, nanostructuring on 2D materials and nanowires will be discussed along with electrical and optical device performance for nanowire and 2D material-based devices fabricated using the NanoFrazor.

Keywords: thermal scanning probe lithography(tSPL). nanofrazor. nanofabrication, integrated DLS module, integrated topography sensor.

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Keyword：thermal scanning probe lithography (tSPL), Nanofrazor, nanofabrication, integrated DLS module, integrated topography sensor

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最终交流类型: Keynote

Effect of Interlayer and interfacial coupling on lattice vibrations of twisted two-dimensional materials

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The interfacial coupling at the interface makes the van der Waals heterostructures (vdWHs) exhibit many unique properties that cannot be realized in its constituents[1]. Such a study usually starts with a twisted stack of two flakes exfoliated from the same layered materials to form twisted multilayers, in which the impact of interfacial coupling on the low-frequency interlayer modes had been well understood[2]. However, it is not clear how interfacial coupling affects the high-frequency intralayer modes of twisted multilayers. Herein, we perform high-resolution resonance Raman spectroscopy of the high-frequency intralayer modes in twisted multilayer MoTe2 (tMLM)[3]. All the Davydov entities of the out-of-plane intralayer mode are observed and distinguished at 4 K. It is found that the out-of-plane intralayer modes in tMLM are sensitive to its interfacial layer-breathing coupling so that the out-of-plane intralayer modes in tMLM do not show a direct relationship with those of the two constituents. However, the case is quite different for the in-plane intralayer modes in tMLM, whose spectral profile can be fitted by those of the corresponding modes of its constituents. This indicates that the in-plane intralayer modes are localized within the constituents in tMLM because of its negligible interfacial shear coupling at the interface. All the results can be well understood using the vdW model in which only the nearest neighbor interlayer/interfacial interaction is considered. This work directly builds the relationship between the Davydov splitting of the high-frequency intralayer vibrations and the low-frequency interlayer vibrations in tMLM, which can be further extended to other twisted materials and the related vdWHs.

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Keyword： interfacial coupling, twisted multilayer flakes, Raman spectroscopy, Davydov splitting

最终交流类型: Keynote

van der Waals layered magnetic semiconductors

Young-hee Lee
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Ferromagnetism in van der Waals two-dimensional (2D) materials has been reported recently. Intrinsic CrI3 and CrGeTe3 semiconductors reveal ferromagnetism but the Tc is still low below 60K. In contrast, monolayer VSe2 is ferromagnetic metal with Tc above room temperature but incapable of controlling its carrier density due to metallic nature. Difficulty arises from lack of right ferromagnetic semiconductors. Historically, diluted magnetic semiconductors (DMSs) have been introduced by doping the minute amount of magnetic dopant such as Mn, in III-V or II-VI semiconductors has been introduced as an alternative. Moreover, the long-range ferromagnetic order in doped diluted chalcogenide semiconductors has not been demonstrated at room temperature. The key research target here is to realize the long-range order ferromagnetism, Tc over room temperature, and gate tunability. In this talk, we introduce magnetic dopant, vanadium in semiconducting WSe2 and manifest Tc at room temperature and gate tunability at low doping concentration. This could be realized via strong spin orbit coupling and strong COulomb interaction in van der Waals layered transition metal dichalcogenides, for example, WSe2 layer. We further explore different doping concentrations including highly degenerate regime and demonstrate unconventional magnetic order by random telegraph spin noises via interlayer coupling at low doping concentration limit and strange metal if time is allowed.

Keyword： Diluted magnetic semiconductor, ferromagnetism, long-range magnetic order, Curie temperature, gate-tunability

最终交流类型: Invited

Wafer-Scale Syntheses and Application Explorations of Semiconducting Transition Metal Dichalcogenides

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Two-dimensional (2D) semiconducting transition metal dichalcogenides, most with a formula of MX_2 (M=Mo, W; X=S, Se, *etc.*), have emerged as promising channel materials for next-generation integrated circuits, considering of their dangling bond-free surfaces, moderate bandgaps, and relatively high mobilities, etc. Wafer-scale preparation of 2D MX_2 films should hold fundamental significance for propelling their applications. Herein, we report the direct synthesis of 6-inch uniform monolayer MoS_2 on unique soda-lime glass through an elaborately designed “face-to-face” metal-precursor supply route. The growth system is featured with large domain size and high growth efficiency, thus providing novel insights into the batch production and green transfer of highly uniform monolayer MX_2 films. Also, we have realized the epitaxial growth of inch-scale monolayer MoS_2 single crystals on vicinal Au(111) thin films, as achieved by melting and resolidifying commercial Au foils. By utilizing onsite scanning tunneling microscope (STM) characterizations combined with first-principles calculations, we have clarified the epitaxial mechanism from the viewpoints of adlayer-substrate lattice matching effect and substrate-step-edge guiding effect. More intriguingly, we have made significant progress on the inch-scale preparation of some vicinal facets to Au(111), and other low-symmetry Au single-crystal substrates like Au(101). On such surfaces, we have accomplished the growth of mono-oriented monolayer MoS_2 striped patterns or triangular domains, respectively, and wafer-scale uniform monolayer MoS_2 single crystals. This series of work should provide some in-depth understanding of the epitaxial mechanism of monolayer MX_2 single crystals on some metal or insulating substrates, thus paving ways for their applications in fabricating multifunctional devices (*e.g.*, photodetectors, sensors) and constructing non von Neumann architectures.

Keyword： Two-dimensional materials, Wafer-scale growth, Characterization techniques, Single crystal, Electronic devices

最终交流类型: Invited

The synthesis of bilayer borophene

陈岚
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The 2D sheet of boron named borophene has sparked an enormous research effort including theoretical predictions of its properties and its experimental preparation on metal surfaces. Several polymorphs of monolayer borophene have been grown on metal surfaces. Bilayer borophene was predicted to be more stable than the monolayer borophene due to the bonding between the two layers, and is a candidate material for a wide range of applications ranging from nodal-line semimetal, to superconductors and anodes in lithium-ion batteries. However, bilayer or few-layer borophene has not been synthesized so far due to the passivation of metal substrates by monolayer.

In this presentation, I will introduce the molecular beam epitaxy growth of boron on Cu(111) surface. The scanning tunneling microscopy experiments together with theoretical calculations reveal the formation of unique boron clusters on monolayer borophene on a Cu(111) surface. The boron clusters tend to selectively bind to specific sites of monolayer borophene with covalent boron-boron bonds in the periodic arrangement. The close-packed adsorption of boron clusters would facilitate the synthesis of bilayer borophene, which is proven by the further epitaxy of boron atoms on cluster/monolayer samples. As a result, the bilayer borophene is formed on Cu(111) surface, which consists of two monolayers and is held together by covalent intra- and interlayer boron–boron bonding. The formation of bilayer borophene is associated with the significant transfer and redistribution of charge in the first boron layer on Cu(111), which provides additional electron density for the bonding of additional boron atoms, enabling the growth of the second layer. The bilayer borophene is shown to possess metallic character, and be less prone to being oxidized than its monolayer counterparts.

Keyword： elemental 2D materials, borophene, scanning tunneling microscopy

最终交流类型: Keynote

2D Materials as Quantum Light Source & Single-Element Ferroelectric Monolayer

Andrew T.S. Wee
National University of Singapore, Singapore

I will begin by showing our typical work on layer-dependent electronic structure of 2D transition metal dichalcogenides, using PtSe2 as an example [1]. I will next report a van der Waals crystal, niobium oxide dichloride (NbOCl2), featuring vanishing interlayer electronic coupling and monolayer-like excitonic behaviour in the bulk form, along with a scalable second-harmonic generation intensity of up to three orders higher than that in monolayer WS2 [2]. To our knowledge, this is the first SPDC source unambiguously demonstrated in two-dimensional layered materials, and the thinnest SPDC source ever reported. Our work opens an avenue towards developing van der Waals material-based ultracompact on-chip SPDC sources as well as high-performance photon modulators in both classical and quantum optical technologies.

In the third part, I report the observation of a single-element ferroelectric state in a black phosphorus-like bismuth layer, in which the ordered charge transfer and the regular atom distortion between sublattices happen simultaneously [3]. Instead of a homogenous orbital configuration that ordinarily occurs in elementary substances, we found the Bi atoms in a black phosphorous-like Bi monolayer maintain a weak and anisotropic sp orbital hybridization, giving rise to the inversion-symmetry-broken buckled structure accompanied with charge redistribution in the unit cell. As a result, the in-plane electric polarization emerges in the Bi monolayer. Using the in-plane electric field produced by scanning probe microscopy, ferroelectric switching is further visualized experimentally. This emergent single-element ferroelectricity broadens the mechanism of ferroelectrics and may enrich the applications of ferroelectronics in the future.

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Keyword： 2D Materials, Quantum light source, ferroelectric monolayer

最终交流类型: Invited

Nonreciprocal second harmonic generation of 2D magnet

吴施伟
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Second harmonic generation is not only of technological importance for nonlinear optical devices, but also a powerful tool for the investigation of symmetry related physical phenomena that are otherwise challenging to probe. The power of this technique lies in its sensitivity to inversion-symmetry breaking, which is the prerequisite for non-vanishing SHG under the electric dipole approximation. While this SHG technique is usually used to study noncentrosymmetric crystallographic materials, the spin structure in magnetic materials may also break the space-inversion symmetry and lead to a nonreciprocal SHG signal. Recently we found the layered antiferromagnetism induced nonreciprocal SHG in CrI3 bilayer is several orders of magnitude larger than that in bulk magnetic crystals. In this talk, I will report our latest studies on various two-dimensional magnetic materials and discuss the related technique issues with this novel SHG technique.

Keyword： 2D magnet, second harmonic generation, symmetry breaking, magneto-optics, nonreciprocal devices

最终交流类型: Invited

High performances two dimensional materials-based photodetectors

张永哲

Beijing University of Technology, China

Photodetection on intensity, polarization and frequency of lights are significant and widespread in modern society scientific research and industrial production. The current instruments are usually bulky and expensive, especially for the polarization and frequency probing. Two-dimensional (2D) materials based optoelectrical devices have attracted lots of attention in next generation of high-performance optoelectronics integrated applications due to the perfect dangling bond-free surface, external field tunability and natural anisotropy. This provides more opportunities to achieve multi-dimensional light detection upon low cost, low power consumption and ultra-miniaturized size. We hence put forward a series of 2D heterogeneous integration design based on energy band engineering and external field modulation. First, a concept of in memory sensing is implemented, where highly sensitive detection and storage for UV light are realized. Secondly, switchable photoelectrical response mechanism is developed, which enables the on-chip full linear polarimetry. Thirdly, electrically tunable interlayer exciton absorption is explored, based on which an ultra-miniaturized near infrared spectrometer with footprint <10 μm is demonstrated.

Keyword： Van der Waals heterostructure; Spectrometer; Polarization; In-Memory Photodetection; 2D materials

最终交流类型: Oral

Deep ultraviolet hydrogel based on 2D cobalt-doped titanate

许友安
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Birefringent optical elements that work in deep ultraviolet (DUV) region become increasingly important these years. However, most of the DUV optical elements have fixed birefringence which is hard to be tuned. Here, we invent a birefringence-tunable optical hydrogel with mechano-birefringence effect in the DUV region, based on two-dimensional (2D) low-cobalt-doped titanate. This 2D oxide material has an optical anisotropy factor of 1.5×10^{-11} $\mathrm{C^2\ J^{-1}\ m^{-1,}}$ larger than the maximum value obtained previously, leading to an extremely large specific magneto-optical Cotton-Mouton coefficient of $3.9 \times 10^{6}\ \mathrm{T^{-2}\ m^{-1}}$. The extremely large coefficient enables the fabrication of birefringent hydrogel in a small magnetic field with an ultra-low concentration of 2D oxide material. The hydrogel can stably

and continuously modulate 303 nm DUV light with large phase tunability by varying the strain (compression or stretching) from 0 to 50%. Our work opens the door to designing and fabricating new proof-of-concept DUV birefringence-tunable elements, as demonstrated by optical hydrogels capable of DUV modulation by mechanical stimuli.

Keyword: 2D material, liquid crystal, hydrogel

最终交流类型: Oral

"Spin Polarization" in Transport Study of Chirality-Induced Spin Selectivity

Tianhan Liu
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Chirality-induced spin selectivity (CISS) is a recently discovered effect that structural chirality can result in different conductivities for electrons with opposite spins.(1) Spin polarization (SP) describes the fraction of spins generated along the chiral axis of chiral media originating from non-spin-polarized currents. In the CISS community, SP is the most widely used physical quantity to describe the efficiency of spin filtering/polarizing process. Experimentally, the CISS effect has been studied mainly in chiral bioorganic molecules, such as double-stranded DNA and peptides, via photoemission, chemical reactions, and transport measurements.(2) Many other organic and inorganic chiral systems have also been explored and large SPs have been reported.(3)

However, the methods of defining, calculating, and analyzing SP have been inconsistent across various studies, hindering advances in the field. It is imperative to define and to calculate SP physically and consistently to avoid confusion and to enable direct comparisons between experiments. We identify the physical quantities that describe the CISS effect across different assemblies rather than focusing exclusively on SP. We will briefly relate the relevant history of the use of SP and focus on the discussion of its determination in different contexts, i.e., photoemission and transport measurements. We propose a more practical and meaningful figure of merit for quantitative analysis in CISS.

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Keyword： chirality-induced spin selectivity, spin polarization, transport, spin-valve

最终交流类型: Invited

Narrow-gap 2D Semiconductors for Infrared and Terahertz Optoelectronics

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Narrow-gap semiconductors like III-V/II-VI materials and their superlattices boost the infrared (IR) and terahertz (THz) technologies and play a critical role in the fields of security inspection, bio-medical imaging, free-space communication, gas detection, and so on. Nowadays, conventional IR and THz devices encounter great challenges referring to the complex structures and expensive epitaxy growth, incompatible with silicon chips, etc. The rising of two-dimensional (2D) materials, with the advantages of atomic thickness, van der Waals integration and fantastic physical characteristics, paves the way for the evolution of advanced optoelectronics. For this end, we have paid our continuous effort on the growth and band engineering of novel narrow-gap 2D semiconductors, representatively as black phosphorus[1-5] and their applications in IR & THz devices, especially for lasers and photodetectors[6-10].

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Keyword： Two-dimensional materials；Black phosphorus；Infrared & Terahertz; Photodetector; Laser

最终交流类型: Oral

Direct-writing atomic-thick two-dimensional semiconductor thin film

李立宏
中国科学院化学研究所

Two-dimensional (2D) semiconductor crystals offer the opportunity to further extend Moore's law to the atomic scale. For practical and low-cost electronic applications, directly printing devices on substrates is advantageous compared to conventional microfabrication techniques that utilize expensive photolithography, etching, and vacuum metallization processes. However, the currently printed 2D transistors are plagued by unsatisfactory electrical performance, thick semiconductor layers, and low device density. Herein, we demonstrate a facile and scalable 2D semiconductor printing strategy utilizing the interface capture effect and hyperdispersed 2D nanosheet ink to fabricate high-quality and atomic-thick semiconductor thin-film arrays without additional surfactants. Printed robust thin-film transistors using 2D semiconductors (e.g., MoS2) and 2D conductive electrodes (e.g., graphene) exhibit high electrical performance, including a carrier mobility of up to 6.7 cm2·V-1s-1 and an on/off ratio of 2×106 at 25 °C. As a proof of concept, we printed 2D transistors with a density of ~47,000 devices per square centimeter. In addition, this method can be applied to many other 2D materials, such as NbSe2, Bi2Se3, and black phosphorus, for printing diverse high-quality thin films. Thus, the strategy of printable 2D thin-film transistors provide a scalable pathway for the facile manufacturing of high-performance electronics at an affordable cost.

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Keyword： 2D materials, Direct-writing, Atomic-thick, Transistors

最终交流类型: Invited

Two-dimensional electronic devices towards intelligent vision sensors

Zhenxing Wang
National center for nanoscience and technology, Beijing, China

Artificial intelligence technology has become the core driving force for the new round of technological and industrial revolutions in the information age. After more than 70 years of development, the performance potential given by the von Neumann architecture has almost reached its limit. With the physical limit of size reduction faced by Moore's law, the progress of integrated process nodes has slowed down, which further magnifies the problems faced by the von Neumann architecture, such as low intelligence, high energy consumption, and low fault tolerance. Exploring new computing architectures and intelligent electronic devices has become the focus of attention.

Due to the weak Van der Waals force between the layers of two-dimensional layered materials, the heterostructure construction is not limited by the interface lattice, polarity, thermal expansion coefficient and other physical mismatches. It can realize the heterostructure construction of any kind of materials, different stacking sequences, different stacking angles and thicknesses, showing unique physical properties and potential in building new structural devices.

In this report, I will focus on our research progress in new structure electronic devices based on two-dimensional materials in recent two years, including two-dimensional ferroelectric semiconductor sensing computing integrated devices and memristor devices.

Keyword： Ferroelectric semiconductor, neuromorphic device, computing in sensor, Memristor

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最终交流类型: Oral

Third-order Nonlinear Hall effect

赖岫
澳门大学

The nonlinear Hall effect can be used to study the geometric properties of the energy band under the condition of time-reversal symmetry and is a powerful means to explore the physical properties of materials. The second-order nonlinear Hall effect was first realized experimentally in 2019, but it requires the breaking of the inversion symmetry of the test system, which limits its application range. In 2021, we and our collaborators observed a third-order nonlinear Hall effect [1] in a system not constrained by space inversion symmetry and carried out detailed characterization and analysis. Through the combination of experimental tests and theoretical calculations, it was verified that the physical source of this phenomenon is the "Berry connection polarization tensor", and in the follow-up work, the third-order nonlinear Hall effect at room temperature was realized. This series of works laid the foundation for the practical device application of the nonlinear Hall effect.

Keyword： nonlinear Hall effect, energy band, time-reversal symmetry, inversion symmetry, Berry connection

最终交流类型: Oral

Two-dimensional transition metal chalcogenides with tunable electronic and magnetic properties

黄玉立
天津大学福州国际联合学院

Two-dimensional (2D) transition metal chalcogenides (TMCs), a class of strongly correlated materials, have exhibited a wide variety of novel electronic and optical properties, and more recently magnetism. Being atomically thin, they are significantly differing from their bulk counterparts due to the quantum confinement effect. Among the most interesting properties of 2D TMCs is the high tunability of the electronic and magnetic properties with their atomic structures, thickness, defects, interfaces, and so on. Here, we will firstly present our recent progress achieved in the defect engineering of 2D TMDs with tunable electronic band gaps. This strategy could also be used to induce room temperature ferromagnetism in non-magnetic 2D materials. Secondly, the realization of intrinsic 2D ferromagnetisms for next-generation electronic and spintronic devices will be discussed. The underlying driven mechanisms have also been understood via density-functional theory calculations.

Keyword： 2D materials, scanning tunneling microscopy, molecular beam epitaxy

最终交流类型: Invited

Rational design of gate configuration for high-performance 2D transistors

Xingqiang Liu
Hunan University

Scaling down the gate dielectric on two-dimensional semiconductors while maintaining high-quality interface is challenge. Herein, a 5.3 Å van der Waals (vdW) gap with supersaturated oxygen is formed between dielectric and channel, which is afforded by the initial HfS_2/MoS_2 vdW contact interface. The HfO_2 dielectric is derived from HfS_2 flake by a mild ozone treatment. The experimental data and density functional theory (DFT) calculation results indicate the vdW gap can decouple the interaction between dielectric and channel, and thus can largely persevere the intrinsic properties of dielectric and channel in the transistors. The MoS_2 vdW-gap-gated (VGG) transistors present a negligible hysteresis of 10 mV with ideal average steep subthreshold slope of 63.1 mV/dec, very close to the physical limit of 60 mV/dec. Moreover, logical NOT, OR and AND gates are constructed based on the superior saturation performance of VGG transistors. The present strategy is alternative for fabricating high-quality dielectric on two-dimensional semiconductors with suppressed scattering. Therefore, it is promising for the design of high-performance low-power electronics.

Keyword： MoS2 transistor; interface; subthreshold swing

最终交流类型: Invited

Atomic Lego for Future Computing

缪峰
南京大学

Van der Waals (vdW) heterostructures (“Atomic Lego”) are formed by stacking layers of different 2D materials and offer possibilities to design new atomic structures with rich physics and functions. In this talk, I will show how these heterostructures provide unprecedented opportunities to explore new physics and realize device applications in the field of future computing, including quantum simulation and neuromorphic computing. I will first present our observation of tunable quantum criticalities in an experimental simulator of the extended Hubbard model with spin–valley isospins arising in chiral-stacked twisted double bilayer graphene [1]. The results demonstrate a highly tunable solid-state simulator

with intricate interplay of multiple degrees of freedom for exploring exotic quantum critical states and behaviors. vdW vertical heterostructures can also be exploited to realize neuromorphic computing devices, such as highly robust memristors based on graphene/$MoS_{2-x}O_x$/graphene vdW heterostructure [2]. Our experimental results on a prototype reconfigurable neural network vision sensor based on a WSe_2/BN heterostructure [3], and in-sensor broadband convolutional processing using a band-alignment-tunable $PdSe_2$/$MoTe_2$ heterostructure [4] will also be presented. In the last part of the talk, I will discuss our preliminary explorations on new computing schemes based on these novel devices [5-6], and share our outlook for the future of this emerging field.

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Keyword： atomic lego, van der Waals heterostructure, future computing, neuromorphic computing

最终交流类型: Invited

Epitaxial Growth and Quantum Properties of Noevel 2D Materials & Heterostructures

Yeliang Wang
Beijing Institute of Technology

The novel properties of graphene honeycomb structure have spurred tremendous interest in investigating other two-dimensional (2D) layered structures beyond graphene for nanodevices. In this talk, I will mentioned the fabrication and properties of several monolayer 2D materials such as silicene, antimonene, semiconducting MoTe2, magnetic VSe2, superconductor transition-metal-trichalcogenide HfTe3, and charge density wave NbSe2, as well as their quantum properties for nanoelectronics and valleytronics will also be introduced. The precise structural configurations at atomic-resolution of these materials will also be introduced, based on the measurements by several advanced techniques like LEED, STM/STS and STEM.

Keyword： 2D Materials, transition-metal-dichalcogenide, quantum properties, STM/STS

最终交流类型: Invited

Design and Realization of 2D Quantum Materials with Topological Flat Bands

杜轶
北京航空航天大学

The energy dispersion of fermions or bosons vanishes in momentum space if destructive quantum interference occurs in a frustrated Kagome or Lieb lattice with only nearest-neighbor hopping. A discrete flat band (FB) without any dispersion is consequently formed, promising the emergence of fractional quantum Hall states at high temperatures. In this talk, I will report the experimental realization of the frustrated lattices (kagome, Lieb, breathing kagome, distorted colouring-triangle) in a two dimension. Because of the unique frustrated and two-dimensional structure, the electrons are localized in the frustrated lattices because of quantum destructive interference, and thus, their kinetic energy is quenched, which gives rise to an FB peak in the density of states. A robust and pronounced one-dimensional edge state has been revealed at the Kagome edge, which resides at higher energy than the FB. For epitaxial buckled Lieb lattice, it indicates a partially broken nodal line loop protected by its mirror reflection symmetry and a topologically nontrivial insulating state with a spin-orbital coupling (SOC) effect in the band structure of this Lieb lattice. Our observations of Kagome and Lieb lattices together with their electronic properties open up the possibility that fractional Chern insulators could be realized experimentally.

Keyword： two dimensional, frustrated lattices, flat band, scanning tunneling microscopy, angle-resolved photoemission spectroscopy

最终交流类型: Invited

Integrated Memristor Networks and Chips for Neuromorphic Computing

杨玉超
北京大学

As Moore’s law slows down and memory-intensive tasks get prevalent, digital computing becomes increasingly capacity- and power-limited. In order to meet the requirement for increased computing capacity and efficiency in the post-Moore era, emerging computing architectures, such as in-memory computing and neuromorphic computing architectures based on memristors, have been extensively pursued and become an important candidate for new-generation non-von Neumann computers. Here we report an optoelectronic synapse that is based on α-In2Se3 and has controllable temporal dynamics under electrical and optical stimuli. Tight coupling between ferroelectric and optoelectronic processes in the synapse can be used to realize heterosynaptic plasticity, with relaxation timescales that are tunable via light intensity or back-gate voltage. We use the synapses to create a multimode reservoir computing system with adjustable nonlinear transformation and multisensory fusion, which is demonstrated using a multimode handwritten digit recognition task and a QR code recognition task. We also realize a multiscale reservoir computing system via the tunable relaxation timescale of the α-In2Se3 synapse, which is tested using a temporal signal prediction task.

Keyword： Memristor, Neuromorphic computing, in-memory computing

最终交流类型: Invited

Bioinspired vision sensors with 2D semiconductors

Yang Chai
Hong Kong Polytechnic University

According to the projection by Semiconductor Research Corporation and Semiconductor Industry Association, the number of sensor nodes exponentially increases with the development of the Internet of Things. By 2032, the number of sensors is expected to be ~45 trillion, which will generate >1 million zettabytes (1027 bytes) of data per year. The massive data from sensor nodes obscure valuable information that we need it most. Abundant data movement between sensor and processing unit greatly increases power consumption and time latency, which poses grand challenges for the power-constraint and widely distributed sensor nodes in the Internet of Things. Therefore, it urgently requires a computation paradigm that can efficiently process information near or inside sensors, eliminate redundant data, reduce frequent data transfer, and enhance data security and privacy. We propose bioinspired in-sensor computing paradigm to reduce data transfer and decrease the high computing complexity by processing data locally. By using two-dimensional (2D) semiconductors, we demonstrate the in-sensor computing at the device and array levels. The unique sensory response characteristics of 2D semiconductors lead to computing functions at sensory terminals. In particular, bioinspired device characteristics enable the fusion of the sensor and computation functionalities, providing a way for intelligent processing sensory information.

Keyword： Bioinspired vision sensors

最终交流类型: Invited

Tailoring Ultrafast Dynamics of Emerging Semiconductor Materials for Photonic Devices

王枫秋
Nanjing University

Low-dimensional materials enabled photonics and optoelectronics are rapidly becoming a preferred avenue for next-generation information devices, promising both significant performance improvement and the potential for disruptive, novel-concept devices. Understanding the photocarrier dynamics, which is fundamentally linked to many of the figures of merits of photonic devices, is the key to develop high-performance devices and also one of the most fundamental tasks of ‘light-matter interaction’ research.

While it is highly desirable to be able to customize the photocarrier dynamics of low-dimensional materials to adapt to various device applications, approaches developed for conventional bulk semiconductors (i.e. III-V compounds) are not directly applicable and such a task remains a significant experimental challenge. In this talk, recent progress in controlling the photocarrier lifetimes in three representative material classes (including graphene-like Dirac materials, 2D transition-metal dichalcogenides, as well as 2D semiconductor heterostructures) will be presented. Photonic applications of these emerging materials in ultrafast optical switches, high-speed photodetectors, opto-spintronic devices will also be touched upon.

Keyword： ultrafast photonics, ultrafast spectroscopy, ultrafast dynamics, ultrafast detectors

最终交流类型: Invited

Light-Matter Interplay in Exciton-Photon Hybrid Systems of TMDC Nanostructures

Jianbin Xu
The Chinese University of Hong Kong

In this study, we concentrate on the interaction between nanophotonic cavities with monolayer/multilayer transition metal dichalcogenides (TMDCs), a family of semiconductors accommodating room-temperature (RT) excitons. The optics of a hybrid system composed of a few-layer (1L–3L) TMDC and open plasmonic cavity system is investigated. By theoretically calculating their optical scattering or reflection spectra, two physical processes are unveiled. In addition to the well-known Rabi-splitting process due to the energy transfer between constituent components, a Fano interference process is shown, resulting in the pronounced Fano-type asymmetry in the spectrum even at zero detuning. Through transferring different layers of WSe2 (one of the TMDC materials) onto the gold disk array, we confirm that the Fano process is not merely determined by the exciton-plasmon interaction, but also highly dependent on the driving field excitation.

Thanks to the significant Ohm losses of the conventional plasmonic cavity, especially at optical frequency, Mie resonators based on the dielectric nanostructures have arisen and attracted increasing attention in nanophotonics in recent years. Here we propose and develop a bottom-up method to grow the TMDC nanostructures with chemical vapor deposition, which is scalable. These TMDC nanostructures show high-quality Mie resonances and self-coupled polaritons due to the coupling between Mie modes and the excitons inside.

Finally, we leverage on the optical interference of two Mie modes with opposite parity, i.e., electric dipole (ED, odd parity) and magnetic dipole (MD, even parity), to achieve the directional scattering of the TMDC resonator. That is, the backward or forward scatterings become vanished when the equal-amplitude ED and MD modes are in-phase (phase difference is zero) or out-of-phase (phase difference is π), also known as Kerker's effects or scatterings. Moreover, through coherent interaction of the exciton, Kerker scattering could be tuned by tailoring the coupling between the exciton and Mie modes.

Keyword：light-matter interactions, 2-dimensional materials, transition metal dichalcogenides, Fano and Rabi resonances, Mie scatterings

最终交流类型:

Two-dimensional organic-inorganic van der Waals heterojunctions

耿德超
Tianjin University, China

Two-dimensional (2D) materials have gained significant attention in recent decades ascribed to their exceptional optoelectronic properties. To meet the growing demand for multifunctional applications, 2D organic-inorganic van der Waals (vdW) heterojunctions have become increasingly popular in the development of optoelectronic devices. These heterojunctions demonstrate an impressive capability to synergistically combine the favourable characteristics of organic and inorganic materials, thereby offering a wide range of advantages. Herein, an ultralow-power vertical transistor is demonstrated based on transition-metal carbides/nitrides (MXene) and organic single crystal. The transistor exhibits a high JON of 16.6 mA cm−2 and a high JON/JOFF ratio of 9.12 × 105 under an ultralow working voltage of −1 mV. Furthermore, it can successfully simulate the functions of biological synapse under electrical modulation along with consuming only 8.7 aJ of power per spike. It also permits multilevel information decoding modes with a significant gap between the readable time of professionals and nonprofessionals, producing a high signal-to-noise ratio up to 114.15 dB. This work encourages the use of vertical transistors and organic single crystal in decoding information and advances the development of low-power neuromorphic systems

Keyword：two-dimensional, van der Waals heterojunctions, organic-inorganic

最终交流类型:

Low-dimensional Semiconductor Materials for Stretchable Electronics and Tactile Sensing

潘曹峰
中国科学院北京纳米能源与系统研究所

Emulation of human senses via electronic means has long been a grand challenge in research of artificial intelligence as well as prosthetics, and is of pivotal importance for developing intelligently accessible and natural interfaces between human/environment and machine.

In this talk, we present a novel design of nanowire LED arrays, which can be used to directly record the strain distribution by piezo-phototronic effect with a resolution as high as 2.7 μm, which is published in Nat. Photonics. Such sensors are capable of recording spatial profiles of pressure distribution, and the tactile pixel area density of our device array is 6250000/cm2, which is much higher than the number of mechanoreceptors embedded in the human fingertip skins (~ 240/cm2).

When the device is under pressure, the images unambiguously show that the change in LED intensity occurred apparently at the pixels that were being compressed by the molded pattern, while those were off the molded characters showed almost no change in LED intensity. Instead of using the cross-bar electrodes for sequential data output, the pressure image is read out in parallel for all of the pixels at a response and recovery time-resolution of 90 ms. Furthermore, our recent studies achieve such piezo-phototronic effect induced strain mapping in a flexible n-ZnO NWs/p-polymer LEDs array system. This may be a major step toward digital imaging of mechanical signals by optical means, with potential applications in touch pad technology, personalized signatures, bio-imaging and optical MEMS.

This research not only introduce a novel approach to fabricate Si-based or polymer-based flexible light-emitting components with high performances, but also may be a great step toward digital imaging of mechanical signals using optical means, having potential applications in artificial skin, touch pad technology, personalized signatures, bio-imaging and optical MEMS, and even and smart skin.

Keyword： Low-dimensional Semiconductor Materials

最终交流类型:

Two-dimensional Inorganic Molecular Crystals.

Tianyou Zhai
Huazhong University of Science and Technology, China

Two-dimensional (2D) materials such as graphene are bound by van der Waals (vdW) forces between layers and strong chemical bonds within the layers. In contrast, the two-dimensional (2D) inorganic molecular crystals (IMCs) we report are consisting of cage-like small molecules without dangling bonds, which are bound by vdW forces in three dimensions. We first proposed a new concept of 2D IMCs, developed a surface passivation growth method in chemical vapor deposition, realized the controllable synthesis of 2D IMCs Sb2O3, and explored the microscopic process and mechanism of its phase transition [1]. Through spectroscopic experiments combined with theoretical calculations, the physical properties and the origin of strong intermolecular interactions in inorganic molecular crystals (P4Se3) were thoroughly studied, and its significant impact on intermolecular charge transport are revealed [2]. By design and synthesis of 2D inorganic bimolecular crystals (SbI3 and S8), the central inversion symmetry of molecular crystals is broken and its application potential in nonlinear optics is demonstrated [3]. We also prepared wafer-scale Sb2O3 vdW dielectric film by thermal evaporation. Via reducing the interface scattering of carriers and increasing the gate capacitance, we have significantly improved the mobility of 2D FETs and greatly reduces the operating voltage of the device. It provides a novel approach for the large-scale integration of high-performance, low-power, two-dimensional electronic devices [4]. We furthermore developed a hybrid dielectric layer consisting of IMC seeding layer and high-κ dielectric layer, which can form a high-quality interface with 2D semiconductor while maintaining high dielectric properties. The EOT of the gate dielectric layer is reduced to 0.67 nm and a record-high gating efficiency is achieved [5]. The vdW encapsulation of 2D optoelectronic devices is realized by using Sb2O3 thin films, which significantly improves the stability of the devices and promotes the practical application of 2D devices [6]. Our works on 2D IMCs not only enriched the concept of 2D materials, but also opened up a new avenue for the study of the properties of inorganic molecules and the application of devices.

Keyword：2D materials, inorganic molecular crystals, field-effect transistor, vdW interaction

最终交流类型:

Nanoscale photodetectors for infrared sensing and intelligent recognition.

Weida Hu
Shanghai Institute of Technical Physics, CAS

Infrared photodetectors based on traditional thin-film semiconductors such as InGaAs, InSb, HgCdTe, and QWIP as well as novel type-II superlattice exhibit highly sensitive detection capability. However, these devices always need to work at low temperature, resulting in an additional large and expensive cooling system. Recently, two-dimensional (2D) materials and Van der Waals heterostructures have attracted tremendous attention owing to their bandgap tunability and potential optoelectronic applications. Nevertheless, as a photoconductive detector, the signal-to-noise ratio could be very low without the suppression of dark current. Meanwhile, the performance of 2D photodetectors in including phototransistors, photoconductors with photogating, and photodiodes, is strongly affected by surface states resulting in the restricted electron-hole separation efficiency and low speed, and intrinsic ultrathin absorption thickness for 2D photodetectors suffers the low quantum efficiency. Here we report the progress on novel uncooled infrared photodetectors and their smart chips based on 2D materials and Van der Waals heterostructures manipulated by localized fields. We fully exploit the detection ability of 2D materials by introducing localized-field, including ferroelectric filed, vertical heterojunction field, p-n junction photovoltaic field and so forth. With a strong induced localized-field, high performance infrared photodetectors. Our study opens a new avenue for controllable fabrications of localized field in 2D optoelectronic devices, which is a prominent challenge in 2D material research.

Keyword： Nanoscale photodetectors

最终交流类型:

Evolution of Low-Dimensional Phosphorus Allotropes on Ag(111)

王一贺
天津大学福州国际联合学院

Elemental two-dimensional (2D) materials exhibiting intriguing properties have great potential applications in next-generation electronics. However, controlling single-phase synthesis might be challenging due to the existence of various allotropes with comparable stability. Here, low-dimensional phosphorus (P) is used as a prototype for the understanding of the competition among a series of 0D−2D

allotropes upon adsorption. With a combination of theoretical calculations and scanning tunneling microscopy, we find that the formation of P allotropes significantly depends on the bond angle, coordination number, and atomic density. As a result, P atoms tend to form black phosphorene (BP)-like chains and pentamer molecules at low atomic density and 2D buckling blue phosphorene at high density.

In particular, a trigonal nanoribbon-like phase is observed with the confinement of the BP-like chains. The comprehensive understanding of the evolution of the elemental allotropes in low dimension could provide fundamental guidance for the construction of polymorphic quantum materials with novel functionalities.

Keyword： Low-dimensional phosphorus, STM, epitaxial growth

最终交流类型: Invited

Ferroelectric field effect transistors for electronics and optoelectronics.

Xudong Wang
University of Wisconsin-Madison

Ferroelectrics have shown great value in the modern semiconductor industry and are considered important function materials due to their high dielectric constant and tunable spontaneous polarization. Ferroelectrics have some basic properties including high dielectric constant, piezoelectricity, pyroelectricity, and ferroelectricity. Ferroelectrics gained attention for their high dielectric constant at first, which has been proved to be related to ferroelectricity.

A ferroelectric field effect transistor (FeFET) is a field effect transistor (FET) with ferroelectric polarization field introduced to regulate carriers in semiconductors. With the coupling of ferroelectric and semiconductor, FeFETs are attractive for advanced electronic and optoelectronic applications, including emerging memories, artificial neural networks, high-performance photodetectors, and smart sensors. In this report, representative research results of FeFETs are reviewed from the perspective of structures and applications. Here, the background and significance of ferroelectrics and FeFETs are given. Furthermore, methods of building FeFETs in different structures and physical models describing the characteristics of FeFET are introduced. Important applications of FeFETs in electronics and optoelectronics are presented, with a comparison of performance between FeFETs and FETs without ferroelectrics, including memories and memristive devices, photodetectors, negative capacitance FETs, sensors, and multifunctional devices.

With the development of quantum physics and nano materials, low-dimensional ferroelectrics have attracted much attention. With dimension reduction, symmetry breaking causes out of-plane and in-plane ferroelectricity. Technologies of van der Waals integration provide flexibility and convenience to build FeFETs with perfect interfaces, which is difficult for modern semiconductor technologies to achieve. This will help to reduce the degradation of properties caused by interfacial defects. Outstanding performance, unique functions, and low power consumption indicate that FeFETs have tremendous potential in advanced electronic and optoelectronic devices.

Keyword： ferroelectrics; optoelectronics; highly sensitive photodetector; multifunctional devices

最终交流类型: Invited

Growth of wafer-scale MoS2 and sub-10 nm channel devices

Luojun Du
Institute of Physics, Chinese Academy of Sciences, China

Monolayer MoS2, an emergent two-dimensional (2D) semiconductor, holds great promise for transcending the fundamental limits of silicon electronics and further scaling transistors to the end of roadmap, because of their atomic thicknesses, dangling-bond-free flat surface, excellent electrostatic control, low in-plane dielectric constants, ultra-low standby current, and superior immunity to short channel effects (SCEs). Indeed, isolated monolayer MoS2 devices have been successfully demonstrated to perform well at ultra-scaled sub-10 nm physical channel lengths or gate lengths, which are inconceivable in the framework of traditional silicon with scaling gate length limit of ~12 nm. Monolayer MoS2 transistors have also been identified by Intel as one of three breakthrough technologies to break the scaling limit of silicon. To realize its full potential and high-end industrial applications, it is of utmost importance and a prerequisite to product wafer-scale monolayer MoS2. In this report, I would introduce our recent progress on the growth of wafer-scale monolayer MoS2, fabrication of high-quality sub-10 nm channel transistors and inverters.

Keyword： MoS2,sub-10 nm channel devices

Topical Sessions =》5. Nano-composites and applications

最终交流类型: Oral

Nano-Engineered Cementitious Composites for Sustainable Infrastructures

韩宝国

大连理工大学

Earth’s human-made mass has exceeded the overall global biomass. Cementitious composites, being the most used human-made substance, have become one of the most obvious manifestations of humankind's physical footprint on the Earth. The use of cementitious composites changes the world, promotes the rapid development of human society, and shapes the human civilization. Moreover, cementitious composites are still indispensable in the foreseeable future, and their application room is constantly expanding.

However, some inherent weaknesses and the existing performances of cementitious composites make them unable to fully meet the demands of constructing and creating future human living infrastructures. Additionally, the massive production and application of cementitious composites have an enormous impact on resources, energy as well as environment on the Earth. Nano science and technology can change the “gene” of cementitious composites at a more fundamental level. It provides a transformative approach to solve the above issues and boosts the emergence and rapid development of nano-engineered cementitious composites with sustainable characteristics (e.g., high mechanical performance, long service life, perfect multifunctionality/smartness, easy fabrication, low environmental footprint, strong resilience, and low life-cycle cost).

In the past two decades, the rapid development of nano science and technology build up a fundamental for comprehensively understanding the genomic code of cementitious composites in nature, featuring the blueprint to describe, predict, and tailor performance of cementitious composites from the bottom-up (i.e., from nanoscale to micro-macro-scale) approach, and providing guide for design, fabrication, and applications of cementitious composites. In this manner, research on nano science and technology in cementitious composites reach a very active period. Much work indicated that the big gains in mechanical, durable and functional/smart properties of cementitious composites were achieved by using nanotechnology. The enhancement/modification mechanisms of nano-engineered cementitious composites can be attributed to nano-core effect including intrinsically excellent mechanical, electrical, thermal and electromagnetic properties and morphology features (high aspect ratio); and promoting cement hydration, optimizing C-S-H gel structure and forming ultrafine and compact crystals, improving interfacial transition zone and pore structure, controlling nano-scale cracks, autogenous curing, improving early strength and decreasing autogenous shrinkage.

This report will present both fundamentals and applications, with emphasis on the design and principles, fabrications, characterizations, performances (including mechanical properties, durability, function/intelligence) and mechanisms, and applications of nano-engineered cementitious composites, deliver current groundbreaking science advances and technical innovations in the field of nano-engineered cementitious composites, and deploying the road map to tackle the future development challenges of nano-engineered cementitious composites.

Keyword：Nano；Cementitious composites；Principles; Practices; Sustainable Infrastructures

最终交流类型: Keynote

Advanced Functional Nanocomposite Fibers by Thermal Drawing

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Advanced multimaterial fibers offer a novel degree of freedom to engage applications spanning smart and flexible electronics, nanorobotics, the next generation of sensors and transducers, biomedical diagnosis/therapy, and prosthetics. Advanced multimaterial fibers have experienced rapid development in the past two decades owing to the high scalability, uniformity, and material and structure compatibility of the thermal drawing technique. Fiber drawing from a preform has traditionally been exploited to produce with high precision and reliability the extended lengths of optical fibers that today span the globe, deliver telecommunications, and enable the internet. One limitation of the current state of the art, however, is that the current fiber drawing has been limited to drawing of a single material and

to features no smaller than several microns. Recently, fiber-drawing approaches have been extended to a new class of multi-material fibers containing functional structures that enable the development of optoelectronic fibers. This new class of fibers centers on a method so-called preform-to-fiber fabrication by thermally drawing a macroscopic solid-state preform into extended lengths of uniform fibers. Unlike the traditional optical fiber fabrication, this method features with three key elements in resulting fibers: (1) combining a multiplicity of solid materials with disparate electrical, optical, and mechanical properties into a single fiber, (2) realizing arbitrary nanometer-scale geometries in fibers with low-scattering interfaces, and (3) producing long lengths of fibers through the simple and scalable process of thermal drawing. This talk presents various multimaterial nanocomposite fibers based on different functional structures and their applications in disparate fields. We present representative demonstrations of engaging nanocomposites such as MXene for extended functionalities. Additionally, we summarize the current progress on creating surface structures on thermally drawn fibers, as well as the fabrication of soft and stretchable functional fibers. All these reported applications indicate that this fast innovated interdisciplinary area is of great potential in fiber sensing, soft electronics, functional fiber integration, wearable devices, and smart textiles.

Key Words Nanocomposite fibers, thermal drawing, sensing, wearable electronics, smart textiles

最终交流类型: Oral

Polymer-Brush-Based Nanocomposites

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Attempts to combine properties of two distinct materials on nano/molecular scales may trace back to the Roman empire and the Mesoamerican culture in the 7th century. Modern forms of composites emerged over 100 years ago in an effort to prepare better and more durable materials. Since the dawn of nanotechnology in mid-1900s, numerous tools to prepare nanocomposites with high precision have arisen, among which include the advancement of polymerization techniques, especially controlled radical polymerization, since the end of last century. A variety of unprecedented polymer architectures have been

enabled. One of these architectures, nanoparticles grafted with polymer brushes, a.k.a. particle brushes, are an emerging class of nanocomposites/hybrid materials that merge functionalities of inorganic nanomaterials and processability/assembly behaviors of polymeric materials. Polymer brushes dominate the interfaces with many properties of inorganic nanoparticles preserved. These materials find potential applications in mechanical reinforcement, electromagnetic modification, biomedicines, and power storage.[1] Three major approaches were developed to prepare particle brushes, including the straightforward "grafting-onto" approach, the "grafting-from" approach which requires prior surface-functionalization with initiating moieties, and a "templated synthesis" approach that converts nanoparticle precursors in nanoreactors. An "grafting-from" approach based on surface-initiated atom transfer radical polymerization (SI-ATRP) has been proven to be one of the most powerful tools for the preparation of particles brushes, thanks to the readily accessible surface initiating sites (alkyl halides), rich choices of monomer functionalities, and tunable grafting densities and molecular weight distributions.[2] In the past years, we employed various surface-modification techniques, particularly SI-ATRP, in the preparation of particle brushes with diverse inorganic nanoparticles and sophistically designed chemical compositions, molecular weight distributions, and grafting densities of polymer brushes. Carboxylate-based tetherable initiators enable the surface functionalization of a variety of functional metal oxide nanoparticles. Partial deactivation of growing chains provided a precise manipulation of molecular weight distributions. Catalyst concentrations and its reactivity simultaneously determines the molecular weight distributions and grafting densities. A broad range of potential applications of these nanocomposites were explored. We recently examined the chemical safety aspect in the research practice of difficult-to-etch particle brushes. In this presentation, we discuss the evolution of polymer-inorganic nanocomposites, preparation techniques, the structural control, and some possible applications of particle brushes. We further look at the current obstacles and future opportunities in this field.

Keyword： hybrid materials, nanocomposites, polymer brushes, surface-initiated polymerization, ATRP

最终交流类型: Oral

Extreme Properties of Carbon Nanotubes and Their Applications

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Carbon nanotubes (CNTs) have excellent mechanical, electrical and thermal properties and have great potential to be used in many cutting-edge applications. In terms of extreme mechanical properties, we established a non-contact acoustic resonance testing system to study the mechanical properties of a single defect-free ultralong CNTs. Single CNTs are super-durable and their fatigue strength exceeds any other engineering materials. The fatigue fracture is dominated by the time to creation of the first single-bond-sized defect. A gas flow focusing method was introduced to in-situ fabricate the CNT bundles with centimeters long, defect-free, uniform oriented and continuous structure. After releasing the initial stress to a narrow distribution using a "synchronous tightening and relaxing" strategy, the tensile strength of CNT bundles was increased to more than 80 GPa. With CNT bundles as the flywheel material, the obtained energy density and power density would be as high as 8571 Wh/kg and 2 GW/kg. Here we also report the welding of CNTs for the first time by a fast chemical-vapor-deposition self-assembly (FCVDS) technique using TiO2 nanoparticles as the solder. It has advantages such as simpleness, economy, high speed, applicable to ambient conditions and welding samples with macroscale length like biological missiles (targeted welding). The weld junction can have a mechanical strength over 100 GPa, the highest strength achieved by cold welding so far. The solder mass can be only ~1wt% of welded CNTs. In terms of extreme electrical properties, the application of CNTs in lightning striking protection of large aircrafts was studied.

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Keyword: Extreme properties, Carbon nanotubes, CNT bundles, Flywheel energy storage, Lightning striking protection

最终交流类型: Invited

Flexible Wearable Polymer Nanocomposite-Based Electronic Sensing Device

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北京化工大学

Flexible wearable electronic sensors prepared from versatile functional polymer nanocomposites, are attracting enormous research attention in multifunctional electronic skins, smart human-machine interaction, and wearable intelligent medical diagnosis and treatment for their reliable flexibility, excellent portability, and real-time wearable sensing capability.[1-5] A nacre bionic intercalated MXene nanocomposite film is successfully prepared from the facile assembly of MXene/poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS)/polyvinyl alcohol (PVA) nanocomposite on the polyethylene (PE) film substrate by subsequent facile solvent-evaporation-induced self-assembly, demonstrating nacre-like "brick-and-mortar" microstructure and excellent mechanical strength, which could be assembled as flexible wearable electronic sensor for ultrasensitive human healthcare monitoring and multi-responsive smart actuation.[3] The as-assembled flexible wearable electronic sensor from the nacre bionic intercalated MXene nanocomposite film, exhibited faster sensing response time/recovery time, wide sensing range (up to 166.7 kPa), highly sensitive sensing performance for large scale human motions (for example, finger tapping and finger bending) and tiny electrophysiological signals (for example, electrocardiogram (ECG) signal and electromyogram (EMG) signal), and efficient Morse code message demonstration by touching the sensor. Moreover, the intelligent human-machine interfacing and the smart gesture recognition could be successfully realized by attaching the flexible wearable electronic sensors onto the fingers of a manipulator wirelessly controlled by a volunteer's hand for sensing hand gestures, such as "paper", "scissors", and "rock" respectively. Furthermore, the as-obtained multi-responsive smart actuator displayed excellent actuating performance under external humidity stimuli and near infrared (NIR) light irradiation from the nacre-like intercalated MXene nanocomposite and the polyethylene film

substrate with distinct difference in hygroscopic performance under external moisture stimuli, and different thermal expansion coefficient. And the as-obtained multi-responsive smart actuator could be assembled as the humidity/light-responsive intelligent curtain for reversibly switching the window under external moisture/NIR light irradiation. Thus, this line of research work shows versatile potential in human healthcare monitoring, medical diagnosis, human-machine interfacing, and smart soft robots.

Keyword： nacre-like MXene nanocomposite, wearable human-machine interfacing, epidermic sensor, multi-responsive actuation, flexible electronic device

最终交流类型: Invited

Ultrastrong MXene films via the synergy of intercalating small flakes and interfacial bridging

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Titanium carbide MXene is an emerging two-dimensional transition metal carbide with excellent mechanical properties, high electrical conductivity, and low infrared (IR) emissivity. Interest in assembling MXene flakes into high-performance macroscopic films has recently grown due to promising applications in flexible electrodes, electromagnetic interference (EMI) shielding, and thermal camouflage, among many others. Because of their higher aspect ratio, large MXene flakes have proven to be better than small ones for making high-performance MXene films. A blade-coating method has been developed to effectively align large MXene flakes, greatly increasing their tensile strength and electrical conductivity. However, the weak interlayer interactions prevent further improvement of the mechanical properties. Moreover, the voids in thick films decrease their properties, thereby limiting many practical applications.

The abundant surface functional groups, such as –F, =O, and –OH, allow for chemical crosslinking, including hydrogen, ionic, and covalent bonding, to improve the interfacial strength of adjacent MXene flakes. Although traditional crosslinking strategies can diminish the voids, the electron transport between MXene flakes is usually disrupted by the insulating polymer bonding agents, reducing the electrical conductivity. Thus, it is still challenging to integrate high mechanical and electrical properties into MXene films.

Here we demonstrate a sequential densification strategy to synergistically remove the voids between MXene flakes while strengthening the interlayer electron transport. Small MXene flakes were first intercalated to fill the voids between multilayer large flakes, followed by interfacial bridging of calcium ions and borate ions to eliminate the remaining voids, including those between monolayer flakes. The obtained MXene films are compact and exhibit high tensile strength (739 MPa), Young’s modulus (72.4 GPa), electrical conductivity (10,336 S cm-1), and EMI shielding capacity (71,801 dB cm2 g-1), as well as excellent oxidation resistance and thermal camouflage performance, showing applicability to conditions involving a humid environment and more demanding mechanical loading, such as flexible wearable devices and military stealth cloaks. The presented strategy provides an avenue for the high-performance assembly of other two-dimensional flakes.

Keyword： MXene, films, synergistic densification, intercalating small flakes, interfacial bridging

最终交流类型: Invited

Biomimetic Nanofiber Networks for Bio-Integrated Flexible Devices

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Nanofiber networks are essential structures in natural biological tissues, which exhibit a combination of mechanical flexibility, fracture resistance, and mass permeability to enable many important physiological functions. Inspired by natural soft tissues, we exploit biomimetic nanofiber networks as building blocks for the construction of a variety of bio-integrated soft devices. A key component in these materials and devices is aramid nanofiber (ANF). With appropriate solvent-based processing steps, the ANFs self-organize into hyperconnective networks, which capture some of the key features of load-bearing soft tissues. They also exhibit tissue-mimetic physical properties and microstructural reconfigurability, which are beneficial for device applications. The composites can be functionalized with bioactive molecules or soft electronic components for interfacing with cells and tissues. In this presentation, I will introduce some of our recent works ranging from electroconductive hydrogels and wearable devices to theoretical modeling and meso-structural designs. These works address the fundamental physical mismatches between

biomedical devices and biological soft tissues, paving the way for the development of advanced wearable human-machine interfaces, implantable electronics, tissue engineering platforms, and other biomedical systems.

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4. H. He†, X. Wei†, B. Yang, H. Liu, M. Sun, Y. Li, A. Yan, C.Y. Tang, Y. Lin*, and L. Xu*, “Ultrastrong and Multifunctional Aerogels with Hyperconnective Network of Composite Polymeric Nanofibers” Nature Communications 13, 4242 (2022).

Keyword： biomimetic materials, nanofibers, soft electronics, hydrogels, nanocomposites

最终交流类型: Keynote

Linear and non-linear rheology of polymer nanocomposites

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The mechanical properties of polymer nanocomposites are strongly related to the size, the shape of nanoparticles, and their interaction with polymers. Although many efforts have been devoted to this topic, the quantitative relation between the structure and rheological properties remains obscure. In this work, we studied morphology (Figure 1a), rheological behaviors, and dynamics at different time scales in model polymer nanocomposites filled with agglomerated nanoparticles. We adopted synchrotron small-angle X-ray scattering (SAXS), ultra small-angle X-ray scattering (USAXS), and Transmission Electron Microscopy (TEM) to reveal the hierarchical structure of nanoparticles both in the real space and in the reciprocal space. A new method was suggested to obtain the aggregate and hole sizes from TEM images. We suggested an iso-frictional correction to eliminate the effect of the varying frictional environment due to nanoparticles. We found that the increase of rubbery plateau modulus depends on the effective surface area, which is ascribed to the adsorption-induced entanglements. Such a mechanism is similar to that in polymer nanocomposites with good dispersity. The increase of rubbery plateau modulus implies an increase of the entanglement density, correspondingly an increase in the terminal relaxation time of polymer chains. At a longer timescale, the mechanical enhancement is ascribed to the particle motion or relaxation of agglomerates. A model was suggested to quantitatively describe the linear viscoelasticity of polymer nanocomposites over a wide range of timescales (Figure 1c), where the interplay between the relaxation of nanoparticles and polymer chains is reasonably coupled. We also studied the evolution of morphology and rheology under different shear histories (Figure 1d)1, 2. Percolation diagrams were obtained for nanocomposites under different shear histories (Figure 1e), which indicated that the percolation concentration of nanoparticles increased with the applied shear rate 1 or shear stress 2. These results give more insights into how particle structure forms and evolves under the flow field in a polymeric matrix.

Keyword：polymer nanocomposites, rheology

最终交流类型: Keynote

Fiber Power Systems

彭慧胜

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With the boom of many new important fields such as flexible electronics, wearable technology and smart health management, it is necessary to make the next-generation electronic devices like power systems as thin as possible, which may produce a revolution in the world. However, there remains intrinsic challenges that seem very difficult to be overcome according to the planar structure. To this end, we have explored a new family of fiber energy harvesting devices including perovskite solar cells and fluidic generators, fiber energy storing devices including lithium-ion batteries, lithium-sulfur batteries and metal-air batteries, mainly based on the use of polymer electrolytes. These fiber power systems can be

highly integrated into flexible textiles or other structures for large-scale applications with high efficiency, good safety and low cost. Fiber lithium-ion batteries (FLIBs) have been demonstrated here.

FLIBs are pioneering as flexible power solutions because they can be woven into textiles. Textile batteries offer a convenient and seamless way to power future wearable electronics. However, current FLIBs are only centimetres long because longer FLIBs are difficult to produce and they are thought to have significantly higher internal resistances that compromise electrochemical performance. Here, we unexpectedly discovered that FLIB internal resistance has a hyperbolic cotangent function relationship with fiber length, where it firstly decreases before leveling off as length increases. Systematic studies confirm this is true for different fiber batteries. We produced meters of high-performing FLIBs via an optimized industrial process. Our mass-produced FLIBs had a certified energy density of 85.69 Wh/kg (typical values are <1 Wh/kg) based on the total weight of a lithium-cobalt-oxide/graphite full battery including packaging. Its capacity retention reaches 90.5% after 500 charge/discharge cycles and 93% at 1 C rate (compared with 0.1 C capacity), which is comparable to commercial batteries like pouch cells. Over 80% capacity can be maintained after bending for 100,000 cycles. We show FLIBs woven into safe and washable textile by industrial rapier loom can wirelessly charge a cellphone or power a health management jacket integrated with fiber sensors and textile display.

Keyword：wearable technology；energy harvesting；fiber；textile

最终交流类型: Invited

Ion-Selective Polymer Nanofiber Composites for Lithium Metal Batteries

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Lithium metal batteries (LMBs) with high theoretical capacity and energy density, are still seriously restricted by the "shuttle effect" of lithium polysulfides (LiPSs) and dendrite growth in practical applications. As a vital component in batteries, the separators fundamentally determine the interfacial structure and internal resistance of batteries.

Compared with the traditional porous polymer separators, ion-selective polymer nanofiber separators with precisely directed ion diffusion paths are expected to achieve higher electrolyte wettability and ionic conductivity. In particular, the facile electrospinning technique has been applied to realize the controllable regulations of surface charge and porous structures of the fibrous membranes in this work. The introduced functional groups like carboxyl groups and oxygen radicals, as well as precisely tuned porous structures, can construct a uniform and negative electric field on the surface of separators to effectively suppress the "shuttle effect" of polysulfides and lithium dendrite formation. As a result, the LMBs demonstrate significantly improved cycle stability and rate performance. This work provides new ideas for the general design of advanced composite membranes with typical surface ion selectivity in applications of high-performance LMBs.

Keyword：Polymer Nanocomposites; Nanofibers; Precisely Constructed Porous Structures; Lithium Metal Batteries

最终交流类型: Invited

Multifunctional and efficient thermal management materials and devices

马儒军

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Nowdays, the increasing integration of electronic devices leads to more and more prominent thermal failure problems, and the traditional cooling technology can no longer meet the cooling needs of electronic devices. Here we focus on three aspects to achieve thermal management effects with maximum efficiency: 1. Efficient transfer of heat from working electronic devices through efficient, environmentally friendly, miniaturized solid-state refrigeration devices based on the electrocaloric effect to keep the electronic devices in the optimal operating temperature range and maintain their efficient operation [1-4]. 2. The transferred part of the heat is converted into electrical energy using highly reliable, environmentally friendly, noiseless high-performance thermoelectric devices to achieve waste heat recycling [5-7]. 3. The unused heat is quickly dissipated through zero-energy, environmentally friendly, and easy-to-process radiative cooling devices to further reduce the device temperature [8-10]. The three research aspects are closely integrated and complementary; electrocaloric cooling and radiative cooling provide a greater temperature difference between the hot and cold ends of the thermoelectric devices, which can convert more heat into electricity and provide some of the electrical energy needed for cooling the electrocaloric devices; radiative cooling accelerates heat transfer and improves the efficiency of electrocaloric cooling.

Keyword： Thermal management, Solid-state cooling, Electrocaloric effect, Radiative cooling, Thermoelectric

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最终交流类型: Invited

Assembled Nanowire Thin Films and Flexible Smart Device

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As nanotechnology developed, significant advancement has been made to create and construct well-defined ordered nanowire superstructures or complex architectures for desired properties. Natural biomaterials often show ordered nanowire structures which display unique structural color or optimized fracture toughness avoiding their inherent brittleness. Meanwhile, plenty of modern nanodevices with ordered nanowire structures have flourished with activities focused on both basic and applied research.

In this presentation, we will delve into the latest advancements in transforming nanowires from a disordered state to a hierarchically ordered structure, achieved through diverse assembly strategies, resulting in captivating and extraordinary chemical and physical properties. Also, we will overview the recent developments and highlight the latest achievements in our group of smart electronics composed of integrated nanowire structures. Different assembly strategies for 1D, 2D and 3D nanowire assemblies, especially NW co-assembly processes, and their applications for flexible electronics will be described in details. Finally, a short summary and outlook for future challenges and perspectives in this field are presented. Although great achievements have been made during the past few decades, it is necessary to realize that the large-scale production of nanowires and their precisely controlment remains a major issue in this field. We do believe that all of these challenges and opportunities can be addressed in future efforts, and we can expect the emergence of reliable and efficient nanowire assembled based flexible devices.

Keywords: Nanowire; Nanowire assemblies; Self-assembly; Smart device

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最终交流类型: Invited

Carbon networks for wearable piezoresistive physical sensors

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Wearable piezoresistive physical sensors have attracted tremendous attention due to their broad applications in human-machine interfaces, robotics, health-monitoring, personalized medicine and therapeutics. Conventional metal- and semiconductor-based strain sensors are rigid, fragile, and opaque, restricting their applications in wearable electronics. Among various nanostructured materials that have been explored to construct stretchable piezoresistive sensors, carbon-based structures show the potential of achieving higher flexibility and transparency. We present several novel carbon-based interconnected structures including carbon nanofiber, graphene woven fabric, graphite nanoplatelet welded carbon nanotube networks, wrinkled and crack-bridging graphene film, unidirectional graphene aerogel, and graphene foam as highly sensitive, flexible, and stretchable strain sensors capable of detecting human motions. The synthesis strategies of carbon-based sensing structures, including 1D fibers, 2D planar networks and 3D interconnected nanoarchitectures are summarized. By bridging the technological gap between signal collection, processing and transmission and allowing data transmission to a smartphone via a custom-developed application consisting of a user-friendly interface, several wearable applications including wireless wearable musical instrument prototype, human motion detection and switch controls are demonstrated. The novel approaches reported here offer a wide range of practical applications, including medical diagnosis, health monitoring, early warning systems for structural failure, and wearable displays. With the development of new strategies and technologies as well as a deeper understanding of wearable sensor systems, we believe that carbon-based flexible electronics will play an increasingly more important role in driving the development of a wide range of emerging applications in biomedicine, healthcare, robotics, artificial intelligence and entertainment technologies.

Keyword： Carbon networks, Strain sensors, Pressure sensors, Directional Sensors, Wearable devices

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最终交流类型: Oral

Multifunctional biomass-based composite aerogels

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With the rapid development of the modern electronic industry, especially the advent of the 5G network era, electronic appliances and radio communications have been widely used. While bringing communication convenience to people, electromagnetic interference (EMI) and the resulting electromagnetic (EM) pollution problems have also attracted more attention. EM waves not only affect electronic or communication devices, but also cause serious damage to people's health in the EM environment for a long time. Therefore, it is urgent to explore effective strategies to alleviate the EM pollution problem we are currently facing. EMI shielding is the most effective and convenient way to eliminate EMI. In order to achieve the purpose of controlling EMI from the source, EMI shielding materials with high shielding performances are generally utilized to block the propagation of EM waves by reflecting EM waves back or confining them inside the shield. Recently, high-performance porous polymer-based functional materials have attracted tremendous interests in various applications. However, it is a challenge to develop efficient EMI shielding materials

integrating multiple functions without losing the advantages of being light, porous, green and so on. Herein, we designed a conductive aramid nanofiber (ANF)/cellulose nanofibril (CNF)/silver nanowire (AgNW) (ACA) composite aerogel film by directional freeze-drying and moderate compressing. The ACA aerogel film obtained an ideal electromagnetic interference shielding efficiency of 34.54 dB while maintaining a high electrical conductivity of 10.81 S/m. On the other hand, the surface saturation temperature of the aerogel film reached 111 °C under a low applied voltage of 1.6 V. More importantly, a single-electrode triboelectric nanogenerator (TENG) was assembled by ACA aerogel film and polytetrafluoroethylene film. The open-circuit voltages, short-circuit currents, and maximum instantaneous power density of the TENG exhibited a spectacular value of 104 V, 1.52 μA, and 694 mW/m^2, respectively, which could light up 23 LED lights at the same time. This novel multifunctional ACA aerogel film holds great application potentials for electromagnetic protection, energy harvesting, and thermal management.

Keyword： Aerogel; Nanocellulose; Electromagnetic interference shielding; Flexible sensing

最终交流类型: Invited

Soft Elastic Polymer/Carbon Based Thermal Conductive Composite

秦盟盟

天津大学

With the rapid progress of electronic information, aerospace and other technologies, equipment is constantly developing towards miniaturization, integration, and high-power. The heat aggregation problem gradually becomes the key to restrict the improvement of device performance. Because the surface of the device or material exists the uneven structure, the actual contact area is very small, resulting in a large contact thermal resistance. Composites with high thermal conductivity and flexibility can fill the pores of the interface, and eliminate air, then promoting the efficient thermal dredging of the interface. In recent years, with the increase of device power density and the use environment increasingly complex, interface usually undergo deformation, gap change, and warping. Traditional flexible silicone with plasticity is difficult to realize rebound, and thermal conductive composite gel will also lose resilience during cyclic compression, which is difficult to adapt to the new interface cooling demand.

To solve these problems, we propose new thermal interface materials with high thermal conductivity, low modulus and resilience. We carried out the structural design of composite from the perspective of polymer matrix and thermal conduction fillers, respectively. Forming a continuous thermal conductive network can promote the reduction of thermal resistance between thermal conductive fillers, thereby improving the utilization efficiency of the fillers. Reducing the content of fillers can also reduce the elastic modulus. In addition, a continuous network structure can also promote the improvement of rebound performance. By designing the molecular structure and chemical bond type of polymer, the low modulus, self-healing and resilience of polymer can be achieved.

A stiff and tough supramolecular frameworks of PBA-PDMS were established using a chain extender with double amide bonds in a side chain to extend prepolymers through copolymerization. Then, by introducing the copolymer into a folded graphene film (FGf), a highly thermally conductive composite of PBA-PDMS/FGf with self-healing capacity was fabricated. The ratio of crosslinking and hydrogen bonding was optimized to ensure that PBA-PDMS could completely self-heal at room temperature in 10 min. Additionally, PBA-PDMS/FGf exhibits a high tensile strength of 2.23 MPa at break and high thermal conductivity of 13 W/mK, of which the self-healing efficiencies were 100% and 98.65% at room temperature for tensile strength and thermal conductivity, respectively. The excellent self-healing performance comes from the efficient supramolecular interaction between polymer molecules, as well as polymer molecule and graphene. This kind of thermal conductive self-healing composite has important application prospects in the heat dissipation field of next generation electronic devices in the future.

Keyword： Thermal interface materials, Soft elastic, Thermal conductivity, Graphene, Thermal resistance

最终交流类型: Invited

Preparation and Recycling of High-Performance Thermoset Epoxy/Carbon Fiber Composites

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Achieving carbon peaking and carbon neutrality goals, wind turbine generator with the larger and lighter blades will grow rapidly, and thermoset carbon fiber reinforced polymer composites (CFRPs) will be used widely and potentially in wind turbine blades. Blades waste will reach 38,000 tons per year in 2030 after end-of-life. Currently, only 5% of CFRPs are recycled into lower-value secondary products. High-efficiency and high-value closed-loop recycling of matrix and CF poses an important challenge as well as high mechanical strength of composites. Here, we report a sustainable approach for the closed-loop recycling of the resin and fiber from CFRPs. Thiol-functionalized carbon fiber (TCF) obtained by functionalization with a thiol-ended hyperbranched polymer, and then an epoxy-ended degradable hyperbranched polymer (HTn, n=3, 6, 9, 12) are used to prepare HTn/TCF composites, which show considerable acid resistance and mechanical performance. The effects of HTn molecular weight and resin content on mechanical strength of HTn/TCF composites were investigated in detail. The result suggested that the mechanical properties of HTn/TCF composites containing a moderate molecular weight of HTn and a medium resin content of 57 vol% possesses the extraordinary performance. Compared with the corresponding performance of diglycidyl ether of bisphenol A (DGEBA)/pristine carbon fibers composites, the tensile strength, tensile modulus, flexural strength, flexural modulus, and interlaminar shear strength of HT12/TCF composites are increased by 112.73%, 169.45%, 227.34%, 346.02%, and 544.33%, respectively. The service life of the HT12/TCF composites is about 200 years at 40 °C by simulating environmental experiments of acid rain and seawater resistance, being much longer than DGEBA/carbon fibers of about 20 years. The cured composites are controllably depolymerized into monomers and oligomers with high recyclability, which can be utilized to prepare HTn and the precursor of crosslinked HTn. After recycling twice, the composites still maintain high mechanical strength, suggesting high efficient renewability of carbon fibers and epoxy resins. This research provides a sustainable approach for preparing high-performance environmentally-friendly epoxy resin/carbon fiber composites capable of upcycling, well-balancing service life and performance.

Keyword： Hyperbranched Polymers; Epoxy resins; Carbon fibers; Composites; Recycling.

最终交流类型: Invited

New enhancement mechanism and large-area fabrication strategy of ultrastrong layered nanocomposites

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Biomaterials like nacre, bones and mollusk shells provide a rich source of inspiration for developing mechanically strong and tough composites. A number of approaches, such as vacuum filtration, cast drying and layer-by-layer assembly, have been developed to fabricate layered nanocomposites with highly aligned microstructures. However, these methods are limited in their ability to continuously fabricate uniformly layered large-area nanocomposites with long range aligned structure. Therefore, it remains an open issue how to produce highly strong, tough composites in a viable, scalable manner.

Herein, a new method for the fabrication of layered nanocomposite films based on superspreading shear-flow was developed, which solved the problem that layered composite materials cannot be continuously prepared in large area. The superspreading shear flow can drive nanosheets to align rapidly along the flow direction. The aligned nanosheets can be conserved by calcium ions (Ca^{2+})-induced crosslinking of alginate. An elegant setup was developed for the continuous fabrication of such layered structures. By optimizing the content of polymers and nanofillers, a series of layered nanocomposite films that exhibited high uniformity and the highest mechanical properties to date were prepared. The nanocomposites based on nanosheets of graphene oxide and clay exhibit a tensile strength of up to 1,215 ± 80 MPa and a Young's modulus of 198.8 ± 6.5 GPa, which are 9.0 and 2.8 times higher, respectively, than those of natural nacre (mother of pearl). When nanosheets of clay are used, the toughness of the resulting nanocomposite can reach 36.7 ± 3.0 MJ/m^3, which is 20.4 times higher than that of natural nacre; meanwhile, the tensile strength is 1,195 ± 60 MPa. The movement limitation of polymer chains in the confined space between layered nanosheets was the scientific mechanism leading to the ultra-high mechanical properties of these nanocomposites. Furthermore, this superspreading strategy is generalizable and scalable, which could be achieved the alignment a variety of two-dimensional nanofillers and the large-scale continuous fabrication of layered nanocomposite films by using many different kinds of polymerization of other covalent and non-covalent polymers systems. This work provides a new strategy for the structural design and large-scale production of bionic layered materials.

Keyword：biomimetic materials, high strength and toughness, nanocomposites, layered structure

最终交流类型: Invited

Peeling by Pulling: Characterizing the Mechanical Behavior of NanoFilms

戴兆贺

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The flexible and clinging nature of ultra-thin films require the understanding of their elastic and adhesive properties in a wide range of circumstances from fabrications to applications. Simultaneously measuring both elastic and adhesive properties, however, is extremely difficult as the film thickness diminishes to nanoscales. In this talk, I will show our recent work that addresses such difficulties through peeling by vertically pulling thin films off from the substrates (we thus refer to it as “pull-to-peel”). Particularly, we perform in-situ pull-to-peel of graphene and MoS2 films in a scanning electron microscope (SEM) and achieve simultaneous determination of their Young’s moduli and adhesions to gold substrates. This is in striking contrast to other conceptually similar tests available in the literature, including indentation tests (only measuring elasticity) and spontaneous blisters (only measuring adhesion). Furthermore, we show a weakly nonlinear Hooke’s relation for the pull-to-peel response of two-dimensional materials, which may be harnessed for the design of nanoscale force sensors or exploited in other thin-film systems. Lastly, we also discuss the general theories that can be used to give an adhesive criterion when dealing with the adhesion problem of thin films and plates that are even wrinkled due to external compression.

Keyword：Blister test, Thin films, Adhesion, Indentation, in situ SEM

最终交流类型: Oral

Magnetoelectric core-shell nanoparticles as an efficient electroactive platform for noninvasive biomedical applications

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Introduction. Magnetoelectric (ME) nanoheterostructures offer an excellent opportunity as minimally invasive surgical tools because of their strong towing force and functionality. As compared to magnetic nanoparticles (NPs), ME nanoheterostructures can be precisely delivered (magnetic properties) at low Reynolds number (Stoke’s flow regime) and induce the electrical stimulation (ME effect) of surrounding biological microenvironments using safe magnetic fields with a low-strength [1, 2]. These properties of ME NPs are explained by their composition, which consist of magnetostrictive and piezoelectric phases.

Despite the advantages of ME NPs, the attention should be addressed to several challenges, such as biocompatibility, determination of the bio-safety profile, and reproducibility. For instance, mainly ME NPs were fabricated using toxic Co [3, 4], Ni [2], etc. Furthermore, ME NPs are complex structures with many functions, thereby their synthesis often can include a combination of several methods, leading to reducing reproducibility. Thus, the development of technological approach for the fabrication of novel ME NPs based on biocompatible materials is challenging.

Materials and methods. ME core-shell NPs based on the biocompatible MnFe2O4 (MFO) and ferroelectric Ba(1-x)CaxZryTi(1-y)O3 (BCZT) were obtained by using two-steps microwave-assisted hydrothermal method. First, magnetic MFO cores were fabricated with in-situ surface functionalization using CA at 175°C for 30 min. Secondly, the BCZT shell on cores were formed at 225°C for 3 h. To exclude non-magnetic phases, all NPs after the formation was washed out using magnetic separation

The formed magnetic and ME core-shell NPs were extensively studied using atomic force microscopy (AFM), transmission electron microscopy (TEM), X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy, and magnetometer. The cytotoxicity study was performed using MTT-test with and without external AC magnetic field exposure with different parameters (frequency and strengths) to induce ME effect in NPs.

Results and Discussion. The analysis of the morphology revealed quasi-spherical MFO cores and ME core-shell NPs (Figure 1A-B). TEM analysis confirmed the formation of epitaxial BCZT shell for ME NPs. XRD patterns and Raman spectra demonstrated the presence of the typical spinel and perovskite structure for MFO and BCZT, respectively. The MFO/BCZT phase ratio in ME NPs was 39%/61%, respectively. At the same time, the BCZT shell resulted in the increased coercivity force and reduced saturation magnetization of ME core-shell NPs from 46±3 Oe to 69±5 Oe and from 41.4±1.2 emu/g to 6.1±0.2 emu/g as compared to MFO cores (Figure 1C), respectively. MTT-test demonstrated the absence of the toxicity of the developed ME NPs on the cells, such as fibroblasts and cancer cells.

Figure 1. (A, B) AFM images of (A) MFO cores and (B) ME core-shell NPs; (C) Hysteresis loops of MFO cores and ME core-shell NPs.

Conclusion. The developed novel biocompatible ME core-shell nanoheterostructures with a pronounced magnetic behavior can be considered as a promising noninvasive nanotool for the theranostics and regenerative medicine.

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Key Words magnetoelectric, nanoparticles, core-shell, heterostructure, biomedical applications

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最终交流类型: Invited

Mechanics of 2D Material Blisters

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A variety of out-of-plane deformation patterns have been observed for two-dimensional (2D) materials including ripples, wrinkles, buckles, scrolls, folds, tents, blisters, and so on due to their extra-low bending rigidity. Among them, the micro- and nanoscale blisters were frequently observed, which stemming from the deformation of atomically thin membrane by gases, liquids and solids trapped underneath 2D materials. Generally, the spontaneously formed blisters are viewed as inevitable defects of the transfer process. The presence of blisters may severely deteriorate the performance of 2D material devices because of the impeded charge/phonon transport across the interface. On the other hand, these blisters offer a novel avenue to explore the intrinsic mechanical parameters (e.g., Young's modulus, bending rigidity) of 2D materials as well as their interfacial properties (e.g., shear stress, adhesion energy). Furthermore, the stable and controllable blisters also act as effective knobs to tune the electronic and photonic performance of novel semiconductor devices formed by 2D materials. In the present talk, I will summarize the recent progress on the 2D material blisters in my group, especially focusing on the mechanics of anisotropic 2D materials and potential application in strain engineering field.

Keyword：2D material, blisters, mechanical properties, interface, strain engineering

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最终交流类型: Keynote

Electrospun Nanofibrous Aerogels: Controllable Structures and Multifunctionality

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Electrospun nanofibrous membranes, as the forefront of advanced fibrous materials, hold extraordinary potential applications ranging from environmental, energy to biology owing to their integrated advantages of fine diameter, extremely high aspect ratio, and high porosity. Despite their outstanding potential, the major problem associated with electrospun nanofibers is their anisotropic lamellar deposition character, which leads to the bottlenecks in further improving the thickness and porosity of current electrospun nanofibrous materials. Alternatively, three-dimensional nanofibrous aerogels (NFAs) with both high porosity and excellent compressive resilience might open up the possibility of solving the above problem and expand the applications of electrospun nanofibers; however, creating such NFAs has proven extremely difficult. Herein, we demonstrate a novel strategy to create fibrous, isotropically-bonded elastic reconstructed (FIBER) NFAs with a cellular network by three strategies, including fibrous freeze-shaping technique, direct electrospinning, and carding and lapping the fibers. The aerogels exhibited low densities of > 0.12 mg cm-3 and superelasticity. By further regulating the microscopic structures of the aerogels, they could be widely used in the field of sound absorption, warmth retention, and so on. In addition, the superelastic and bendable ceramic nanofibrous aerogels were prepared by using flexible ceramic nanofibers, breaking the mechanical boundaries between ceramics and polymeric materials. The successful synthesis of such fascinating ceramic NFAs will open broad technological implications in thermal insulation, catalyst supports, and flexible electrical devices.

Keyword： electrospinning; nanofibers; aerogels; superelasticity; multifunctionality;

最终交流类型: Keynote

Research on Quantitative Characterization of the Nano-interface and Three-dimensional Dispersion Structure of Elastomer Nanocomposites and Their Relationship with the Viscoelastic Properties

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Filler reinforced elastomer nanocomposites have significant applications in high-performance tires, aerospace, and other industries. The macroscopic performance of these nanocomposites is closely related to the interfacial interaction between filler and elastomer, as well as the dispersion structure of filler in the matrix. However, traditional characterization methods have limited resolution, making it challenging to elucidate the relationship between nanoscale microstructures (interfacial properties, dispersion structure) and the macroscopic performance of nanocomposites. Consequently, it is difficult to provide clear guidance for high-performance material design and preparation. In this study, by virtue of the high-resolution of Quantitative Nanomechanical Mapping Technique of Atomic Force Microscopy (AFM-QNM), a method for quantitatively characterizing the interfacial structure (interfacial thickness, nanomechanical properties) of elastomer nanocomposites is established. To ensure accurate measurements of nanomechanical properties by AFM-QNM, Johnson-Kendall-

Robert (JKR) contact mechanics model that is more suitable for soft materials like rubber have been applied to analyze Young's modulus. The double layer structure of interface was directly identified based on AFM-QNM images and was further directly evidenced by the morphology of bound rubber observed through high resolution transmission electron microscopy [1-4]. Simultaneously, a method for quantitatively characterizing the three-dimensional dispersion structure of fillers in matrix is developed by combining Three-Dimensional Scanning Transmission Electron Microscopy (3D-STEM) with nanoscale resolution and Synchrotron X-ray Computed Tomography (X-ray CT) with a micrometer-level field of view. Using this method, the dispersion structure of fillers that ranges from several nanometers to dozens of microns, including the homogeneity and size of fillers, the compactness of agglomerates, and the branching degree and connectivity of agglomerates and filler networks, were quantified. The reliability of this method is demonstrated through the observation of the Payne effect in elastomer nanocomposites [5-7]. Based on the above quantitative characterization methods, the influence of the properties of rubber and fillers on the multi-scale microstructure (interface properties, dispersion structure) of nanocomposites, as well as their relationship with macroscopic properties, especially their viscoelastic performance, has been further revealed. This study provides valuable guidance for the design and preparation of high-performance elastomer materials.

Keyword： interface; three-dimensional dispersion; quantitative characterization; elastomer nanocomposites; viscoelastic properties

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最终交流类型: Invited

Ionic energy conversion systems based on bioinspired micro-nanopore materials

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In nature, the delicate and intelligent transmission processes in ion channels and ion pumps on cell membranes are closely related to various life activities such as signal transmission, potential regulation, energy conversion and storage. The study of related bioinspired systems is of great significance not only for our understanding of the mass transfer process of living organisms, but also for solving key bottlenecks in related application fields such as salt difference energy conversion. Inspired by the structure and function of ion channels in living organisms, we constructed nanofluidic ion transporting membranes based on bioinspired micro-nanopore materials, and concluded a new strategy that uses the synergistic effect of structure, charge, and interfacial wettability to regulate ion transport and achieve function enhancement. We further introduce the protein-ion-channel based delicate mechanisms into the artificial micro-nano channel, and build a variety of high-performance energy conversion systems.

Keyword： Bioinspired; composite materials; ion transport; energy conversion

最终交流类型: Invited

Interface mechanics in 2D nanomaterials-based nanocomposites

汪国睿

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Two-dimensional (2D) nanomaterials (e.g., graphene, hexagonal boron nitride, Mxene) have been deemed as versatile building blocks to create a novel generation of nanocomposites desired for a variety of commercial applications. Different from that of the conventional fiber-based composites, the enormous interfacial areas, van der Waals forces dominated interface interactions as well as multiple scale load transfer mechanism would greatly impact the mechanical behaviors of 2D nanomaterials-based composites. Besides the widely concerned nanofiller-matrix interface, the filler-filler interface has to be considered in nanocomposites. The main challenge is how to monitor the load transfer process and evaluate load-bearing capability of fillers in composites. Here we present the recent progress in experimental characterization of atomic-scale interface mechanics, and clarify its importance on the reinforcement of nanocomposites. We also highlight the significance of competed mechanism between intrinsic mechanical strength of nanofillers and interfacial shear effect, allowing the delicate design of nanocomposites that deliver desired properties.

Keyword： Nanocomposite; 2D materials; Interfacial mechanics; Shear stress transfer; Raman spectroscopy

最终交流类型: Invited

Inorganic ionic polymerization: a tool for advanced hybrid materials preparation

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In biomineralization, organisms use ionic clusters as precursors for mineral deposition, which endows biomaterials with marvels properties. Inspired by this strategy, we developed inorganic ionic oligomers, which is a molecular scaled ionic precursor, for controllable polymerization for inorganic materials [1]. We named this system as “Inorganic ionic polymerization” for short. The inorganic ionic oligomer is a molecular-scale ionic compound with a size of approximately 1 nm and a composition of 3 to 4 repeated units of its molecular formula. We noted that the inorganic ionic oligomers could act as “inorganic ionic molecules” for the co-assembling of hybrid materials [2]. By using the lacking coordinated structure of cations and anions in inorganic ionic oligomers, we could build strong organic-inorganic interactions between inorganic ionic oligomers and organic molecules. This attributed to the construction of hybrid materials with ultra-high toughness and strength [3-5], which establishes a promising inorganic precursor for advanced mechanical materials synthesis. Moreover, the small molecular assisted inorganic ionic polymerization could regulate the ionic bonding of inorganic structures, which turns brittle inorganic materials to

flexible ones [6]. It enables us to manufacture minerals that behaviors like plastics [7]. In addition, we could functionalize inorganic ionic oligomers with organic molecules to produce organic-inorganic covalent-ionic hybrid molecules, which could assemble to a covalent-ionic bicontinuous network. This structure could combine paradoxical properties: the ceramic-liked hardness, rubber-liked resilience and plastic-liked reprocessibility, into one bulk material. This new matter does not belong to any current classification of materials (e.g. ceramic, rubber, plastic and metal) and we named it as “elastic ceramic plastic” [8]. We emphasize that inorganic ionic polymerization system could fuse the synthetic method of inorganic, organic and polymer chemistry, which could be a promising methodology for the manufacturing of more advanced hybrid materials (Figure 1).

Keyword： Crystal growth, organic-inorganic hybrid materials, inorganic ionic polymerization, inorganic ionic oligomers, elastic ceramic plastic

最终交流类型: Keynote

Interfacial manipulation and performance of rubber composites filled with carbon black

郭宝春

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This report presents some novel strategies to improve the dispersion of carbon black (CB) and enhance interface interaction via interfacial manipulation, aiming at breaking the bottleneck of the performance of CB-filled rubber composites. Low-hysteresis and high-performance CB-filled rubber composites can be manufactured using polyrhodamine-wrapped CB, polysulfide-grafted CB for reinforcement, or newly-developed coupling agents, including amino-functionalized polysulfide, adamantyl-based imine, and 3-hydroxy-N'-(4-methylpentane-2-methylene) naphthalen-2-acylhydrazone for in-situ modification.

Keyword： carbon black, rubber, interfacial manipulation, low-hysteresis, high-performance

最终交流类型: Keynote

Multi-lipid synergy in cartilage-mimicking nanometric lubricating layers: optimizing and predicting nature's solutions

Jacob Klein

Weizmann Institute

Uniquely efficient lubrication of cartilage in the major human joints is essential for its well being and its breakdown is associated with osteoarthritis, a debilitating disease affecting millions. it is believed to be mediated by lipid layers at the cartilage surface acting through the hydration lubrication mechanism. In natural joints however there are over a 100 different lipids and the question is: is this natural redundancy or natural evolution. Here we* present surface force balance studies showing a marked synergy when certain lipid mixtures are used. Moreover, using molecular dynamics simulations we are able to account for this synergy via consideration of the factors promoting hemifusion, the main cause of lubrication breakdown in our experiments.

*Yifeng Cao, Di Jin, Nir Kampf

Key Words biolubrication; hemifusion; lipid mixtures; lipid synergy; cartilage lubrication

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最终交流类型: Oral

Fabrication of dual responsive polymer microgel containing silver nanoparticles with catalytic and antibacterial activity

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Nanocomposites consisting of stimuli responsive microgels fabricated with metal nanoparticles have emerged as efficient, user friendly, recyclable and environment friendly catalysts and antibacterial agents. In this work, preparation of bare poly (N-isopropyl acrylamide-co-vinyl phosphonic acid) [p(NIPAM-co-VPA)] microgel by free radical polymerization and their fabrication with silver nanoparticles by in situ reduction is reported. The prepared bare and composite microgel was subjected to characterization with UV-Visible

spectroscopy, Fourier transformation infra-red spectroscopy, X-ray diffraction, and Laser light scattering. The hydrodynamic diameters of the swollen microgel particles were found in the range of 66-82 nm and a small decrease was noted after the integration of silver nanoparticles. The catalytic potential was demonstrated in the chemical reduction of 4-nitrophenol (4-NP) and 2-nitrophenol (2-NP), eosin Y (EY), and methyl orange (MO) which were chosen as representatives of nitro compounds and dyes. The catalytic activity of the prepared nanocomposite was examined in the chemical reduction of 4-NP, 2-NP, EY, and MO with sodium borohydride in the aqueous medium. The thermodynamics of the catalytic reaction was analyzed by conducting the experiments at different temperatures and corresponding parameters such as activation energy, activation entropy change, activation enthalpy change, and Gibb’s free energy were also calculated. The reduction rates of 4-NP, 2-NP, MO, and EY were calculated as 0.36, 0.24, 0.40, and 0.17 min−1, respectively. For evaluating the antibacterial potential, the prepared nanocomposite was tested against gram-positive bacteria [Staphylococcus epidermidis (ATCC: 14990)], and Gram-negative bacterial strains [Klebsiella pneumonia (ATCC: 4617), and Escherichia coli (ATCC-15224)]. The prepared nanocomposites showed activity against all the selected pathogenic strains with promising zones of inhibition of 17±0.82mm against Staphylococcus epidermidis and 15±0.91 against Escherichia coli and 15±1.52mm against Klebsiella pneumonia.

Key Words Nanocomposite, microgel, silver nanoparticles,catalysis, antibacterial activity.

最终交流类型: Keynote

Fast Large-Stroke Sheath-Run Artificial Muscles and Their Applications

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Electrothermal carbon nanotube (CNT) yarn muscles have demonstrated promising potential in achieving significant strokes during heating-cooling cycles. However, their limited application arises from the slow cooling rate of thermal muscles, particularly due to the inability of large diameter prior-art thermal muscles to undergo rapid cycling. We here describe our new sheath-run artificial muscles (SRAMs), which effectively address the significant challenges faced by CNT hybrid muscles. SRAMs provide solutions for two main issues: (a) the high cost of carbon nanotube yarns and (b) the inefficient actuation contribution from the yarn guest near yarn center. SRAMs employ an actuated guest sheath on a twisted or coiled polymer fiber or yarn, which drives actuation for our new sheath-run artificial muscles. This configuration not only significantly increases muscle power but also allows cost-effective commercialized yarns to replace the expensive carbon nanotube yarns, making the technology more accessible and practical. An electrothermally powered SRAM muscle integrates a CNT sheath with an inexpensive polymer core, delivering significant actuation strokes at different frequencies (14.3% at 1 Hz and 7.3% at 8 Hz in air). Notably, it exhibits rapid cooling compared to prior-art designs and achieves a remarkable average power density of 12 kW/kg, surpassing human skeletal muscle by a factor of 42. This exceptional performance is attributed to the concentrated heating within the muscle sheath, which drives fast actuation cycles. The sheath, being in direct contact with ambient, facilitates efficient cooling, allowing for rapid thermal dynamics. These versatile SRAM muscles can be seamlessly integrated into textiles, opening up a wide range of applications including adaptive clothing, smart structures, and robotics. Their integration provides opportunities for advanced functionalities and enhanced performance in various fields.

Key Words Electrothermal carbon nanotube, Sheath-Run Artificial Muscles

最终交流类型: Keynote

Artificial Muscle Actuation, Mechanical Energy Harvesting, and Refrigeration Using Twisted, Coiled, and Plied Polymer or Carbon Nanotube Yarns

Ray Baughman

University of Texas at Dallas

Similar mechanics involving twist transfer between yarn twist and coiling twist are here used to make powerful thermal and electrochemical artificial muscles, powerful energy-efficient twistron electrochemical mechanical energy harvesters, and compact energy-efficient refrigerators. Coiled artificial muscles can deliver 98 times the output mechanical power of the same weight human muscle, as well as giant tensile muscle strokes. For mechanical energy harvesting between 2 and 120 Hz, our most recent twistron carbon nanotube harvesters have higher gravimetric peak power and average power than previously reported for any prior-art, material-based mechanical energy harvester. We also show that high cooling results from twist changes for twisted, coiled, or supercoiled fibers, including those of natural rubber, NiTi, and polyethylene fishing line. By using opposite chiralities for twist and coiling, supercoiled natural rubber fibers and coiled fishing line fibers result that cool when stretched. The processes we used to make these exceptional yarns are described, as well as important applications, such as harvesting the energy of human motion by weaving coiled yarns into textiles and deploying them for comfort adjusting jackets that are environmentally powered. These discoveries resulted from a collaborative effort with many scientists around the world.

Key Words Artificial Muscle Actuation, Carbon Nanotube

最终交流类型: Invited

Lightweight, High-Performance Nanocomposite for Electromagnetic Interference Shielding

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Shandong University

Lightweight polymer nanocomposites embedded with various conductive nanomaterials such as carbon nanotube, graphene, metal nanowires, and transmission metal carbides/nitrides (MXenes) have attracted increasing attention for addressing emergency electromagnetic radiation or interference. Here, we employed efficient polymers for assisting in building lightweight, robust, and highly flexible EMI shielding composites. Typically, we employed low-dimension cellulose nanofibrils for assisting in building ultralow-density, robust, and highly flexible aerogels with orientated biomimetic hybrid cell walls. High conductivity and introduced interfaces lead to high intrinsic shielding ability of cell walls, which can be amplified by the cellular structures in the aerogels. Taking completely advantage of the biomimetic cell walls and cellular structure, the normalized surface specific shielding effectiveness is up to 189400 dB·cm2/g, significantly exceeds that of other EMI shielding materials reported so far. We have suggested some convenient, facile preparation approaches for constructing high-performance polymer nanocomposite-based EMI shields.

Keyword： lightweight, nanocomposites, porous architectures, polymer, EMI shielding

最终交流类型: Oral

Mossbauer study of the Impact of Process Control Agent on the Structural and Magnetic Properties of Ball-Milled FeCr Alloy: A Case Study Utilizing Ethanol

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Iron Chromium (FeCr) alloys have gained significant attention due to their remarkable resistance to high

temperatures and corrosion [1]. In this study, nanocrystalline Fe86Cr14 alloy was successfully synthesized

using a mechanical alloying technique, employing Ethanol as a process control agent (PCA) at a

concentration of 5 wt.% of the total sample mass. The objective was to investigate the impact of Ethanol on

the structural and magnetic properties of the FeCr alloy. Mössbauer spectroscopy was employed as a

characterization tool to analyze the samples. The results revealed that the addition of Ethanol induced

notable alterations in the ferromagnetic environment of the alloy, leading to the appearance of an additional

paramagnetic phase. This phenomenon can be attributed to the diffusion of chromium (Cr) atoms into the

iron (Fe) matrix. The findings shed light on the effects of process control agents on the structural and

magnetic properties of ball-milled FeCr alloys, contributing to the advancement and comprehension of

these materials

Key Words FeCr alloys; Mechanical alloying; Mossbauer spectroscopy: Magnetic properties; Process control agent; Ethanol.

最终交流类型: Keynote

Synchrotron radiation X-ray study on electrochemical energy storage materials

宋礼

中国科学技术大学

It is high desirable and critical to better understand the real process and mechanism in electrochemical energy storage materials and composites. However, for most of nanomaterials, drastic structural changes during electro-cycles can lead to the formation of new structures or different phases, implying complex and distinctive processes. Based on synchrotron radiation X-ray light source, many state-of-the-art X-ray methods can be developed to probe such dynamitic changes in electrochemical energy storage processes. Herein, I will present some of our recent studies on the development of multiple/operando X-ray techniques for probing typical energy storage materials that applied for electrochemical ion-batteries [1-5]. The outlook of advanced X-ray techniques will be also discussed with new generation light source.

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Keyword：X-ray Characterization, electrochemical energy storage material, mechanism

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最终交流类型: Keynote

Breaking the century-old Leidenfrost effect above 1000°C for efficient thermal cooling

王钻开

affliation

Since the old observation of the Leidenfrost effect, characterized by the levitation of water drops on hot solids upon an insulating vapor film, developing strategies to elevate the critical Leidenfrost point (LFP) for efficient heat transfer has remained a long-standing challenge. However, achieving high LFP and efficient thermal cooling across a wide range of temperatures seems mutually exclusive. Here, we design structured thermal armors (STAs) that block the onset of the Leidenfrost effect and meanwhile preserve efficient heat transfer up to 1150°C. Our design consists of thermally conductive, protruding pillars serving as thermal bridges, an imbedded insulating porous membrane for persistently wicking, and U-shaped channels for evacuating vapor. The key point lies in the coexistence of materials with thermally heterogeneous properties (conductive, insulating) and distinct topography (pillar, membrane), which cooperatively transforms normally uniform temperature and vapor profiles into non-uniform ones and counterintuitively reinforces thermal cooling. The broad range of substrate temperatures for sustained and efficient thermal spray cooling without Leidenfrost effect is only limited by the melting of materials, rather than by the architecture and physical principle of our design. We also fabricate flexible STA that can be closely attached to substrates otherwise challenging to be structured. Our design strategy holds potentials to implement liquid thermal cooling at extremely high temperatures, a property uncharted to date.

Keyword： The Leidenfrost effect, heat and mass transfer, extremely high temperatures, thermally heterogeneous properties, superwettability.

最终交流类型: Invited

Study on the Construction of Functional Coatings on the Surface of Medical Pipelines and the Reduction of Tubing Complications

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四川大学

Tracheal catheter is one of the most commonly used Catheter in clinic, which can deliver oxygen to patients who cannot breathe autonomously and maintain the most basic life activities. However, the process of catheter insertion, retention, and extraction can lead to various complications, including difficulty in pronunciation, sore throat, and swallowing, which can lead to serious life-threatening complications such as tracheoesophageal fistula. To

address the issue of complications caused by mismatch between the surface characteristics of the catheter and human mucosal tissue, we simulated the hydration lubrication coating of the mucosa through intermolecular association of HA based micelles, prepared a highly lubricated coating, reduced friction coefficient and improved anti protein adhesion performance, and lowered the damage of the catheter to the glottis and trachea. In order to enhance the interaction between the coating and the catheter interface, inspired by the mucosal structure and function in nature, a chemically grafted mucosal conformal modification coating was constructed on the surface of the tracheal catheter to reduce catheter damage and pain, and achieve opioid removal. In order to solve the intubation related complications caused by the inner surface of Tracheal intubation, inspired by the epithelial layer, we build a protective barrier coating on the surface of the trachea, which not only has good hydrophilic lubrication performance, but also has excellent anti fouling and bactericidal properties. The corresponding trachea also reduces the risk of air passage blockage while maintaining the lubrication of the outer surface[1-3]. The above research can significantly reduce intubation related complications and provide broad prospects for clinical conversion.

Keyword： Tracheal intubation, Surface modification, Hydration lubrication, Conformal modification, Gas phase fluorination technology

最终交流类型: Invited

Lightweight and ultrastrong pyrolytic carbon nanolattices

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A long-standing challenge in modern materials design is to create low-density materials that are robust against defects and can withstand extreme thermomechanical environments because these properties typically are mutually exclusive: the lower the density, the weaker and more fragile the material. Here we fabricated pyrolytic carbon nanolattices with truss- and shell-based topologies through two-photon lithography and subsequent pyrolysis. For the truss-based nanolattices, the smallest strut size is up to 260 nm. These nanolattices exhibited a compressive strength of ~1.90 GPa at a density of ~1.0 g/cm3. As a result, the nanolattices achieved an exceptional specific strength of 1.90 GPa g-1 cm3, which is 1-3 orders of magnitude higher than those of nearly all micro/nanolattices reported so far. For the shell-

based nanolattices with IWP minimal surface topology, the smallest shell thickness is up to 177 nm. When the density is larger than 0.53 g/cm3, the strength of pyrolytic carbon IWP nanolattices achieved the theoretical limit of porous materials. In addition, these shell-based carbon nanolattices exhibited an ultrahigh strength of 3.52 GPa, an ultralarge fracture strain of 23%, and an ultrahigh specific strength of 4.42 GPa g-1 cm3, surpassing all previous micro-/nanolattices at comparable densities. The high strength and specific strength of pyrolytic carbon nanolattices are attributed to miniaturization of overall structure and optimization of lattice topology. Our study demonstrates a mechanomaterial route to design and synthesize micro/nanoarchitected materials.

Keyword：3D nanolattices, truss-based topology, minimal surface topology, 3D fabrication, mechanical properties

最终交流类型: Invited

Polymer nanocomposites for oil-water separation

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Water pollution arising from the discharge of various oil-water mixtures lead to severe environmental and ecological problems. Therefore, materials that can effectively separate such mixtures are in urgently needed. This paper will present our recent progress on developing polymer-based nanocomposites for efficient recovery of oil and organic liquids in/on water. Nanocomposites derived from the synthetic and natural polymers were prepared, and their morphologies were optimized to endow the materials with controlled dimension, surface property as well as excellent recyclability and stability. Additionally, the unique structure and property of polymer nanocomposites led to the increase on the oil concentration in the liquid, which in turn enhanced the collision of emulsified oil droplets to aggregate into large ones in the emulsion and resulted separation from the water. An aggregation-induced separation (AIS) process was proposed to explain the above phenomenon, and the mechanism was confirmed by studying the distribution of oil droplets in emulsion. The advantages of polymer nanocomposites for oil-water separation are manifested by comparing their cost and applicability with those of commercial products. Based on the verification on the technical

principle of AIS, an industrial-scale setup was performed, targeting on removing highly emulsified oil in wastewater.

Keyword： Polymer nanocomposites, oil-water separation, aggregation-induced separation

最终交流类型: Invited

Defect engineering and anionic conduction in melilites

匡小军

桂林理工大学

Recently the tetrahedral-containing structural types have received growing interest on developing new oxide ion conductors for low temperature solid oxide fuel cells. The tetrahedral units with non-bridging terminal oxygens have been shown to be a key factor for accommodating and transporting oxygen defects via the cooperative mechanisms involving the framework tetrahedral rotation and deformation. We have been working on anionic conduction in two-dimensional tetrahedral layered melilite structures for more than a decade. This talk will present the recent research progress on defect engineering and anionic conduction in melilite-type structures, which includes the localization of oxygen interstitials, chemical bonding and size effect on the interstitial oxide ion conductivity, new metastable interstitial oxide ion conducting melilites from glass-ceramic route using the aerodynamic levitator and laser heating system as well as the mixed anion chemistry.

Keyword： anionic conduction, defect engineering

最终交流类型: Keynote

Multifunctional composite mechanical metamaterials

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The Univeristy of Hong Kong

Composite mechanical metamaterials mainly rely on their microstructure to realize the performance regulation of macroscopic mechanics, which provides infinite possibilities for the realization of high-performance structural design and novel functional design. Here, we demonstrate a thick-panel origami structure prepared by a multimaterial 3D printing method with a wrap-based fabrication strategy, which can effectively improve its support capacity and impact energy absorption capacity. Then, it was proved that by partially pyrolytic carbonizing the 3D printed polymer micro-lattice, a high-strength and high-toughness carbon lattice mechanical metamaterial can be obtained; this kind of rigid and flexible carbon lattice material has a good biological compatibility. Further, by coating its surface with a metal film, it is assembled into a thermoelectric device with excellent mechanical/thermal properties and reliability, demonstrating the ability of mechanical metamaterials to achieve overall mechanical performance regulation by artificially constructing its geometry and material properties. In addition, we took advantage of the microlattice with excellent strength and ductility produced by partial carbonization, combined with the improved thermal impedance effect, to fabricate a thermoelectric generator with a three-dimensional structure, which can exhibit a specific energy absorption of about 30 J/g and a power conversion efficiency of about 10%. In conclusion, composite mechanical metamaterials will lead to new paradigm shifts in high-performance structural design and advanced manufacturing, as well as provide new inspiration for multifunctional applications.

Key Words microstructure; mechanics; mechanical metamaterials

最终交流类型: Oral

Graphene-based Nanocomposites for Safe Out-of-Oven Manufacturing CFRPs

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西北工业大学

Owing to their high specific strength and stiffness, as well as chemical resistance, carbon fibre reinforced polymer (CFRP) composites have been widely used in diverse fields, such as aerospace, automotive, civil, energy, sports, etc. On the other hand, with the increasing consideration on environmental impact, low-/zero-carbon technologies are increasingly demanded. For CFRP composites manufacturing, traditional methods including autoclave and oven-based curing procedures lead to high energy consumption as well as size restrictions. In order to overcome these limitations, our group has performed diverse study in pyroresistive performance of conductive polymer composite and achieved reliable self-regulating heating devices, which can be used for sustainable out-of-oven (OoO) curing [1-5].

The positive temperature coefficient (PTC) effect was used, in which the electrical resistance of the CPC increased with increasing temperature, thus could be used to control the heating procedure and protect the system from over-heating.

Considering the cure cycle of high performance CFRP composites, which commonly consists of the cure and post-cure stages, double or two-step PTC effect is considered in this work. Here, graphene nanoplatelets (GNPs) filled HDPE, PVDF and HDPE/PVDF binary-polymer were fabricated through melt pressing. For GNP/HDPE and GNP/PVDF nanocomposites, single PTC and self-regulating heating behaviour, were achieved owing to the thermal expansion of HDPE and PVDF. For the GNP/HDPE/PVDF ternary system, a double PTC behaviour accompanied with two self-regulating heating stages were achieved at around 120 °C and 150 °C respectively. Afterwards, the graphene-based nanocomposites with a double PTC effect were used for safe and sustainable out-of-oven manufacturing CFRPs, and compared with the composites cured by traditional oven methods. As a result, OoO cured composites show comparable mechanical properties with only 3% energy consumed. Moreover, the integrated CPC layer could also be used for structural health monitoring, anti-/de-icing, etc., to achieve advanced multifunctional lightweight composite structures.

Keyword：graphene nanoplatelet, conductive polymer composite, positive temperature coefficient effect, sustainable manufacturing, out-of-oven curing

最终交流类型:

Shape Memory Polymer Composites: Programmability, 4D Printing and Applications

冷劲松

哈尔滨工业大学

Shape memory polymers and their composites are smart materials with excitation response. They have the ability to maintain temporary shape and return to their original shape under specific external environment excitation. At present, shape memory polymers such as epoxy, cyanate ester, styrene, polyimide, polylactic acid, and polyurethane with adjustable glass transition temperatures have been developed. Smart structures prepared based on shape memory materials have unique shape memory properties and characteristics of lightweight and high strength and have the functions of active deformation, self-sensing and self-repairing. We have developed a variety of shape memory smart structures, which have been initially applied in aerospace, biomedical, 4D printing, and other fields. These materials offer significant promise for future smart products in many areas of science and technology.

Keyword： Shape memory, Nanocomposites, Smart materials

最终交流类型: Invited

Single-Atom Electrocatalysts for Energy Process

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In recent decades, as a new type of clean and sustainable energy system, polymer electrolyte membrane fuel cells (PEMFCs) have been studied extensively due to the limited resources of fossil fuels on earth.[1] One of the major challenges for the large-scale application of PEMFCs, however, is developing highly cost-effective electrocatalysts for cathodic oxygen reduction reaction (ORR).[2] By now, the most efficient ORR catalysts for PEMFCs are still Pt-based ones. However, the increasing price and scarcity of Pt on earth make it one of the main obstacles hindering the large-scale application of fuel cells. Therefore, maximizing the Pt utilization in fuel cells has become urgent.

In the present work, we report a carbon-supported defect-anchored Pt single-atom catalyst (SAC) which presents high ORR performance and a superhigh Pt utilization of 0.09 gPt kW-1 in fuel cells. Further results indicate that single Pt atoms anchored by four carbon atoms in carbon divacancies (Pt-C4 sites) are the main active sites for the observed highly efficient ORR process.[3] We also report some single-atom catalysts for CO2RR and HER. The results show that the modification of the microenvironment also can effectively tune the activity of the nanocatalysts and the synergistic effect between different oxygen-containing groups can lead to much high enhancement of the activity of pure carbon materials for CO2RR process.[4]

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Keyword:single atom catalyst; electrocatalysis; energy; fuel cells
最终交流类型: Invited

Photoelectrocatalysis

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The development of photoelectrocatalytic systems capable of converting the abundant green energy into storable and transportable chemical fuels is one of the promising approach to address energy crisis and global warming. Among various photoelectrocatalytic systems, as-assembled heterostructure electrodes have opened up new realms in electronic and optoelectronic devices. With regards to the efficient utilization of solar energy, direct photoelectrochemical (PEC) water splitting is a promising solution to alleviate the energy and environmental issues. However, the PEC performance is generally limited by poor light harvesting, low charge separation and transfer, and sluggish water oxidation kinetics. To address these bottlenecks, various materials as favorable photoanode, such as TiO2, BiVO4, WO3, Fe2O3, TaON, Ta3N5, GaP, etc, have attracted more attentions for PEC water splitting. Direct photoelectrochemical (PEC) water splitting is a promising solution for solar energy conversion; however, there is a pressing bottleneck to address the intrinsic charge transport for the enhancement of PEC performance. Herein, we report on the synthesis of novel heterostructure electrodes, exhibiting extraordinarily high catalytic performance toward green energy conversion. For instance, a versatile coupling strategy was developed to engineer atomically dispersed Ni-N4 sites coordinated with an axial direction oxygen atom (Ni-N4-O) incorporated between oxygen evolution cocatalyst (OEC) and semiconductor photoanode, boosting the photogenerated electron−hole separation and thus improving PEC activity. This state-of-the-art OEC/Ni-N4-O/BiVO4 photoanode exhibits a record high photocurrent density of 6.0 mA cm-2 at 1.23 V versus reversible hydrogen electrode (vs. RHE), over approximately 3.97 times larger than that of BiVO4 photoanode, achieving outstanding long-term photostability. From X-ray absorption fine structure analysis and density functional theory calculations, the enhanced PEC performance is attributed to the construction of single-atomic Ni-N4-O moiety in OEC/BiVO4, facilitating the holes transfer, decreasing the free energy barriers, and accelerating the reaction kinetics. This work will pave new avenues to the exploration and design of heterostructure photoelectrocatalytic systems towards robust green energy utilization.

Keyword: Photoelectrocatalysis, Solar water splitting

最终交流类型: Invited

Organic semiconductors (OSs) for efficient photoelectrochemical water splitting

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π-conjugated organic semiconductors (OSs) are known to be promising materials for solar cells, field effect transistors, and even photoelectrochemical cells because they are cheap and can be easily tuned at the molecular level to create optical and electrical properties with high carrier mobility. However, their poor stability in an aqueous environment and low solar-to-hydrogen conversion efficiency as photoanodes is a fatal drawback for wide application in water splitting. Here, we explore the suitability of applying a diketopyrrolopyrrole (DPP)-based π-conjugated OS to a Ti doped hematite (Ti-Fe2O3) photoanode for efficient photoelectrochemical water splitting. We employ a PSi as a hole extracting and hole transporting medium between the Ti-Fe2O3 anode and the oxygen evolution catalyst (OEC, NiFe(OH)x). The conformally coated OS, PSi layer on hematite (Psi/Ti-Fe2O3) generates a type-II heterojunction, which induces stiff band bending, resulting in fast hole extraction. We confirmed enhanced electrochemical performances of Psi/Ti-Fe2O3 in the PEC water splitting system due to the efficient hole transport behavior of PSi proved by higher charge carrier mobility than the representative HTL OS (Pod) in FET configuration. After verifying the basic mechanism of PSi-related electrochemical performances with Ti-Fe2O3, we further applied Psi to a highly efficient photoanode, Ge doped porous hematite (Ge-PH). Thanks to the excellent hole extraction and subsequent fast hole transport property of the PSi interlayer, with conformal contact between the Ge-PH and NiFe(OH)x,NiFe(OH)x/PSi/Ge-PH showed a high photocurrent density of 4.57 mA cm-2 at 1.23 VRHE with a cathodic shift of the onset potential (0.735 VRHE) and outstanding stability for 65 hours. Our study demonstrates the successful use of soft but inherently unstable π-conjugated OSs as a hole transport material for photoanodes to effectively resolve the interfacial resistance between two hard materials (Ti-Fe2O3 and the OEC) and the intrinsically low hole transport rate of a hematite photocatalyst, which are the major causes of the limited efficiency of hematite in water splitting.

Keyword: water splitting; photocatalyst; organic semiconductor
最终交流类型: Invited

Mechanistic Analysis of Cu-Catalyzed Electrochemical CO2 Reduction Reaction

徐冰君
北京大学

Electrochemical CO2 reduction reaction (CO2RR) has been widely acknowledged as a key component in the global transition from fossil energy to renewable energy powered society to combat climate change. A prerequisite for wide deployment of CO2RR processes is its economic viability, and thus the development of electrocatalysts capable of producing high value products is a focus of recent research. So far, Cu-based materials have shown unique ability in facilitating selective formation of valuable multicarbon products, however, the mechanistic pathways through which electrochemical transformations occur remain unclear. In this seminar, we will discuss the identification of the rate-determining step, determination of CO adsorption enthalpies at electrochemical conditions, and interception of elusive reaction intermediates in Cu-catalyzed CO2RR via a combination of electrokinetic, in-situ spectroscopic and isotopic labeling investigations in our recent works. A mechanistic framework capable of rationalizing a significant fraction of literature results will be presented, and its implications on the selectivity control will be discussed.

Electrochemical CO2 reduction reaction (CO2RR) has been widely acknowledged as a key component in the global transition from fossil energy to renewable energy powered society to combat climate change. A prerequisite for wide deployment of CO2RR processes is its economic viability, and thus the development of electrocatalysts capable of producing high value products is a focus of recent research. So far, Cu-based materials have shown unique ability in facilitating selective formation of valuable multicarbon products, however, the mechanistic pathways through which electrochemical transformations occur remain unclear. In this seminar, we will discuss the identification of the rate-determining step, determination of CO adsorption enthalpies at electrochemical conditions, and interception of elusive reaction intermediates in Cu-catalyzed CO2RR via a combination of electrokinetic, in-situ spectroscopic and isotopic labeling investigations in our recent works. A mechanistic framework capable of rationalizing a significant fraction of literature results will be presented, and its implications on the selectivity control will be discussed.

Keyword: Electrochemical CO2 reduction, in-situ spectroscopy, kinetic analysis

最终交流类型: Invited

Heterojunction Nanostructured Materials for Photothermal-assisted Photocatalysis

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Abstract: Interest in hydrogen as a zero-carbon energy carrier has increased significantly in recent years, given that hydrogen-based economy is the best energy alternative to the increasing concerns over carbon emissions, energy security, and climate change. At present, green hydrogen is gaining unprecedented business momentum as it drives the next wave of renewable energy investment. Using readily available renewable resources i.e. solar energy and seawater to secure sustainable fuel and freshwater for humanity is an impactful quest. The utilization of photothermal materials with broad solar absorption, in parallel to engineered nanocatalyst, offers new approach to achieve efficient solar light conversion. Hoewever, the incorporation of multimaterials into a unitary photocatalyst configuration for efficient full solar spectrum catalysis with maximized photochemical and photothermal effects is particularly challenging. Here, we have designed solar thermal collector nanocomposites that possess efficient photothermal properties for highly targeted interfacial phase transition reactions that are synergistically favorable for catalytic hydrogen production. The photothermal effect arises from plasmonic metal, semiconductor and carbon nanomaterials exhibit localized interfacial heating which directly triggers surface-dominated catalysis processes, with minimal heat losses, thermal masses and optics implementation. We propose a spectrum-designated solar harnessing photocatalyst that has uncompromised bilateral photothermal and photocatalytic functions. Tailored spectrum photocatalysts whereby high-frequency solar photon is exclusively captured for photochemical, while low-frequency photon is assigned to photothermal effect. The solar thermal collector nanocomposites are photo stable for practical solar conversion to simultaneously produce clean energy and water. Finally, proof-of-concept prototypes demonstrate the viability of sustainable photothermic driven catalysis and desalination under natural sunlight.

Keyword: Photothermal, photocatalysis, membrane distillation, plasmonic

最终交流类型: Oral

Function-coordinated Nanocatalysts for Carbon Dioxide Electroreduction

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华东理工大学

The electrochemical reduction of carbon dioxide enables the storage of intermittent renewable energy in the form of chemical bonds. Further progress is required in the electrocatalysts which facilitate the conversion chemistry. The functional coordination structures of the electrocatalysts have been regarded as important factors for the catalytic performance of carbon dioixde reduction. By using the oxygen-containing functional groups of water-soluble polymers, we have regulated the reaction microenvironment for catalyst synthesis, and created the cluster-sized catalysts with rich oxygen donors [1-3]. We found out that this kind of metal oxide catalysts exhibited excellent activity and selectivity for carbon dioxide reduction. Further, we have proposed a strategy to improve catalyst stability for carbon dioxide reduction, that is, by enhancing the oxygen transfer processes in the micro-region of electrode/electrolyte interface. By optimizing the electrolyte formula to match the catalytic materials, the applicant promoted the stability of the oxygen-containing active sites in metal oxide catalysts, thus achieving a cathode energy efficiency of more than 75% at high current density for carbon dioxide reduction [4-6]. Recently, we have proposed to couple the processes of cathode and anode reactions, and devised a redox-mediated electrocatalytic reactor. This reactor realized the efficient production of ethylene oxide from carbon dioxide with low energy input and high conversion rate [7].

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Keyword: Nanocatalyst, Function coordination structure, Carbon dioxide electroreduction, Value-added chemicals

最终交流类型: Oral

Holey Ruthenium Phosphide Nanosheets as Highly Efficient Electrocatalyst for Hydrogen Evolution

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Yonsei University

The exploration of efficient electrocatalysts has evoked intense scientific efforts because of important role of electrocatalytic reactions in renewable energy technologies. Here we report the synthesis of high-performance 2D nanostructured electrocatalysts of subnanometer-thick holey Ru_2P nanosheets with plenty of crystal defects. The atomically-thin holey Ru_2P nanosheets could be synthesized by phosphidation of monolayered RuO_2 nanosheets. In comparison with non-holey Ru_2P nanoparticles, holey Ru_2P nanosheets delivered much better hydrogen evolution reaction (HER) activity with very small overpotentials of 17 and 26 mV for acidic and alkaline electrolytes, respectively. Thus, they are among the best-performing Ru-P-based HER catalysts reported thus far. Systematic in situ Raman and X-ray absorption near edge structure (XANES) spectroscopic investigations underscored that holey nanosheet morphology enhanced the adsorption of proton/water and the accumulation of adsorbed hydrogen, leading to the increased contribution of Volmer-Tafel mechanism to the HER activity of ultrathin holey Ru_2P nanosheets. The controlled phosphidation for exfoliated metal oxide nanosheets provides an effective means to explore high-performance 2D nanostructured electrocatalysts.

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Keyword: 2D nanosheet, electrocatalyst, in situ analysis, metal phosphide, hydrogen evolution reaction

最终交流类型: Invited

Interface and Defect Engineering of Two-Dimensional Nanosheet-based Catalyst Materials

Seong-Ju Hwang
Yonsei University

Two-dimensional (2D) monolayer nanosheets of layered inorganic solids (metal oxides, layered double hydroxides, metal chalcogenides, metal carbides, metal nitrides, and carbon nitrides) have evoked great deal of research activity because of their unique physicochemical properties and outstanding performances as functional materials. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties and functionalities. The inorganic nanosheets can be used as powerful building blocks for exploring high performance hybrid catalysts. Since the crystal defect and interfacial interaction have profound influence on the catalytic activity of hybrid materials, the energy functionalities of 2D inorganic nanosheet-based hybrid materials can be greatly enhanced by defect- and interface-engineering. In this talk, several classes of 2D nanostructured hybrid materials applicable for renewable energy technology will be presented together with the discussion about the relationship between chemical bonding nature and functionalities. The crucial role of interface/defect engineering in optimizing the catalyst performances of 2D nanosheet-based hybrids will be highlighted.

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Keyword: 2D nanosheet, Electrocatalyst, Defect, Photocatalyst, Exfoliation

最终交流类型: Keynote

Artificial Photosynthesis for Chemical Transformation

吴骊珠
中国科学院理化技术研究所

With the increasing concern over the global energy crisis and the greenhouse effect caused by carbon dioxide emission, the development of carbon-neutral and renewable-energy solutions has attracted considerable interest in both the scientific and industrial communities. Nature long ago figured out how to use photosynthetic complex to capture sunlight and then to store its energy in a chemical form. Artificial photosynthesis is the idea that one might be able to create energy and other useful thing from sunlight, water and carbon dioxide, as plants do. Inspired by the ability of natural photosynthesis to convert solar energy into chemical energy, the scientific community recognized the potential of light-driven reactions (photochemistry) as a powerful approach to chemical synthesis. From the high energy intermediate generated by photoinduced excitation of organic molecules, unique reaction manifolds can be accesses that are generally unavailable to conventional thermal pathways.

Thus photochemical reactions considerably enrich the synthetic repertoire of modern organic chemists. Our group has long engaged in the photochemistry research related to the photoinduced energy transfer, electron transfer and chemical transformation, including artificial photosynthesis, visible light catalysis for organic transformation, and photoinduced electron transfer, energy transfer and chemical reactions in supramolecular systems. In this presentation, we will compile several stories to illustrate photochemical approaches that may be useful in the design of artificial photosynthetic systems for effective chemical transformation. With these joint efforts, artificial photosynthesis will enable versatile and promising opportunities to recycle "wasted" substances such as CO2 into value-added compounds such as C1 fuels, carboxylic compounds, and multicarbon feedstocks, maintaining carbon neutrality for chemical manufacturing. Along this line, artificial photosynthesis will not only match and even outcompete the quantum efficiency, chemo-selectivity, regio-selectivity, stereo-selectivity, and scalability of natural photosynthesis, but also offer energy-economic, step-economic, carbon-neutral, and value-added solutions for sustainable chemical manufacturing in the next few decades.

Keyword: Artificial Photosynthesis; photochemistry; visible light catalysis; election transfer; energy transfer;

最终交流类型: Invited

Novel Materials Chemistry for Applications in Catalysis

Nicola Pinna
Humboldt-Universität zu Berlin, Germany

The current trend in various energy applications, ranging from batteries to electrolizers, lays in the control of structural, physicochemical and morphological properties of materials and their interfaces. During this presentation, recent scalable strategies for nanostructured materials synthesis, targeting energy and environmental applications will be discussed. Especially, we will focus on one-pot strategies for the fabrication of hybrid and complex nanomaterials focusing on the importance of the organic-inorganic and inorganic-inorganic interfaces. Among the examples presented, we will discuss the synthesis of complex nanostructures and the stabilization of metastable phases for applications in catalysis. We will see that nowadays the available strategies allow a control in terms of composition, crystalline structure, morphology and nanostructuration that would have been unimaginable just few years ago. Finally, the open challenges the field is currently facing and possible further developments which are needed to meet the always growing demand for high performing materials will be also discussed.

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Keyword: Catalysis, Sol-Gel Chemistry, Hybrid Materials

最终交流类型: Oral

Atomically controlled catalysts for modular electrosynthesis and beyond

王枫梅
北京化工大学

The huge environmental and energy concerns on the conventional thermochemical routes of manufacturing valuable chemicals derive the quest for an alternative strategy. Electrochemical synthesis driven by the intermittent clean energy electricity from earth-abundant feedstocks (such as biomass, inorganic ions, H2O, and CO2) to valuable chemicals has become one of the most promising alternatives to this process. Until now, several strategies, ranging from developing atomically controlled catalysts to establishing an innovative electrochemical system, have been widely adopted to efficiently synthesize high valued chemicals. In this talk, I will first focus on our recent work on atomically controlled electrocatalysts for high-valued chemical synthesis，including H2O2 from water and O2, 2,5-Furandimethanol (BHMF) from hydroxymethylfurfural (HMF), formic acid from glycerol etc.. Specifically, we designed a single metal atom-doped titanium dioxide (TiO2) electrocatalyst for producing H2O2 via two-electrons water oxidation process. The isolated metal atoms (such as ruthenium and nickel atoms) in the TiO2 matrix could tune the adsorption energetics of OH intermediate to the thermodynamic value of 1.76 eV, providing a high selectivity for hydrogen peroxide synthesis through two electron water oxidation and achieving a superior H2O2 yield at high current densities. We note that this kind of as-synthesized metal-doped TiO2 anode can be paired with the oxidized carbon nanotube cathode to produce H2O2 in the full cell device. Then, I will briefly highlight our recent work on the electrochemical synthesis of high-value chemicals from biomass-based substrates over novel layered naomaterial electrocatalyst. The concurrent production of valuable chemicals is realized by utilizing layered metal phosphorus trisulphide(CdPS3) and MnCo2O4.5 as cathode and anode in one cell device, respectively. Moving beyond this, considering the strong coupling feature between anodic and cathodic reactions, we parallelly design and bulid a novel modular electrochemical synthesis (ModES) system, which utilizes solid-state redox reservoirs and integrate two redox reactions for efficient synthesis of different high-valued chemicals, including hydrogen peroxide (H2O2), sodium hypochlorite (NaClO), sodium persulfate (Na2S2O8) or active chlorine. The designed system can be continuously operated via using electrochemically reversible heterogeneous redox reservoir (RR), which reversibly store and release electrons and ions (e.g., Na+, H+, and OH-), and achieve a complete electrochemical reaction. The ModES concept presented in our works highlights the prospects for using redox reservoirs to enable efficient, modular, and on-demand electrochemical synthesis of valuable chemicals.

Keyword: Modular electrochemical synthesis, atomically controlled catalysts, redox reservoirs, electrochemical synthesis

最终交流类型: Invited

Developing Nanostructured Materials for Hydrogen Oxidation/Evolution Reaction in Alkaline Solution

李彦光
Soochow University, China

There is rapidly growing interest in alkaline membrane fuel cells and alkaline membrane electrolyzers due to their higher energy efficiency and lower manufacturing cost. However, their commercial success hinges on the development of efficient electrocatalysts for hydrogen oxidation reaction (HOR) and hydrogen evolution reaction (HER) in alkaline solution. In alkaline solution the activities of noble metal-based catalysts (such as Pt and Pd) are about three orders of magnitude lower than their activities in acidic solution. Some of them suffer from limited working potential windows. On the other hand, Ni-based materials are also promising candidates and in fact the only non-precious-metal-based candidates for HOR. However, pure Ni metal has relatively strong hydrogen adsorption that essentially limits its electrocatalytic performance. In this talk, we will briefly introduce our recent efforts on developing Ir-skinned Ni nanoparticles and Ni nanoparticles with N doping or Mo alloying. For the former, we find the introduction of atomic layered NiIr alloyed skins on Ni nanoparticles could lower the usage of precious metals, while the electronic effect upon alloying affords the catalyst with high mass activities per noble metal and broad working potential of > 1 V in alkaline solution. The catalyst also demonstrates excellent stability for tens of hours. For the latter, we find that N doping or Mo alloying could alleviate the H adsorption of Ni and lowers the activation barrier for water formation and dissociation. Consequently, the resultant products exhibit excellent mass activities superior to all existing non-precious-metal-based materials and great CO-tolerance for hydrogen oxidation reaction, as well as remarkable activity and stability for hydrogen evolution reaction. Our experimental results are further understood and supported by theoretical simulations. At the end, we would highlight possible efforts in order to further enhance the electrocatalytic performances and to make this technology a reality in the near future.

Keyword: electrocatalysis, hydrogen oxidation, nanostructures

最终交流类型: Oral

Rapid Self-reconstruction of Fe-modified Ni Hydroxysulfide for Efficient and Stable Large-current-density Water/Seawater Oxidation

余颖
华中师范大学

Reasonable design of electrocatalysts with rapid self-reconstruction for efficient oxygen evolution reaction (OER) under commercially demanded current density is highly desired, but really challenging. Herein, ultrathin Fe-modified Ni hydroxysulfide (Fe-NiSOH) nanosheet arrays were grown in situ on Ni foam via a simple two-step oxidation strategy for efficient and stable large-current-density water/seawater oxidation. Systematical insights including experimental and theoretical analysis reveal that in-situ S leaching from the electrode boosts its self-reconstruction, and results in more ready generation of highly active Ni4+ species, which is benefited from their reduced formation energy. Owing to its excellent physical and chemical properties, the Fe-NiSOH catalyst only requires low overpotentials of 207, 240, and 268 mV in alkaline water to deliver current densities of 10, 100, and 500 mA cm-2, respectively, and can work stably for 1100 hours under commercially demanded current density of 500 mA cm-2. Furthermore, it also exhibits excellent seawater oxidation activity and superior resistance to Cl- corrosion since it can run stably at 500 mA cm-2 for over 900 hours. [1] In addition, functional bimetal (Co and Fe) has been designed specifically to modify nickel phosphide (denoted as CoFe-Ni2P) for boosting seawater splitting. These in situ generated CoFe-NiOOH species remarkablely inhibit the adsorption of Cl- ions but selectively adsorb OH- ions, which contributes to excellent performance of the CoFe-Ni2P electrode for large-current-density seawater splitting. Impressively, a flow-type anion exchange membrane electrolyzer assembled by the CoFe-Ni2P/Ni-felt bifunctional electrode is demonstrated to be operated stably at an industrially large current density of 1.0 A cm-2 in 6 M KOH + seawater electrolyte for 300 hours. [2]

Keyword: Water/seawater splitting • Self-reconstruction • Fe-modified Ni Hydroxysulfide • Co and Fe modified Ni2P

最终交流类型: Invited

Solar Hydrogen Production via Overall Water Splitting of Powder Photocatalysts

章福祥
Dalian Institute of Chemical Physics

Solar energy supply is inexhaustible in human terms, and its use is harmless to our environment and climate. Scientists around the world are working towards the goal of developing technologies to harness energy from the sun to produce fuels. Solar hydrogen production using a powder photocatalyst is a potentially clean and renewable artificial photosynthesis solution to convert solar energy into hydrogen fuel. In the past decades, increasing interests in this field have been paid to developing materials to capture and channel sunlight; deepening understanding of photosynthesis; and discovering new catalysts to make the chemistry possible. In this talk, I will present the recent research progress about the solar hydrogen production via overall water splitting of powder photocatalysts in my group. It involves development of photocatalyst/cocatalyst materials, fabrication of overall water splitting under visible light as well as understanding of underlying mechanism. Meanwhile, the strategies of promoting photogenerated charge separation and assembly of efficient solar-chemical conversion systems by crystal engineering, hetero-phase junction or dual cocatalysts etc. will be discussed in details.

Solar energy supply is inexhaustible in human terms, and its use is harmless to our environment and climate. Scientists around the world are working towards the goal of developing technologies to harness energy from the sun to produce fuels. Solar hydrogen production using a powder photocatalyst is a potentially clean and renewable artificial photosynthesis solution to convert solar energy into hydrogen fuel. In the past decades, increasing interests in this field have been paid to developing materials to capture and channel sunlight; deepening understanding of photosynthesis; and discovering new catalysts to make the chemistry possible. In this talk, I will present the recent research progress about the solar hydrogen production via overall water splitting of powder photocatalysts in my group. It involves development of photocatalyst/cocatalyst materials, fabrication of overall water splitting under visible light as well as understanding of underlying mechanism. Meanwhile, the strategies of promoting photogenerated charge separation and assembly of efficient solar-chemical conversion systems by crystal engineering, hetero-phase junction or dual cocatalysts etc. will be discussed in details.

Keyword: Photocatalysis, Visible light, Inorganic Semiconductor, Water splitting

最终交流类型: Invited

Theoretical Study of Nonoxidative Conversion of Methane: From Single-Atom Catalysis to Single-Cluster Catalysis

常春然
西安交通大学/榆林学院

Methane is one of the most important carbon-based energy resources in modern chemical industry. Its efficient conversion and utilization will significantly contribute to the optimization of energy structure and the reduction of air pollution. The nonoxidative conversion of methane on silica-confined single iron sites reported by Bao et al.[1] has attracted extensive attention in the last few years, where the singly-dispersed Fe sites connected with two carbon atoms and one silicon atom (Fe1©SiC2) were assigned as the active center. However, the formation mechanisms of the active centers and the reaction mechanisms of CH4 conversion on them are not fully illustrated. In this talk, I will present our latest theoretical findings on how was the active center formed and the catalytic reaction mechanism over the single-atom center. We find that the formation of Fe1©SiC2 undergoes a series of complex steps from the original oxygen-coordinated single Fe atoms (Fe1©O3). Importantly, during the formation process of Fe1©SiC2 other possible active centers such as Fe1©SiO2, Fe1©SiC, Fe1©SiCO, Fe1©SiC2 may also be generated, which synergistically contribute to the conversion of methane.[2] In addition, we find a novel surface reaction pathway of CH4 coupling to C2 species on Fe1©SiC2 in contrast to the literature-reported gas-phase one.[3] Based on the understandings above, a series of single-atom catalysts three kinds of dual-active-site catalysts were designed and exhibited outstanding performance for the nonoxidative conversion of methane.[4-7]

Keyword: methane, nonoxidative conversion, single-atom, single-cluster

最终交流类型: Invited

Selective C1 Molecule Conversion for Solar-Driven Artificial Carbon Cycle

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University of Science and Technology of China, China

Artificial carbon cycle is a highly important research theme given the increasing global energy demand and carbon dioxide emission. Converting C1 molecules such as carbon dioxide and methane into multicarbon fuels or value-added chemicals with solar energy is one of the keys to constituting artificial carbon cycle. However, the chemical stability of these C1 molecules is relatively high but they could evolve through various reaction pathways once activated. For this reason, it remains a grand challenge to achieve high catalytic activity and product selectivity. In this talk, I will demonstrate how to rationally control the cleavage and formation of chemical bonds for solar-driven CO2/CH4 conversion given that solar harvesting and charge separation are accomplished. Specifically, we leverage the multidisciplinary research at the intersection of controlled synthesis, operando spectroscopy and theoretical simulation. Such a research module allows us to tailor the surface/interface and electronic structures of catalytic materials with atomic precision, and employs time-resolved spectroscopic techniques and simulation methods to discover the dynamic evolution of catalysts and reaction species. Taken together, the controlling means and fundamental understanding pave the way to chemical transformations.

Keyword: carbon cycle; selective conversion; photocatalysis; solar energy; catalytic sites

最终交流类型: Invited

Electrochemical Oxygen Generator With 99.9% Oxygen Purity and High Energy Efficiency

吴宇恩
University of Science and Technology of China, China

Given the escalating probability of long-term coexistence with COVID-19 and the potential for recurrent infections within the broader population, there has been a pronounced surge in demand for safe, portable, and user-friendly oxygen (O_2) generators. This requirement is particularly significant for individuals with persistent cardiopulmonary diseases. At the current stage, the O_2 production industry generally adopts the physical air separation strategy, which mainly relies on the technologies of cryogenic distillation (CD) and pressure swing adsorption (PSA). However, for the demand of general population , the utilization of oxygen produced by CD technology and stored in steel cylinders is deemed impracticable due to the considerable size and weight of steel cylinders, challenges associated with transportation logistics, and the potential hazard of explosions. Meanwhile, the commercial oxygen generator relied on PSA technology still suffers from inherent limitations including low oxygen purity (93±3%), high noise level, and relatively large size and weight. The advent of electrochemical oxygen generation technology enables the rapid and on-site production of medical-grade O_2, offering a more suitable alternative for general application of populace. In our study, we have manufactured an oxygen generation device that relies on electrochemical technology. The performance of the electrochemical oxygen generator (EOG) is remarkably improved to a practically applicable level, achieving long-term (>200 h), stable, and quick production (>1.5 L min^{-1}) of high purity O_2 (99.9%) at high energy efficiency (496

L kW^{-1} h^{-1}), via simultaneous optimization for intrinsic electrochemical reaction mechanisms, electrocatalysts, and external cell structure. The EOG also presents powerful competitiveness in user experience, which finds expression in high portability (4.7 kg), nearly instant O_2 production (<1 s), and a quiet working condition (<39 dB). The EOG shows great potential to substitute commercial PSA O_2 generation devices, which may significantly impact the traditional oxygen production industry.

Keyword: oxygen evolution reaction, oxygen reduction reaction, electrochemical oxygen generation, high oxygen purity, high energy efficiency

最终交流类型: Invited

Photocatalytic biorefineries for H2 production

王峰
Dalian Institute of Chemical Physics, CAS

Photocatalytic biorefineries are deemed as a potential route to sustainably provide carbon resources and green energy vectors. The major interests of photocatalytic biorefineries focuses on treating biomass as sacrificial hole reagents for H2 generation or fragmenting biomass to provide carbon resources. Photocatalysis allows for uphill reactions at room temperature, which is expected to realize the mild conversion of biomass and obtain energy chemicals with high yield[1]. This way of biorefineries extremely rely on photocatalysts for interfacial charge transfer to activate diverse chemical bonds, and for harnessing radicals to control product selectivity[2].

Our research focuses on H2 production via photocatalytic biorefineries. The involved processes can be divided into H2 production and coupled H2 and value-added chemical production. Biomass is widely spread in nature, and its collection and pretreatments contribute greenhouse gas emissions. In the aspect of biorefineries for H2 production, the strategy of "C-C bond scission first" was promoted, targeting of cleaving all the C-C bonds in biomass to maximize H2 production per mass of biomass[3]. Powered by solar energy, refineries of polyols and sugars over a Ta-doped CeO2 allowed the complete fragmentation of radical C-C bonds. The H2 yield from glucose reached 33%, much higher than H2 production by direct biomass photoreforming[4]. In terms of coupled H2 and value-added chemical production from photocatalytic biorefineries, we proposed the strategy of two fuels on one catalyst and realized coproduction of H2 and diesel fuel precursors over a Ru-doped

ZnIn2S4[5]. We also realized the coupled production of H2 and 2,3-butanol from ethanol by controlling the reaction pathways of α-hydroxyethyl radical intermediates[6]. Moreover, through controlling cocatalyst sizes[7], surface structure modification[8], heterojunction construction[9] and facet control[10], sugars and polyols were fragmented via C-C bonds, allowing for CO and H2 production. The above works have realized the coupled conversion of solar energy and biomass energy.

Keyword: Photocatalytic biorefineries, H2, C1 chemical, fuels

最终交流类型: Invited

High-density non-precious metal-nitrogen-carbon active sites for advanced oxygen electrocatalysts

胡劲松
中国科学院化学研究所

Fuel cells and metal air batteries are promising techniques for innovative energy conversion and storage. The commercialization of these techniques requires the earth-abundant efficient and durable electrocatalysts for oxygen reduction reaction (ORR) and/or oxygen evolution reaction (OER). The performance of these electrocatalysts are closely related to the intrinsic activity and the number of the accessible catalytic sites in the electrocatalysts. This presentation will focus on the development of high-density earth-abundant metal-nitrogen-carbon active sites for advanced ORR and OER electrocatalysts. A couple of new strategies will be introduced, including a molecular-based cascade anchoring strategy for general mass production of high-density metal-nitrogen single-atomic catalysts for diverse electrocatalytic applications, metastable rocksalt oxide mediated synthesis of high-density well-armored transition metal nanoparticles for boosting power density and cycling life of zinc-air batteries, etc. These results may give new insights for the rational design and bottom-up synthesis of cost-effective and high-performance electrocatalysts for diverse advanced energy-related devices.

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Keyword: ORR, OER, Fuel cells, Metal air batteries, Non-precious metal

最终交流类型: Invited

Atomic Doping and Surface Adsorption Promotes Activity for Hydrogen Generation

Hongjin Fan
Nanyang Technological University

Electrolysers, fuel cells, and metal-air batteries require efficient and low-cost electrocatalysts that can significantly lower the reaction overpotentials and boost the kinetics. Atomic defects due to doping are proven effective in tailoring local electronic structures and boosting the activities of the catalyst materials. This talk will provide a few example electrocatalysts for water electrolysis: i) activation of the basal plane of MoS2 monolayers by local atomic defects, ii) enhancement of MoS2 activity by biaxial strain, iii) doping metal elements with suitable electronegativity enhances the stability of amorphous MoSxO2-x catalyst for acidic HER.

Keyword: electrocatalysts, water splitting, atomic doping, biaxial strain, electronegativity, surface adsorption, charge transfer

最终交流类型: Invited

Artificial Photosynthesis of Value-added Chemicals and Pharmaceuticals

苏陈良
深圳大学

Today, under the development model of fossil fuel-driven economic growth, we are facing global challenges of environmental degradation and energy security. To provide the solutions, scientists present the “liquid sunshine” roadmap, the vision of converting solar energy to liquid fuels to power the future. In this spirit, solar energy or solar-electricity driven large scale production of fine chemicals as well as pharmaceuticals from sustainable sources are also the actionable pathways. This lecture introduces solar energy-driven redox-reactions to active small molecules to furnish active-species for sequential “dark reaction” to use these active-species for production of value-added chemicals and pharmaceuticals.

Keyword: Artificial Photosynthesis, Semiconductor Photocatalyst, Photo-redox Catalysis

最终交流类型: Invited

Engineering Ta3N5 Thin Film Photoanode for Efficient Solar Water Splitting

李严波
电子科技大学

Tantalum nitride (Ta_3N_5) is a promising photoanode material with a theoretical maximum solar conversion efficiency of over 15% for photoelectrochemical water splitting. However, the highest solar conversion efficiency achieved is still far below its theoretical limit. The presence of deep-level defects in the bulk and at the interfaces is probably the major limiting factor of the efficiency of Ta_3N_5 photoanode [1]. In the past few years, our group has been devoted to improving the efficiency of Ta_3N_5 thin film photoanode via band structure engineering [2], defect engineering [3], interface engineering [4], and co-catalyst modification [5-6]. By constructing a gradient band structure in the bulk of Ta_3N_5 thin film through gradient Mg-doping, we achieved a half-cell solar-to-hydrogen conversion efficiency (HC-STH) of 3.31% thanks to the improved bulk charge separation efficiency in the gradient Mg-doped Ta_3N_5 photoanode [2]. Alternatively, by modifying the interfaces of Ta_3N_5 thin film with an electron transport layer (ETL: In-doped GaN) and a hole transport layer (HTL: Mg-doped GaN), we realized a heterostructure Ta_3N_5 photoanode with an HC-STH of 3.46% [4]. Lately, we demonstrated a heterogeneous doping strategy that combined surface La doping with bulk gradient Mg doping in Ta_3N_5 thin film to decouple light absorption and carrier transport, resulting in a record-high HC-STH of 4.07% for Ta_3N_5 photoanode [3], ten times higher than what we achieved a decade ago (Fig. 1) [7]. These results established Ta_3N_5 as a leading performer among visible-light-responsive photoanodes for PEC water splitting.

Keyword: Tantalum nitride, photoelectrochemical water splitting, defect engineering, interface engineering, oxygen evolution co-catalyst

最终交流类型: Invited

Spontaneous Polarization Driven Water Splitting

Haitao Huang
Hong Kong Polytechnic University

Over the past few years, due to high atom utilization efficiency, outstanding selectivity, and stability, single-atom catalysts have been an extremely hot topic in heterogeneous catalysis, which is often governed by the linear scaling relation. By adding more atoms on the neighboring site of the single-atom, one may break this scaling relation and achieve significant improvement in catalytic activity for water splitting. Here, the well-dispersed ruthenium (Ru) based clusters with adjacent Ru single atoms (SAs) on layered sodium cobalt oxide (Ru/NC) is demonstrated to be a superb electrocatalyst for alkaline HER. The Ru/NC catalyst manifests an activity increase by a factor of two relative to the commercial Pt/C. Operando characterizations in conjunction with density functional theory (DFT) simulations uncover the origin of the superior activity and establish a structure-performance relationship, that is, under HER condition, the real active species are Ru SAs and metallic Ru clusters supported on the NC substrate. The excellent alkaline HER activity of the Ru/NC catalyst can be understood by a spatially decoupled water dissociation and hydrogen desorption mechanism, where the NC substrate accelerates the water dissociation rate, and the generated H intermediates would then migrate to the Ru SAs or clusters and recombine to have H2 evolution. More importantly, comparing the two forms of Ru sites, Ru cluster dominated the HER activity due to the more fluent migration of H* and its more favorable adsorption-desorption energetics towards H intermediates. This study highlights the importance of combining metal oxide support and Pt-group metal catalyst to create spatially decoupled water dissociation and hydrogen desorption towards efficient alkaline HER. Moreover, the more favorable activity of Ru cluster than Ru SA would inspire new direction in designing noble metal based catalysts with excellent performance for alkaline HER and beyond.

Keyword: Water splitting, HER, Single-atom catalyst; Clusters

最终交流类型: Oral

Tailoring the molecular interfaces for boosted CO2 reduction

叶汝全

香港城市大学

Carbon dioxide reduction to produce various fuels and chemical products can simultaneously fix carbon dioxide and convert renewable electrical energy into chemical energy storage, making it an attractive route to achieve a closed-loop carbon cycle. Metal complexes are an important class of catalysts with the advantages of well-defined and controllable structures. However, due to the molecular aggregation and leaching effects in the catalytic process, the low conversion frequency, low electron transport rate and poor stability in the heterogeneous catalytic process are encountered. This talk will summarize our group's recent progress on carbon dioxide reduction based on metal-organic molecular catalysts, and mainly discuss the influence of catalyst interface aggregation effect on catalytic mechanism and product selectivity; this includes the in-depth understanding of interface electron transport and molecular configuration evolution, which change the product turnover and even selectivity. We demonstrate that interfacial aggregated state realizes efficient and controllable two-electron and multi-electron reduction.

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Keyword: CO2 reduction, molecular catalysts, interface engineering

最终交流类型: Oral

Graphitic Carbon Nitride Photocatalysts

余慧军

东南大学

Artificial photocatalysis, mimicking the photoreactions widely exists in nature, provides a rational and effective solution to renewable energies. Currently, it is still a great challenge

to develop photocatalysts with high yield and selectivity, especially for systems without sacrificial reagents. Here, we develop a new strategy to synthesize carbon nitride photocatalyst with tunable band structures, which greatly improved the capture and conversion of solar energy in water splitting reaction. In addition, we construct two more carbon nitride base nanostructures, providing efficient ways to the photoreduction of CO2. We believe these results would provide new opportunities to carbon nitride based photocatalysts and pave the research in artificial photocatalysis.

Keyword: Photocatalysis, hydrogen evolution, carbon dioxide reduction, carbon nitride, polyoxometalate

最终交流类型: Invited

Photo- and electrocatalyst development for catalytic oxidation of organic molecules to value-added chemicals

Menny Shalom
Ben Gurion University of the Negev

Photoelectrochemical cells (PECs) have been developed as environmentally friendly systems that can directly utilize photogenerated electron-hole pairs for water splitting, fuel production, conversion of carbon dioxide, and pollutant degradation. Most reports on the photocatalytic or PEC hydrogen (H2) evolution via water splitting have focused on the H2 reduction half-reaction by generating on the photoanode non-valuable oxygen or using sacrificial agents to consume the generated h+, resulting in a significant waste of energy. Lately, much effort is invested into synthesizing valuable chemicals on the photoanode while retaining the production of H2 on the cathode.

Over the past few years, polymeric carbon nitrides (CN) attract widespread attention due to their outstanding electronic properties, which have been exploited in various applications, including photo- and electro-catalysis, heterogeneous catalysis, CO2 reduction, water splitting, light-emitting diodes, and PV cells. CN comprises only carbon and nitrogen, and it can be synthesized by several routes. Its unique and tunable optical, chemical, and catalytic properties, alongside its low price and remarkably high stability to oxidation (up to 500 °C), make it a very attractive material for photoelectrochemical applications. However, only a few reports regarded CN utilization in PECs due to the difficulty in acquiring a homogenous CN

layer on a conductive substrate and our lack of basic understanding of the intrinsic layer properties of CN.

This talk will introduce new approaches to growing CN layers with altered properties on conductive substrates for photoelectrochemical applications. Growth mechanism and their chemical, photophysical, electronic, and charge transfer properties will be discussed. I will show the utilization of PEC with a CN-based photoanode as a stable and efficient platform for the oxidation of organic molecules to added-value chemicals, with hydrogen co-production. The talk's second part will focus on the electrocatalytic oxidative upgrading of organic molecules by NiFe-oxide into valuable chemicals.

Keyword: Carbon nitride, photocatalysis, electrocatalysis

最终交流类型: Invited

Rational Design of Two-Dimensional Hybrid Photocatalysts

曹少文
武汉理工大学

Excessive consumption of fossil fuels is the key contributor to climate change. Solar-powered artificial photosynthetic conversion of CO2, potentially direct from diluted sources, into value-added products is considered as a promising strategy to alleviate the problem. The exploitation of low-cost, sustainable, and highly active photocatalysts is critical to improve CO2 photoreduction for practical applications. Hybrid photocatalytic systems on the basis of two-dimensional (2D) materials have shown great potential in this field. Constructing an interface with intimate contact and strong interaction is of vital importance for achieving highly efficient 2D material-based hybrid photocatalytic systems, which essentially promoting the charge transfer across the interface. Herein, we introduce the rational design of 2D material-based hybrid photocatalytic systems via various strategies. (1) Carbon nitride/single-atom metal 2D/0D systems are constructed via strong coordination, which establishes directional charge transfer channels through a built-in electric field and enhances the photocatalytic CO2 reduction and H2 production. (2) Polymer/quantum dot 2D/0D systems are constructed via electrostatic adsorption–in situ growth, which generates interfacial electric field to promote charge transfer across the interface for enhanced photocatalytic inactivation of bacteria and H2 production. (3) Graphene/crystalline carbon nitride 2D/1D system is constructed via dissolution-recrystallization–in situ growth, which shows remarkable improvements of light absorption, exciton splitting, and charge transport, enabling the efficient photochemical reduction of wet CO2 in the gas phase and without any sacrificial agent.

Keyword: Artificial photosynthesis, CO2 reduction, H2 evolution, 2D hybrid photocatalyst, Charge transfer

最终交流类型: Oral

Wet-chemical synthesis of metal nanomaterials with unconventional crystal phases and their catalytic properties

陈也
香港中文大学

Metal nanomaterials have excellent intrinsic catalytic activity, high electrical conductivity and high stability, making them promising catalyst materials. However, conventional colloidal synthesis mainly focuses on the morphology and composition control of nanocrystals. This talk will introduce some interesting discoveries we have recently made in the aspect of crystal phase control of metal based nanocatalysts and their enhanced catalytic performances. For example, traditional Au nanomaterials have the same face-centered cubic (fcc) crystal structure as bulk gold, while we have developed unconventional 4H/fcc heterogeneous Au nanorods with high yield. Au nanorods in these unconventional crystal phases have high thermal stability and can serve as high-quality seeds for epitaxial growth. Therefore, we further prepared unconventional 4H/fcc core-shell nanostructures, in which Au was coated with other catalytically active metals (such as Pd and Cu). The catalytic performances of these new crystal phase metal nanomaterials in ethanol electrooxidation, and carbon dioxide electroreduction were studied. In a latest work, we used Pd-based nanocrystals of different crystal phases as seeds, further deposited Pt surfaces of different crystal phases by colloidal epitaxial growth, and carried out phase-dependent performance analysis of Pt surfaces in heterogeneous selective hydrogenation reaction. The Pt surfaces with unconventional crystal structures show better selectivity and durability compared to conventional fcc Pt. These works demonstrate a new strategy to design and synthesize the

crystal phase of metal nanomaterials by wet-chemical method, and explore the effect of crystal phase regulation on various properties of metal nanomaterials.

Keyword: Metal nanomaterials, unconventional crystal structures, epitaxial growth, nanocatalysis, phase engineering

最终交流类型: Invited

Water oxidation with metal porphyrins

曹睿
Shaanxi Nornal University

Developing highly efficient catalysts for water splitting and oxygen reduction reaction has attracted increasing attention in the past decades. Dr. Rui Cao focuses on illustrating the reaction mechanisms of water splitting and oxygen reduction and also on developing novel porphyrin-based molecular catalysts for these reactions. By demonstrating several H-H and O-O bond formation/cleavage processes, revealing the crucial effects of the electronic structure and proton transfer on these bond formation/cleavage processes, and by establishing structure-function relationships at the molecular level, in the past five years, Dr. Rui Cao has obtained significant achievements in hydrogen and oxygen evolution and oxygen reduction reactions, including: (1) demonstrated three different H-H bond formation mechanisms for the hydrogen evolution reaction (HER); developed highly efficient porphyrin-based molecular catalysts with the state-of-the-art performance for HER; (2) disclosed two O-O bond formation mechanisms for the oxygen evolution reaction (OER); rationally designed and developed highly efficient porphyrin-based molecular catalysts for OER; and (3) controlled and improved the O-O bond cleavage for the oxygen reduction reaction (ORR); developed porphyrin-based molecular ORR electrocatalysts with promising applications in new energy conversion and storage devices.

Keyword: metal porphyrin, water oxidation, O-O bond formation

最终交流类型: Invited

Single-Atom Catalysts: Emerging Multifunctional Materials towards Sustainable Energy Conversion

huabin zhang

king abdullah univeristy of science and technology

Increasing demand for sustainable energy has accelerated research on various renewable technologies. Developing catalytic energy conversion technologies for replacing the traditional energy source is highly expected to resolve the fossil fuel exhaustion and related environmental problems. Exploring stable and high-efficiency catalysts is of vital importance for the promotion of these technologies. Single-atom catalysts (SACs), containing single metal atoms anchored on supports, represent the utmost utilization of metallic catalysts and thus maximize the usage efficiency of metal atom.1 However, with the decreasing of particle size, the surface free energy increases obviously, and tends to aggregate into clusters or particles. Selection of an appropriate support is necessary to interact with isolated atoms strongly, and thus prevents the movement and aggregation of isolated atoms, creating stable, finely dispersed active sites. Furthermore, with uniform single-atom dispersion and well-defined configuration, SACs afford great space for optimizing high selectivity and activity.

Our research interest focuses on the development of single-atom catalysts with the particular configuration for sustainable energy conversion, including photocatalysis, electrocatalysis, and thermal catalysis.2 His research also extends to the operando investigation for monitoring the structural evolution of the reactive centers, as well as the mutual interaction between the reactive center and reactant in the catalytic process. The widespread adoption of SACs in diverse catalytic reactions will be comprehensively introduced.3, 4 By presenting these advances and addressing some future challenges with potential solutions related to the integral development of catalysis over SACs, we expect to shed some light on the forthcoming research of SACs for catalytic energy conversion.

Keyword: Single-atom catalysis; electrocatalysis; photocatalysis

最终交流类型: Invited

Surface Modified Ag@Ru-P25 for Photocatalytic CO2 Reduction with High Selectivity over CH4 Formation

SUIL IN
DGIST

Systematic optimization of the photocatalyst and investigation of the role of eachcomponent is important to maximizing catalytic activity and comprehending thephotocatalytic conversion of CO2 reduction to solar fuels. A surface-modifiedAg@Ru-P25 photocatalyst with H2O2 treatment was designed in this study toconvert CO_2 and H_2O vapor into highly selective CH_4. Ru doping followed by Agnanoparticles (NPs) cocatalyst deposition on P25 (TiO_2) enhances visible lightabsorption and charge separation, whereas H_2O_2 treatment modifies the surfaceof the photocatalyst with hydroxyl (–OH) groups and promotes CO_2 adsorption.High-resonance transmission electron microscopy, X-ray photoelectron spectroscopy, X-ray absorption near-edge structure, and extended X-ray absorption finestructure techniques were used to analyze the surface and chemical compositionof the photocatalyst, while thermogravimetric analysis, CO_2 adsorption isotherm,and temperature programmed desorption study were performed to examine thesignificance of H_2O_2 treatment in increasing CO_2 reduction activity. Theoptimized Ag1.0@Ru1.0-P25 photocatalyst performed excellent CO_2 reductionactivity into CO, CH_4, and C_2H_6 with a ~95% selectivity of CH_4, where theactivity was ~135 times higher than that of pristine TiO_2 (P25). For the first time,this work explored the effect of H_2O_2 treatment on the photocatalyst thatdramatically increases CO_2 reduction activity.

Keyword: gas-phase CO_2 reduction, H_2O_2 treatment, plasmonic nanoparticles, solar fuel photocatalyst, surface modification

最终交流类型: Invited

Electrochemical CO2 Reduction Chemistry over Model Single Atom Catalysts

Bin Liu
City University of Hong Kong

Noble-metal and transition-metal based materials have been demonstrated as promising catalysts for selective electrochemical CO_2reduction reaction (CO2RR), however, neither the detailed structures of catalytic intermediates nor the key surface species have been unambiguously identified. In this work, a series of single transition-metal atom catalysts with well-defined structures were developed as model systems to explore the electrochemical CO2RR chemistry. Employing a combination of operando X-ray absorption spectroscopy, attenuated total reflectance surface enhanced infrared absorption spectroscopy, Raman spectroscopy and Mössbauer spectroscopy, we successfully captured the dynamic evolution of the catalytic centers during the CO2RR process.

Keyword: CO_2 reduction; Single atom catalysis; in-situ/operando; reaction pathway

最终交流类型: Invited

Tuning semiconductor–metal single atom interaction for artificial photosynthesis

郭少军
Peking university

Metal single-atom (MSA) catalysts with 100% metal atom utilization and unique electronic properties are attractive cocatalysts for efficient photocatalysis when coupled with semiconductors. Owing to the absence of a metal–metal bond, MSA sites are exclusively coordinated with the semiconductor photocatalyst, featuring a chemical-bond-driven tunable interaction between the semiconductor and the metal single atom. This semiconductor–MSA interaction is a platform that can facilitate the separation/transfer of photogenerated charge carriers and promote the subsequent catalytic reactions. In this talk, we will introduce the fundamental physicochemistry and their application in artificial photosynthesis of the semiconductor–MSA interaction.

Keyword: Photocatalysis; Artifical Photosynthesis

最终交流类型: Invited

Raman Spectroscopy for Microstructure Study: From site identification to Quantitative Analysis

刘睿
Research center for Eco-environmental Sciences, CAS

Understanding the microstructure of the reactive species, c.a., the catalysis center, is of great significance for process and mechanism study. The up to 10-3 eV energy resolution of Raman spectroscopy/surface enhanced Raman Spectroscopy (SERS) makes this technology an ideal tool for atomic structure study. Combining with spherical aberration correction electron microscopy and X-ray absorption spectroscopy (XAS), we developed a SERS-spectra of chemisorbed 2,6-DMPI based new method for the interrogating the atomic-scale structure of the Pd reactive centers and quantitatively estimated their relative abundance. Up to five catalogues of Pd site were spectroscopically identified on Au@Pd surface, $Pd_{-isolated}$, $Pd_{-interface}$, $Pd_{-ensemble}$, $Pd_{-elongated}$ and $Pd_{-island}$.

In the catalyzed Suzuki–Miyaura coupling reaction, we found that strained sites with elongated Pd bonds are >100 times more active than unstrained sites. SERS spectra and theoretical simulations reveal that changes in bond lengths influence the electronic state of Pd atoms more profoundly than substituting coordination atoms or reducing coordination numbers. Further, we discovered that Pd growth begins as a continuous atomic chain rather than a single atom as thought previously.

Furthermore, combined by charge-analysis and I-labeling based elemental analysis, the relative abundance of all the Pd sites was quantified. By deconvoluting and linear regressing the overall catalysis performance, the activity and selectivity of all Pd sites involved in the reduction of 4-nitrophenol and chemoselective hydrogenation of 4-chloronitrobenzene was determined. The catalysis process was stimulated on different Pd sites, and the theoretic rate constant aligned perfectly with the experimental data. The mutual corroboration of theoretical and experimental results strongly supports rationality of our Pd site identification and quantification method. This enables us to treat the heterogeneous process as a weighted linear combination of various reactive sites rather than an elusive black box. Additionally, it provides valuable guidance for the design of Au@Ag_{ML}@Pd as a highly active/selective catalyst.

Keyword: Surface Enhanced Raman Scattering, Environmetal Catalysis, Structure activity relationship

最终交流类型: Invited

Leveraging Renewable Energy: Transforming CO2, CO, and Beyond into Valuables

钟苗
Nanjing University

Utilizing electrical or solar power to convert low-cost CO2, CO, and N2 into high-value chemical feedstocks presents a promising solution for storing energy derived from intermittent renewable sources in chemical bonds. Despite significant efforts in this field, certain crucial reactions still face challenges in achieving the desired combination of high selectivity, activity, energy efficiency, and stability. This report focuses on exploring the critical roles of catalysts, interfaces, and reaction microenvironments in influencing the reaction kinetics. We present the results of fundamental studies, including computational analyses and in situ spectroscopic observations, which help identify active catalyst sites and their interactions with intermediates to enhance reaction selectivity. We also discuss synthetic approaches to in situ stabilize these identified active sites at reaction interfaces, and show new routes to engineer the reaction microenvironment, enabling the enhancement of reaction activities and stabilities up to levels relevant for industrial applications. By providing insights into the fundamentals and practicality of catalysts and systems, our findings are expected to contribute to the development of sustainable technology for the production of chemicals and fuels from renewable energy.

Keyword: electrolysis, CO2 reduction, nanocatalysts, reaction kinetics, catalyst and interface

最终交流类型: Keynote

Induced Catalytic Active Sites over Nano-structures

Shik Chi (Edman) Tsang
University of Oxford

As generally known, the elucidation of active sites' structure in solid nanocatalysts under real reaction conditions is one of the most important challenges facing the scientific community. There is an increasing amount of evidence by the in situ/operando characterization that active sites can be generated by the interaction of substrate molecules with the inorganic nanocatalysts as akin to enzyme-substrate interaction, which can result in the significant promotion of catalytic performance. In addition, surface rearrangement could occur under reaction conditions, which may cause dynamic changes in the active sites. Therefore, the real active sites under working conditions could be significantly different from those characterized under ex situ conditions. Yet, current limitations in state-of-the-art characterization techniques regarding spatial, temporal and temperature/pressure gaps are sometimes unable to provide the answers for the understanding. In-situ/operando characterization using modern designated synchrotron offers exciting possibilities. Hence, in this meeting, some examples how Frustrated Lewis Pair (FLP) sites on solid nanostructure will be given, which offer to catalyse a wide range of chemical reactions. It is hoped that this talk could stimulate new science/new instrumentation in catalysis and other disciplines in future.

Keyword: Nanostructure; active sites; substrate; modification; operando

最终交流类型: Keynote

Low temperature catalytic water activation and hydrogen production

马丁
北京大学

Water molecules (H2O) are the most abundant molecules on the Earth's surface and serve as a plentiful green hydrogen source. With the advancement of the hydrogen economy, efficient production and transportation of hydrogen gas have become critical frontiers in catalytic research. However, due to the high thermodynamic stability of water molecules, activating and breaking the O-H bonds in water at low temperatures, and designing catalytic cycles for low-temperature hydrogen activation, remain significant challenges. Therefore, the development of a novel catalyst system for mild water molecule activation and stable hydrogen evolution is of paramount importance.

By altering the carbon interstitial content of molybdenum carbide and tuning its band structure, a cubic-phase α-MoC catalyst has been successfully prepared, capable of dissociating water at room temperature, cleaving the O-H bonds of water molecules, and stabilizing metastable hydroxyl species. In situ characterization and theoretical calculations have revealed the unique properties of the α-MoC catalyst, including low-temperature dissociation of water molecules and dynamic equilibrium of metastable -OH and O species. The newly constructed metal/α-MoC catalyst system has surpassed the low-temperature limit and activity ceiling of water-gas shift and methanol-water reforming processes, achieving the highest level of hydrogen production catalytic performance to date. Additionally, a multi-active site ordered composite catalyst of metal-carbide was designed, enabling the direct coupling of hydrogen production from water and highly selective hydrogenation to valuable oils and chemicals. This resulted in efficient synthesis of C5+ oils, polyols, aniline derivatives, and other new catalytic processes without the need for external hydrogen under CO+H2O conditions.

Keyword: Water, hydrogen, Pt, molybdenum carbide

最终交流类型: Invited

Electrochemical CO2 Reduction Reaction in Acid for High Carbon Utilization

王莹
香港中文大学

Developing high-efficiency carbon dioxide capture, storage, and conversion technologies has received extensive attention. Renewable electricity-powered CO2 conversion offers an attractive means to produce low-carbon-footprint fuels and chemicals. In the past few decades, significant progress has been made in advancing CO2RR technology under industrial-relevant current densities (> 100 mA/cm2). One of the remaining critical challenges is to improve the carbon utilization efficiency of CO2RR. Due to the hydroxide ion produced at the electrode interface during electrolysis, a significant amount of CO2 will be converted to carbonate rather than reduced to targeted products. The maximum carbon conversion efficiency of CO2-to-CO is only 50% for the current neutral/alkaline CO2RR electrolyzer. This efficiency will further drop for multi-electron transfer products, such as ethylene (25%) and ethanol (25%). We are working on developing acidic CO2RR electrolyzers for high carbon conversion efficiency to multicarbon products (C2+). Converting CO2 to C2+ in acid requires overcoming the competition from the hydrogen evolution reaction and the CO2-to-C1 pathways. Understanding the electrode process, including charge transfer and mass transport, is essential in developing efficient catalysts and electrolyzers for CO2RR in acid.

Keyword: Electrocatalysis, Electrochemistry, Bimetallic Catalyst, CO2 Reduction Reaction, Carbon Neutrality

最终交流类型: Keynote

Toward Atomically Precise Heterogeneous Catalysis via Single-Cluster Catalyst (SCC)

李隽
Tsinghua University

Catalysis science is essential for chemical industries, biological transformation, atmospheric processes, environment, energy, and human health. In recent years, heterogeneous single-atom catalysts (SACs) and single-cluster catalysts (SCCs) have aroused

significant interest in the catalysis community [1-3]. In this talk, we will provide an overview and perspective of atomically precise heterogeneous catalysis via SACs and SCCs.

Keyword: atomically precise heterogeneous catalysis; single-atom catalyst; single-cluster catalyst

最终交流类型: Invited

Solar hydrogen production by photoelectrochemical water splitting

李朝升
南京大学

Recently, solar hydrogen production by photoelectrochemical water splitting has attracted intensive interest. Unfortunately, there is lack of low-cost, environment-friend, efficient and stable photoanodes. In this talk, we will introduce the latest research progress of solar hydrogen production in our research team. The main progresses include:

(1) Constructing a Turing structured ZnFe2O4/Fe2O3 photoanode significantly improves its charge separation efficiency, thereby increasing the performance of photoelectrochemical water splitting for hydrogen production.

(2) Sn doping is used to not only increase the carrier concentration of metastable β-Fe2O3 photoanodes, but also inhibit the loss of the active site during the process of photoelectrochemical seawater. Therefore, Sn-doped β-Fe2O3 photoanodes exhibit long-term stability over 3000 h for efficient hydrogen production by photoelectrochemical seawater splitting (Fig. 1).

(3) A new type of electrocatalyst for efficient and stable decomposition of seawater for hydrogen production has been obtained.

Keyword: Photoelectrochemical water splitting, Photoanode, Turing structure, Charge separation efficiency, Seawater splitting

最终交流类型: Keynote

Metal-organic frameworks for catalysis and energy

徐强
南方科技大学

Recently, we have successfully synthesized a number of porous metal-organic frameworks (MOFs) and developed their new applications as catalysts, as supports for metal nanoparticles and as templates/precursors for synthesis of nanostructured materials.[1] Porous carbons and carbon composite materials have been synthesized by using MOFs as templates/precursors and the resultant materials display high specific surface areas and excellent electrochemical properties as electrode materials for electric double-layered capacitor (EDLC) and as electrocatalysts for various reactions. This talk will discuss the catalytic and energy applications of MOF-derived nanomaterials.

References:

[1] For recent reviews, see: (a) S. Dang, Q.-L. Zhu, Q. Xu, *Nat. Rev. Mater.*, **2017**, *3*, 17075. (b) R. Zhao, Z. Liang, R. Zou, Q. Xu, *Joule*, **2018**, *2*, 2235. (c) Z. Liang, R. Zhao, T. Qiu, R. Zou, Q. Xu, *EnergyChem*, **2019**, *1*, 100001. (d) Y.-S. Wei, M. Zhang, R. Zou, Q. Xu, *Chem. Rev.*, **2020**, *120*, 12089.

Keyword: metal-organic frameworks, MOFs, catalysis, energy storage, energy conversion

最终交流类型: Invited

Chainmail Catalysis: From Fundamentals to Applications

邓德会

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After nearly 190 years of development, the discipline of catalysis has established basic concepts represented by "reaction activation energy", "surface adsorption", "active center", etc., laying a theoretical foundation for the design and development of catalysts. However, for the development of catalysts for practical applications, an important indicator is high stability and durability. So far, the development of highly stable catalysts has basically remained in a trial-and-error stage, and there has been no unified understanding. The reporter team creatively encapsulated non precious metal nanoparticles in the "chainmail" formed by the curling of two-dimensional materials such as graphene through the innovation of synthesis strategy, and found that highly stable two-dimensional materials can protect non-precious metals from the etching of harsh environments such as strong acids, strong bases and other mediators, while free electrons of non-precious metals can be transferred to the surface of the two-dimensional material "chainmail" and stimulate catalytic activity. Based on this, the concept of "chainmail catalysis" was for the first time proposed internationally. The "chainmail catalyst" has successfully operated with high activity and stability in the catalytic system including fuel cell, water electrolysis, hydrogen sulfide electrolysis, carbon dioxide conversion, etc. under harsh conditions such as strong acid, strong base, high temperature, etc., providing a new way for the design of high stability and high activity catalyst under harsh conditions. Based on this concept, a monolithic non-precious metal "chainmail catalyst" was developed and applied to water electrolysis, solving the dual challenges of low activity and poor stability of non-precious metal catalysts in water electrolysis. On this basis, we have successfully developed a high-performance, long-life, low-cost water electrolysis-based hydrogen and oxygen production device and system, and realized its application in industrial green hydrogen and life health and other fields.

Keyword: Chainmail catalysis, Two-dimensional material, Non-precious catalyst, Penetrated electron, Water electrolysis

最终交流类型:

Protease-Activatable Nanozyme with Photoacoustic and Tumor-Enhanced Magnetic Resonance Imaging for Photothermal Ferroptosis Cancer Therapy

秦文
华中科技大学

Despite the promise of ferrotherapy in cancer treatment, current ferrous therapeutics suffer from compromised antitumor ferroptosis efficacy and low specificity for tumors. Herein, a protease-activatable nanozyme (Fe_3O_4@$Cu_{1.77}Se$) is reported for photoacoustic and tumor-enhanced magnetic resonance imaging (MRI)-guided second near-IR photothermal ferroptosis cancer therapy. Fe_3O_4@$Cu_{1.77}Se$ remains stable in physiological conditions, but disintegrates to increase reactive intratumoral ferrous supply for elevated hydroxyl radical generation by Fenton reaction and GSH depletion in response to overexpressed matrix metalloproteinases in tumor microenvironment, leading to amplified ferroptosis of tumor cells as well as enhanced T2-weighted MRI contrast. Further integration with second near-IR photoirradiation to generate localized heat not only triggers effective photothermal therapy and photoacoustic imaging but more importantly, potentiates Fenton reaction to promote ferroptotic tumor cell death. Such synergism leads to the polarization of tumor-associated macrophage from the tumor-promoting M2 type to the tumor-killing M1 type, and induces the immunogenic cells death of tumor cells, which in turn promotes the maturation of

dendritic cells and infiltration of cytotoxic T lymphocytes in tumor, contributing to significant tumor suppression. This study presents a novel activatable ferrous nanotheranostics for spatial-temporal control over antitumor ferroptosis responses.

Keyword: truncated tissue factor, Nanogel, TACE, TVI, local blood coagulation

最终交流类型: Invited

Single Atom Catalysts: From Fundamental Understanding into Industrial Applications for Heterogeneous Hydroformylation of Olefins and Carbonylation of Alcohols

丁云杰
中国科学院大连化学物理研究所

Single-atoms catalysts of precious metal often possess outstanding catalytic performance better than that of corresponding nanoparticle catalysts. However, supported single-atoms catalysts have even greater challenges that are prone to aggregate or sinter when increasing the metal loading, especially at the practical reaction conditions. Herein we show that an absolutely new methodology for immobilization of homogeneous catalysis has been developed in our research team (DNL0805, DICP), in which the single-atomically active sites for olefins hydroformylations and alcohol carbonylations form on the surface of bi-functional porous organic polymers (POPs) or porous ionic polymer (PIPs) as supports and ligands respectively, therefore, this kind of the immobilized catalysts show very high performance of hydroformylations of olefins and carbonlation of alcohols with various carbon chains, the first commercial plant of heterogeneous hydroformylation of ethylene will be commissioned in the end of this year in Ningbo China. In addition, the very interesting phenomena of atomic dispersion of mosth precious metals nanoparticles with more than 5 wt. % loading of noble metals into single-atomically active complexes on the surface of carbon materials during reaction, which display very high activity, selectivity and stability of the heterogeneous carbonylation of alcohols, have been discovered. A mononuclear complex route to prepare stable single-atomically dispersive Rh catalysts with metal loading up to 5 wt. % on the surface of activated carbon (AC) was discovered and developed. The formation and migration of mononuclear complex (Rh(CO)xIy(O-AC), O-AC represents oxygen-containing groups on the surface of AC) originated from the reaction of metallic Rh nanoparticles with a mixture of CH3I/CO, with the promotion effect of some functional group with isolated phenol or adjacent phenol-carbonyl pair on the surface of AC carrier and the iodine free radicals in the breakage of Rh-Rh bonds, led to the single-atomic dispersion. The obtained atomically dispersed Rh1/AC catalyst exhibited quite high activity in heterogeneous alcohols carbonylations. A stable space-time-yield (STY) of more than 3000 mol-methyl acetate/mol-Rh·h-1 for time on stream of over 100 h was observed in methanol carbonylation. The first pilot plant test (5 liters catalyst loading) heterogeneous carbonylation process of methanol to methyl acetate has been done in 2016.

Keyword: Single Atom Catalysts

最终交流类型: Invited

The Electrolyte Materials and Interface in Lithium Metal Batteries

赵勇
Henan University, China

Lithium-metal battery with high theoretical energy density is one kind of promising energy storage and power battery, which has attracted wide attention. However, lithium metal battery is facing the problems of low actual energy density and poor cycle stability, which has become the bottleneck of its practicality. In the cycle process of lithium metal battery, it is not only challenged by lithium dendrite growth and continuous side reaction at the interface of cathode lithium metal and electrolyte, but also by the low reaction rate and stability at the interface of cathode and electrolyte. Therefore, deeply understanding the mechanism of the influence of electrode and electrolyte materials on the interface reaction process, and developing the high-performance electrode and electrolyte materials to improve the rate and stability of the battery interface reaction, is the key to build a high energy density lithium metal battery.

In this talk, we will introduce the basic principle of electrode interface reaction of electrochemical energy conversion devices, and discuss the key challenges of lithium metal batteries, the mechanism and difficulties of interface reactions with one-electron and multi-electron transfer pathway, and the key scientific issues of interface reaction. On this basis, the research work of our group in "Electrolyte design and interface reaction control of lithium metal batteries" is introduced, which mainly includes the following contents: (1) the mechanism of solid-liquid two-phase synergetic catalysis of positive electrode interface reaction is proposed, which promotes the efficiency of electron transfer and ion transport for interface reaction at positive electrode, and improves the stability of interface reaction; (2) the construction strategy of the advanced SEI layer on the lithium metal surface is developed, and the SEI layer with high lithium ion transport rate was obtained, which improved the stability of the interface reaction at negative electrode; (3) a new two-phase electrolyte system is constructed to inhibit the diffusion of functional components from the positive electrode to the negative electrode, and simultaneously improve the reaction stability of the positive and negative interface.

Keyword: Electrolyte, Interface, Battery, Electrochemical reaction

最终交流类型: Invited

Protection strategies of alkali metal anode for high performance alkali metal batteries

余彦
University of Science and Technology of China, China

Alkali metal batteries have been considered as the most promising energy storage systems because of their high theoretical capacity and high energy density. However, alkali metal anodes are faced with severe issues. However, the practical application of alkali metal anodes faces many challenges in terms of unstable SEI structure, dendrite growth and huge volume expansion during the plating and stripping process, which may cause the structure damage of electrode and poor electrochemical performance of alkali metal batteries. To address the above key problems, we have developed some effective strategies including: 1) designing three-dimensional conductive skeleton can reduce local current density and induce uniform deposition of alkali metal ions in the surface of alkali metal. For example, we design the Ni3S2/Ni3P heterostructure with high work function, which can reduce the Fermi level and effectively inhibit the continuous electrolyte decomposition after the long-term sodiation process. 2) constructing the artificial interface protective layer on the surface of alkali metal anode could not only improve the mechanical toughness and ion diffusion ability, but effectively reduce the nucleation overpotential of metal ions, thus realizing high performance alkaline metal batteries. For example, according to density functional theory calculation and ab initio molecular dynamics simulation, we predict that Na2Te shows lower Na+ diffusion barrier and higher diffusion coefficient, indicating that the Na2Te is beneficial to migration of Na+ and suppresses the Na dendrite growth more effectively. 3) modifying the electrolyte and separator can also induce uniform metal ions deposition process and suppress the dendrite growth. For example, we find that NaBr has the lowest diffusion barrier and the highest diffusion rate among various NaX (X= F, Cl, Br and I) based on the First principles computation, and is expected to be ideal SEI component to induce uniform Na deposition, thus inhibiting dendrite growth. Our research may provide scientific guidance to promote the commercial development and application of alkali metal batteries.

Keyword: Alkali metal batteries; Alkali metal anode; conductive skeleton; artificial interface layer;

最终交流类型: Oral

Two-dimensional nanomaterials composite membrane for energy storage device

胡静
浙江大学

Energy is an essential material basis for human survival and development. To cope with the energy demands of the ever-increasing global population, the storage and utilization of renewable energy have become extremely urgent. Zinc-based flow batteries (ZFBs) show very promising prospects in the field of stationary energy storage due to their high security and high energy density in recent years. However, the challenges from zinc dendrites and accumulation of ZFBs, considerably impede their wide application. In this regard, series composite membranes modified with two-dimensional nanomaterials with different functions were designed and fabricated, and in-depth research on the regulation mechanism of composite membrane on the zinc deposition morphology was carried out. Specifically, boron nitride inorganic nanoparticles (BNNSs) were successfully introduced on the surface of polymer to prepare BNNSs composite membrane. Its high thermal conductivity and excellent mechanical properties induced the uniform deposition of zinc, which greatly improved the stability of the ZFBs. [1] High-performance layered double hydroxides (LDHs) composite membrane by spary-coating the LDHs nanomaterials on the porous substrate to afford the ZFBs high energy efficiency. The hydroxide ions transport through LDHs via vehicular (standard diffusion) & Grotthuss (proton hopping) mechanisms is uncoverd, which offers an in-depth understanding of ions transport in LDHs and further inspires their applications in other energy-related devices. [2] Then the nano LDHs were in-situ growth on the substrate to enable a fast OH− transport and high areal capacity of zinc deposition. Owing to the high hydroxide ion conductivity and ion selectivity nature of LDH nanosheets, specifically, the precise control of directional ion transport in vertical arrangement LDHs, a superior battery performance can be realized. Moreover, the defect-free LDHs layer serves as a buffer layer to

enable a uniform Zn deposition, which effectively enhances the areal capacity of the battery.[3] Overall, Porous two-dimensional materials exhibit excellent permeability and selectivity, which opens a new way for the construction of efficient membrane materials for energy storage device.

Keyword: Two-dimensional nanomaterials, composite membrane, flow battery, ion transport mechanism

最终交流类型: Invited

Electronic Interface Catalysts for Energy Conversion

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Metal and semiconductor components were integrated together as efficient electrocatalysts. With respect to such a kind of heterojunction-based hybrids, metal particles and supports are not independent systems. Electrons will flow until the Fermi level on both sides of the metal-semiconductor interface is the same. This effectively creates a charged interface, with electrons or a negative space charge on the more noble side, while the less noble side is positively charged and depleted in electrons.

The influence of electronic interface is essentially a change of electron density at the catalytically active centers and thus enhanced catalytic activity for electrocatalysis, organic synthesis and artificial photosynthesis. On the one hand, the conventional aspect of interface engineering has focused on the nanostructures of binary metal-semiconductor systems for better dispersion of possible active sites and facilitating mass diffusion efficiencies. On the other hand, “interface engineering” of Schottky heterojunctions also leads to enhanced charge redistribution driven by the Schottky barrier, generating more pronounced electron-rich and electron-deficient regions on the two sides of the interface.

As the third aspect of an electronic interface catalyst composed of metal and semiconductor components, the interface indeed dominates their synergy between the two components for specific catalytic applications. A rectifying contact at the interface may generate new electron states and transitions, resulting in a dyadic system with novel/enhanced physicochemical properties not part of any of the components. As a result, the synthesis of an invisible interface holds the key to boosting the activity of Mott Schottky catalysts to surpass the original activity of the metal and/or semiconductor. The tunable electron density of the metal or semiconductor component affords us the ability to control the redox power of the metal-semiconductor dyad and also extend the functionality of these charged spaces as Lewis acid-base pairs or a built-in electric field for selective fixation and/or activation of certain reactants.

Keyword: heterojunction, electronic interface, catalysis

最终交流类型: Invited

Nanowire Energy Storge Materials and Devices

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One-dimensional nanomaterials can offer large surface area, facile strain relaxation upon cycling and efficient electron transport pathway to achieve high electrochemical performance. Hence, nanowires have attracted increasing interest in energy related fields. We designed the single nanowire electrochemical device for in situ probing the direct relationship between electrical transport, structure, and electrochemical properties of the single nanowire electrode to understand intrinsic reason of capacity fading. The results show that during the electrochemical reaction, conductivity of the nanowire electrode decreased, which limits the cycle life of the devices. We have developed a novel assembled nanoarchitecture was also presented, which consists of V2O3 nanoparticles embedded in amorphous carbon nanotubes that are then coassembled within a reduced graphene oxide network. The naturally integrated advantages of each subunit exhibit highly stable and ultrafast sodium-ion storage. In addition, we demonstrated a 3D nitrogen-doped graphene/titanium nitride nanowire (3DNG/TiN) composite as a freestanding electrode for Li–S batteries. The highly porous conductive graphene network provides efficient pathways for both electrons and ions and TiN nanowires attached on the graphene sheets have a strong chemical anchor effect on the polysulfides. As a result, the 3DNG/TiN cathode exhibits an initial capacity of 1510 mAh g−1 and the capacity remains at 1267 mAh g−1 after 100 cycles at 0.5 C. A commercial polypropylene (PP) separator decorated with TiO2 nanosheets with oxygen acancies (OVs-TiO2@PP) is fabricated to enhance the fast lithium-ion penetration and the high energy density of the whole cell. We also develop a bilayer-structured vanadium oxide (Mg0.3V2O5·1.1H2O) with synergistic effect of Mg2+ ions and lattice water as the cathode material for magnesium-ion batteries (MIBs). The pre-intercalated Mg2+ ions provide high electronic conductivity and

excellent structural stability and the lattice water enables fast Mg2+ ions mobility because of its charge shielding effect. As a result, the Mg0.3V2O5·1.1H2O exhibits excellent rate performance and an unprecedented cycling life with capacity retention of 80.0% after 10,000 cycles. Moreover, a K+/vacancy disordered P3-type structure is designed and synthesized by simply modulating the K+ contents in Mn/Ni-based layered oxides. The K+/vacancy disordered K0.7Mn0.7Ni0.3O2 exhibits much better rate performance and higher discharge capacity. Our work presented here can inspire new thought in constructing novel one-dimensional structures and accelerate the development of energy storage applications.

Keyword: One-dimensional nanomaterials; nanowire; energy storge

最终交流类型: Invited

Exploration of multi-site synergistic rare earth catalysts for energy applications

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The state of the catalytic active centers directly determines the activity, selectivity and stability of catalytic materials. In recent years, a new type of catalytic material structure: dual active sites with different functions coupled in the same structural element, i.e., dual-site catalytic materials, has been attracting attention because of their superior performance that is significantly different from traditional single-site catalytic materials. Dual sites can be composed of different elements or different fugitive states of the same element. By synergizing with each other, they can effectively improve the electronic state on the surface of catalytic materials, improve the adsorption of substrate molecules, migration of reactive intermediates or desorption of product molecules, and promote the positive reaction. We have pioneered a series of efficient synthesis techniques and prepared a variety of new nanocatalytic materials with two-site synergy, which have been successfully applied in catalytic reactions such as triple-action catalysis, CO2 selective reduction, and liquid-phase selective hydrogenation.

For example, we discover a unique “two-way synergistic effect” between Fe and Pt atoms anchored on CeO2 support, which can significantly boost the RWGS reaction efficiency. The Fe atoms play a crucial role of surface-state regulator in decreasing the electron density of Pt atoms, contributing to the increased CO generation rate. More importantly, the excess active hydrogen species generated over Pt atoms can activate the inert Fe atoms, making them as active sites for intermediate transformation. The obtained Fe-Pt/CeO2 dual-site single atom catalyst shows a high turnover frequency of 65,131 h-1 based on Pt atoms which is superior to most of the currently-reported noble metal-based catalysts. We believe that this study can represent one of the major breakthroughs in RWGS reaction, opening up the possibilities for industrial production of syngas from CO2. Our strategy of creating dual sites and utilizing “two-way synergistic effect” towards the performance enhancement also paves a new way for catalyst upgrading in a wide range of applications.

Keyword: Rare earth catalysts

最终交流类型: Invited

Design, regulation and application of spinel-based electrocatalysts

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With the continuous advancement of social progress, the human demand for energy has increased dramatically, however, because the excessive consumption of energy has sounded the alarm for mankind, the sustainable development has caused widespread concern. The energy conversion technology based on electrocatalysis conforms to the national green development strategy of "carbon neutrality" and its conversion efficiency is directly related to the selection and design of electrocatalysts. Benefiting from the stable structure and adjustable active sites, spinel oxides (AB2O4) are desirable multifunctional electrocatalysts for the substitution of the traditional precious metal (Pt-, Ru-, and Ir-based) materials. However, due to the low conductivity, small specific surface area, and strong binding energy with oxygen, the intrinsic electrocatalytic activity of current spinel oxides is very low-efficient and dissatisfactory for the large-scale applications. In response to the key challenges mentioned above, we have carried out a series of related work, which mainly includes the following three aspects: (1) Construction of carbon-based spinel composite materials. A novel idea of coupling spinel oxide from "commercial carbon nano tubes (CNTS)" to "heteroatom modified CNTS" to " autocatalytic CNTS" has been proposed. (2) Site modulation of spinel oxides. A series of new strategies for the regulation of spinel sites (A, B, O) are explored by using Co3O4 as an original model. (3) Interface - vacancy engineering of spinel oxides. The new mechanisms for optimizing catalytic performance through various interfaces and vacancies have been revealed. Finally, the above highly efficient electrocatalytic materials are applied to the fields of energy conversion, such as zinc-air batteries and hydrogen production from water electrolysis, and exhibit exceptional feasibility of industrialization energy conversion. Our findings provide new ideas for the design and synthesis of highly active spinel-based electrocatalysts for electrocatalytic energy conversion technologies, and supplies theoretical support for the development of sustainable electrocatalytic energy conversion technologies.

Keyword: Spinel; Electrocatalysis; Zinc-Air battery; Hydrogen production from water electrolysis

最终交流类型: Invited

Piezo-phototronic effect and Flexible Micro LED

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Group III nitrides (GaN, InN, AlN and their alloys) are the third-generation semiconductor materials, which have important applications in many fields, such as lighting, display, power electronic devices and so on. Especially, GaN Micro LED is a highly anticipated next-generation display technology. The crystal structure of group III nitrides is lack of the central inversion symmetry, and then they have strong spontaneous polarization/piezoelectric polarization characteristics. The piezotronic effect proposed by Prof. Z.L.Wang in 2006 points out that the piezoelectric polarization electric field can effectively modulate the band structure of the device, which affects the key physical processes such as quantum transition, recombination and carrier transport, thus restricting the performance of electronic and optoelectronic devices. With the rapid development of human-computer interaction technology and wearable electronic devices in recent years, piezoelectric polarization effect provides a new way to realize effective, flexible and seamless interaction between micro nano electronic/optoelectronic devices and external mechanical strain, which has potential application value in intelligent sensing, environmental monitoring, Internet of things, human-computer interaction and other fields.

We have developed the theory of force-electric-light-thermal multi-fields coupling in GaN LEDs and proposed an external stress compensation technology, which compensates the light intensity of Micro LEDs from 67.8% to 104% at high temperatures, and enhances the competitive suppression of non-radiative recombination by 47.6% for heat accumulation [1]. And then, we developed a Micro LED massive preparation transfer technology to fabricate a massive (200 × 200), high-precision (deviation less than 0.5 micrometers), semi-floating Micro LED arrays [2]. Finally, we fabricated the micro-LED display with super flexibility and high biological affinity, such as hydrogel contact lens display and fabric wearable display. These new display technologies are expected to achieve a deeper, seamless, and secure integration between machine vision and humans themselves, promoting the deep integration of information carriers such as humans and the environment, machines, and virtual AI.

Keyword: Piezo-phototronic effect, Micro LED, GaN, hydrogen, display

最终交流类型: Invited

Controllable liquid transfer for making high-performance thin-film devices

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In recent years, with the in-depth development of the precision thin-film devices in various types, higher requirements have been put forward for the quality of micro-patterned thin-films. Usually, the solution approaches of fabricating thin-films are preferred choice in view of the cost of preparation and the simplicity of the process. Controlled liquid transfer, especially that at micro-/nanoscale, is an important process for fabricating micro-patterned thin-films, which directly affects the uniformity, ordering, and physicochemical properties of the as-prepared micro-patterned thin-films. And it is a key process from functional liquids to thin-film devices, therefore have been widely used in making high-performance thin-film devices. Here, we proposed that the fibrous system can be used to manipulate liquid in a well-controllable manner. By in-depth research on the interfacial physicochemical phenomenon, we clarified that the dynamic balance of liquid under multiple driving forces imparted by the unique structures of fibers is the key for realizing the controllable liquid transfer. Both the conical structure, the fibrous elasticity, and the topology of the fiber array are key parameters. Taking advantageous of the fibrous system, we developed a facile strategy of controllable liquid transfer that enables controllable transport of various functional liquids (1D nanowires/polymers, 0D nanoparticles, etc.) at the micro-/nano scales, by which various micro-patterns have been prepared by direct writing with a width resolution up to ~ 1 μm. We also demonstrated various its applications in making high quality functional thin films. Specifically, the oriented and ultra-smooth micro-patterned thin-films have been fabricated using the 1D nanowires/polymers and 0D nanoparticles as inks, respectively. Consequently, various high performances thin-film devices have been developed, including organic thin film transistor (OTFT), transparent flexible electrode, flexible mechanical sensor and quantum dot light emitting diode (QLED). We envision that the result offers a low-cost, facile, and practically applicable solution-processing approach for fabricating high-performance thin-films devices.

Keyword: liquid transfer; conical fibers; micro-patterns; thin-film devices

最终交流类型: Oral

Ultrathin self-standing COF membrane boost the electrochemical performance of nanofluidic osmotic energy generator

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Energy crisis and environmental pollution urgently call for the acquisition of abundant and clean energy. The huge osmotic energy is considered to be completely green and pollution-free, and it can be easily obtained from the salinity gradient energy conversion between seawater and freshwater. Nanofluidics is promising in the construction of highly-efficient osmotic energy generator, but it is still a challenge to develop large-scale and high-performance nanofluidic membranes. Reverse electrodialysis (RED) is currently the most promising technology for harvesting osmotic energy, which highly depends on permselective membranes. However, commercial permselective membranes usually face problems of high membrane impedance and poor ion selectivity, thus leading unsatisfied osmotic energy conversion efficiency. Therefore, developing high-performance permselective membranes with low impedance and high ion selectivity is of great significance for boosting osmotic energy harvesting. The emerging nanofluidic technology provides a good platform for constructing high performance permselective membranes with both high ion selectivity and high permeability, which is of great significance to high-efficient osmotic energy harvesting. The emerging covalent organic frameworks (COFs) provide a desirable platform to create

nanofluidic membranes with high ion selectivity and permeability towards effective osmotic energy conversion. Herein, an ultrathin self-standing COF nanofluidic membranes based on terephthalaldehyde-tetrakis(4-aminophenyl)methane is developed to construct high-efficiency nanofluidic osmotic energy generator. Benefiting from the nano-confined channels (1.4 nm) and negative surface charges, the COF based nanofluidic membrane demonstrates both excellent cation selectivity and high ion conductance. Moreover, an ultrathin thickness of ~1.5 μm significantly reduces the membrane resistance. Consequently, the nanofluidic osmotic energy generator based on COF membrane could deliver a high output power of 5.31 W m−2 under a 50-fold salinity gradient simulating natural river/sea junction, which is superior to most reported systems and reaches the industrial level. More importantly, such a COF nanofluidic membrane exhibits excellent stability in response to various environmental factors, including wide saline solution concentration, temperature and pH ranges. This work is anticipated to highlight the great potential of 1D COF nanofluidic membranes towards highly-efficient osmotic energy generators.

Keyword: COF membranes, one-dimensional nanochannels, ion selectivity, osmotic energy harvesting

最终交流类型: Oral

Engineering High-Performing Thermoelectric Materials for A Sustainable Future

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Roughly 50% of primary energy worldwide is rejected as waste heat over a wide range of temperatures. Techno-economic analysis shows that thermoelectrics (TE) can cost-effectively convert waste heat and compete with other zero carbon and waste heat conversion technologies. However, commercial deployment of TE is still eluding due to many challenges such as efficiency, manufacturing scalability, reliability, and chemical stability.

On the one hand, organic-inorganic hybrids have recently emerged as a class of high-performing thermoelectric materials that are lightweight and mechanically flexible. However, the fundamental electrical and thermal transport in these materials has remained elusive due to the heterogeneity of bulk, polycrystalline, thin films reported thus far. In this work, we systematically investigate a model hybrid comprising a single core/shell nanowire of Te-

PEDOT:PSS. We show that as the nanowire diameter is reduced, the electrical conductivity increases and the thermal conductivity decreases, while the Seebeck coefficient remains nearly constant—this collectively results in a figure of merit, ZT, of 0.54 at 400 K.1 The origin of the decoupling of charge and heat transport lies in the fact that electrical transport occurs through the organic shell, while thermal transport is driven by the inorganic core. This study establishes design principles for high-performing thermoelectrics that leverage the unique interactions occurring at the interfaces of hybrid nanowires.

On the other hand, waste heat above 573 K has the highest Carnot potential (>50%) to be converted to electricity due to higher Carnot efficiency. Among different high-temperature thermoelectrics materials, silicon nanowires possess the combined attributes of cost effectiveness and mature manufacturing infrastructures. Despite significant breakthroughs in silicon nanowires based thermoelectrics for waste heat conversion, the ZT or operating temperature has remained low. Here, we report the synthesis of large-area, wafer-scale arrays of porous silicon nanowires with ultra-thin Si crystallite size of ~4 nm.2 Concurrent measurements of thermal conductivity (κ), electrical conductivity (σ), and Seebeck coefficient (S) on the same nanowire show a ZT of 0.71 at 700 K, which is more than ~18 times higher than bulk Si. This ZT value is more than two times higher than any nanostructured Si-based thermoelectrics reported in the literature at 700 K. Experimental data and theoretical modeling demonstrate that this work has the potential to achieve a ZT of ~1 at 1000 K.

Keyword: thermoelectric, porous nanostructure, hybrid material, organic-inorganic structure, waste heat recovery

最终交流类型: Oral

Controlling the Crystallization Kinetics of Lead-Free Tin Halide Perovskites for High Performance Green Photovoltaics

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Tin halide perovskites are promising candidates for lead-free perovskite solar cells (PSCs) not only due to their low-toxicity, but also due to their ideal energy bandgap, high charge carrier mobility, and long hot carrier lifetime. The certified efficiency of tin halide

PSCs has now reached over 10%, but this is still far from the theoretical expectation. Much of the efficiency gap relates to the poor quality of tin halide perovskite films due to the lack of in-depth understanding about the crystal nucleation and growth mechanisms for such films. This recognition motivates the present review, which is focused on the crystallization kinetics of tin halide perovskites. In particular, starting from a germane discussion on crystal nucleation and growth theories, several methods that have been used for controlling the rapid crystallization of tin halide perovskites are dissected. Finally, the current challenges and prospects for tin halide PSCs are presented. This comprehensive review summarizes and illuminates the parameter space for the optimization of tin halide perovskite film quality, promoting the future development of ecofriendly PSCs with high efficiency and high stability.

Tin halide perovskites are rising as promising materials for lead-free perovskite solar cells (PSCs). However, the crystallization rate of tin halide perovskites is much faster than the lead-based analogs, leading to more rampant trap states and lower efficiency. Here, we disclose a key finding to modulate the crystallization kinetics of FASnI3 through a non-classical nucleation mechanism based on pre-nucleation clusters (PNCs). By introducing piperazine dihydriodide to tune the colloidal chemistry of the FASnI3 perovskite precursor solution, stable clusters could be readily formed in the solution before nucleation. These pre-nucleation clusters act as intermediate phase and thus can reduce the energy barrier for the perovskite nucleation, resulting in a high-quality perovskite film with lower defect density. This PNCs-based method has led to a conspicuous photovoltaic performance improvement for FASnI3-based PSCs, delivering an impressive efficiency of 11.39 % plus improved stability.

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Keyword: Lead-Free Tin Halide Perovskites, Solar cells

最终交流类型: Invited

Surface-interface structure-activity relationship research for new photoelectric devices

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Organic-inorganic hybrid perovskites as promising light harvesting materials have been the focus of scientific research and development of photovoltaics recently. Especially, metal halide perovskites currently become one of the most competitive candidates for the fabrication of solar cells with record certified efficiency over 25.8% . Despite the high efficiency, many fundamental questions remain unclear and need to be addressed at both the material and device levels, such as weaker stability, poorer reproducibility, easier degradation influenced by water, oxygen, thermal, etc. Base on recently reports, interfacial engineering plays a crucial role in controlling the behaviour of the charge carriers and in growing high quality, defect-free perovskite crystals, therefore helping to enhance device performance and operational stability. However, little attention has been paid to the interface interaction mechanism among carrier transport layers and perovskite active layer. It is extremely urgent to explore the perovskite interfaces in details and to find out how its interfaces structure relative to the efficiency and hysteresis in perovskites solar cells. Based on Shanghai Synchrotron Radiation Facility (SSRF), we have established an advanced perovskite photovoltaic device preparation and in-line test system, developed a series of unique surface diffraction analysis methods based on ex- and in-situ grazing incidence wide-angle X-ray scattering (GIWAXS), and reported many novel synchrotron radiation results on crystallization of the perovskite photovoltaics films. Our main investigations are aim to deeply in-situ study the perovskite films growth dynamics using synchrotron radiation GIXRD technology in combine with a customized mini online glove box (c(H2O, O2)<1ppm) and a temperature-humidity control equipment, etc., which should provide solid theoretical background and point to the useful direction for designing and fabricating high-performance perovskites solar cells. Moreover, a multifunctional joint characterization technology that in-situ GIWAXS simultaneously combines with conventional characterization methods at synchrotron radiation beamline station must be put on the agenda in future research, which greatly promotes much more comprehensive and intuitive understanding of the nucleation, micro-crystallization and degradation mechanisms of perovskite heterojunction films, and therefore further optimizing their chemical synthesis strategies at molecular level for functional materials.

Keyword: GIWAXS; in-situ; Solution spin-coating; Perovskite optoelectronic

最终交流类型:

High Performance Organic Hole Transporting Materials for Inverted Perovskite Solar Cells

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Perovskite solar cells (PVSCs) have made an exceptionally rapid progress in the past decade with the power conversion efficiency (PCE) exceeding 25% already. Like most organic optoelectronic devices, it is necessary to introduce carrier transport layers between the perovskite active layer and the electrodes when fabricating PVSCs, with a purpose of improving the carrier extraction and transport efficiency. In inverted devices, the hole transport layer (HTL) is located below the perovskite layer, so it not only affects the hole extraction and transport at the interface, but also affects the growth and crystallization of the upper perovskites, making the design of the hole transporting materials (HTMs) more challenging. Moreover, the sunlight will first pass through the HTL and then reach the perovskite layer, so that the HTM molecules should be continuously at the photo-excited state during device operation, however its influence on the device interface has been ignored so far. On the other hand, most of commonly-used HTMs for inverted PVSCs such as polytriphenylamine (PTAA) still suffer from high synthetic cost, harmful solvent processing and unwanted chemical doping process, and so on. Aiming at solving the above issues, our group has focused on new molecular design strategies of small molecule and polymer HTMs toward high performance inverted PVSCs. For example, we recently developed a simple but efficient design strategy to modify the PTAA structure by introducing pyridine units into the polyarylamine backbone, which can effectively optimize the bottom interface leading to highly crystalline perovskite films with uniform back contact and reduced defect density. Finally, the resulting inverted PVSCs realized remarkable efficiencies of 24.89% (certified value: 24.50%) for small-area (0.08 cm2) as well as 23.12% for large-area (1 cm2) devices. We also developed a unique star-shaped D-A-D structure for designing green-solvent

processable dopant-free HTMs, affording an impressive PCE of 24.34%. Here, we would like share our encouraging progress.

Keyword: Hole-transporting materials, Inverted perovskite solar cells, Bottom interface engineering, Defect passivation

最终交流类型: Oral

Differentiated Ionic Electroresponse of Asymmetric Bio-hydrogels with an Unremitting Power Output

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The bioelectric signal is fundamental and significant to biological activity and evolution, emerging from multiple levels, the cell survival and propagation,[1–4] signal transmission in the nerve,[5–7] as well as the predation of animals,[8,9] for instance. For most bioelectric signals demonstrated so far, the external stimuli trigger the bio-voltage or current spikes, responding to the surroundings or transferring the information to the next acceptor.[10] The cytomembrane in living cells, typically, is excited by the ions and/or osmotic pressure on account of a number of channel proteins.[11–14] These channel proteins discern and regulate the ions through the cytomembrane-driven transcellular potential, accomplishing a dynamic ionic selectivity (Figure 1ai). Particularly, the water channel protein called aquaporin (AQP) and electrogenic Na^+-K^+ pump (Figure 1aii), recognize and direct respective water molecules and inorganic ions with controlled spatial and flux concentrations, essential for many cell functions.[15] Similarly in biology, the electric eels perfectly deploy the above features in their evolution, in which the arrangement of thousands of ion gradients enables electric discharges of 100 W for incapacitating prey.[16]

Hence, artificially engineered systems that can mimic some of these biological features are not only theoretically fascinating but also promises exciting opportunities for creating new type of material systems and autonomous devices. Inspired by the electric eels, artificial soft power sources mimicking the anatomy of electric eels had been demonstrated using the K^+ and Na^+ hydrogels, generating potential in excess of 100 V for several hours.[9] Another of such artificial system representation, analogously, mimics the proton movement across the membrane is the moist-electric generator (MEG),[16–19] where the released protons induced by adsorbed water molecules exemplify yet a variant of contemporary soft power sources.

However, this otherwise promising MEG discontinuously delivers electric output as the process of water adsorption attains an equilibrium state, presenting its shortcomings of sporadic power generation. Besides, some MEGs face materials integrity issues such as polymer dissolution under high moisture imbibement scenario while others are constrained in operating conditions and structural architecture. Moreover, both dynamic and passive behaviours, mirroring biological behaviour with potential in biomedical application,[20] are hardly integrated into these generators. To take the nature-inspired soft devices to the next level, hybrid dynamic ionic electroresponse and passive unremitting power output should be devised holistically, capitalizing on the materials principle of upcycling biowaste for the circular economy. In addition, the current trends in designing power sources mainly by embedding ever more external energy input and routinely introducing complex non-renewable multi-material constructs, have in fact reduced the opportunities for green, spontaneous, differentiated integration seen in the organism. To our knowledge, little headway to date has been made in the autonomous and synchronous manipulation of biomimetic device that entails both the dynamic and passive wealth of behaviours similar to the cytomembrane in media and signal transportation spatiotemporally. The tunable positive and/or negative voltage response may achieve selective neural excitation or inhibition, unequivocally advantageous to biomedical application.[20]

Herein we demonstrate a minimalist concept of self-propagative flow approach in designing an asymmetric hydrogel, capable of orchestrating dynamically differentiated ionic electroresponse to passively output continuous energy (Figure 1 aiii). Not rigid in conformation, the diffusive nature of the colloid is particularly befitting in providing a versatile and subtle approach to forming ion-selective graded structures. The fluidic nature, structurally dynamic and regulable cation and anion constituents lead to the formation of pervasive p and n analogues within the polymeric networks in conjunction with the adaptability to any conformal geometry (Figure 1b). This work highlights the upcycling of biomass into functional bionic hydrogels that (1) readily render free-form manufacturing via self-propagating colloid diffusion and coacervation reaction; (2) execute reverse and differentiated ionic electroresponse between the cathode and anode; (3) manifest high stability in ambient and salt media and (4) elicit sustainable excitation voltage, in which the power output (135-190 mW m^{-2}) is greater than most soft and green power sources reported previously.

Keyword: ionic selectivity, electroresponse, bio-hydrogel, water, salt media

最终交流类型:

Interface engineering of solid-state Li metal batteries

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Solid state Li metal batteries using solid-state electrolytes (SSEs) offer enhanced safety over conventional Li-ion batteries with organic liquid electrolytes due to the nonflammable nature of SSEs. The superior mechanical strength of SSEs can also protect against Li dendrite penetration, which enables the use of the highest specific capacity (3861 mAh/g) and lowest redox potential (−3.04 V vs standard hydrogen electrode) anode: Li metal. However, contact between the Li metal and SSEs presents a major challenge, where a large polarization occurs at the Li metal/SSE interface. Here, we present a composite strategy for solving this problem. To date, we discovered that two-dimensional materials, such as graphite can be a functional additive to composite Li metal. Moreover, nanosized BN, C3N4, can also be added into Li metal. As a result, the interface contact and interfacial resistance between Li-based composites and garnet dramatically decreased due to the significantly decreased surface tension. Moreover, a writable Li metal ink (LMI) prepared by introducing carbon particles into molten Li has also been demonstrated. LMI is able to directly write on copper foils or other substrates that ultrathin Li foils with a remarkably small thickness (<10 μm) can be achieved. The versatility of LMI is further demonstrated in directly writing LMI on the garnet, which offers a perfect contact and enables an extremely low interfacial resistance of 6 Ω cm2, in sharp contrast to 939 Ω cm2 between the pure Li and the garnet. Most recently, we have addressed these challenges by using a functional gradient Li anode (FGLA), which is formed through a self-regulated reaction between molten Li and AlF3. A composition gradient of Li–LiAl–LiF is spontaneously formed from the reaction of molten Li with AlF3 due to the large difference in interfacial energy between Li/LiAl and Li/LiF, where the LiAl reduces the interface resistance and LiF suppresses Li dendrites. The FGLA not only dramatically reduces the resistance at the FGLA/Li6.5La3Zr1.5Ta0.5O12 (LLZTO) garnet SSE interface to ~ 1 Ω cm−2, but also largely increases the critical current density (CCD) to over 3.0 mA cm−2 at room temperature.

Keyword: solid state, interface, garnet

最终交流类型:

High Mobility Conjugated Polymers: Design, Synthesis and Structure-Properties Correlation

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Tianjin University, China

High mobility conjugated polymers (CPs) have found various applications in printable electronics. The development of CPs with high mobility, good solubility, and ease of synthesis relies on the development of new building blocks, new synthetic protocols as well as the understanding of structure-properties correlation. In the current report, I will introduce the recent progress in our group on direct arylation polycondensation (DArP) to high mobility CPs and structure modulation of high mobility CPs for high performance electronic devices.

Currently, most of high mobility CPs are synthesized via transition-metal-mediated cross-couplings such as Stille polycondensation. These protocols are characterized by low atom-economy and may produce toxic byproducts. DArP is an emerging method to synthesize CPs, but is suffered from low reactivity and selectivity of C-H bonds. To address these problems, we developed multi-halogenated thiophene derivatives as highly reactive C-H monomers for C-Br/C-H DArP, and a series of high mobility CPs have been developed. We also found that the structures of both C-Br and C-H monomers had influences on DArP results. In view of the atom economy and straightforwardness, C-H/C-H oxidative DArP (Oxi-DArP) would be the most ideal approach to synthesize CPs. Via the rational design of monomer, we also successfully synthesized a diketopyrrolopyrrole (DPP)-based n-type CP via Oxi-DArP.

Charge carrier mobility of CPs in organic thin-film transistors (OTFTs) are influenced by many factors. Two classes of high mobility CPs based on DPP and isoindigo were selected to study the effect of side chains and molecular weights, respectively, on the performance of OTFTs fabricated via bar-coating. We found that the preaggregation structures of the polymers in solution are key parameters to determine their film microstructures and morphology. The highly aligned and ordered films could be prepared via bar-coating when the polymers formed one dimensional rod-like aggregates with aspect ratio of ca. 20. Consequently, high mobility n- and p-type OTFTs with electron and hole mobilities up to 4.10 and 13.8 cm2 V-1 s-1, respectively, were successfully fabricated.

Keyword: Conjugated polymers, Direct arylation polycondensation, Charge carrier mobility, Organic thin-film transistors, Structure-property correlation

最终交流类型:

Automatic Roll-to-Roll Experiments and Fully Roll-to-Roll Fabricated Perovskite PV Modules

Doojin Vak
CSIRO

Organic-inorganic hybrid perovskite photovoltaics (PePV) are a promising next-generation solar technology with a rapidly increasing record power conversion efficiency (PCE). One of the main advantages of PePV is its ability to be solution processed, making it suitable for cost-effective industrial roll-to-roll (R2R) manufacturing processes. However, most advancements in PePV technology have been made through spin coating, a laboratory-based process that cannot be easily transferred to R2R processes. Therefore, only a small fraction of the processes developed through spin coating can be applied to R2R fabrication, requiring additional optimization for large-scale PePV production using R2R techniques. Recognizing this challenge, the Commonwealth Scientific and Industrial Research Organisation (CSIRO) has been working on developing R2R fabrication methods since the first demonstration of slot die coated PePV in 20151 and the first R2R fabrication of PePV in 2017.2

Despite the development of various fabrication techniques and improvements in PCE, many reports claiming to be fully R2R processed still rely on costly vacuum deposition methods for metallic back-electrode deposition. However, integrating vacuum deposition into a conventional printing line is not economically viable. As a result, the development of R2R-printable back electrodes has been recognized as a significant obstacle in achieving low-cost R2R manufacturing of large-scale PePV panels. To address this challenge, an approach has been developed to successfully demonstrate fully R2R-fabricated PePV cells, eliminating the need for vacuum deposition. Fully R2R-processed cells utilizing carbon electrodes have achieved an impressive PCE of over 15%. This process has been translated to industrial R2R printers, enabling PCEs exceeding 10% on 10 cm × 10 cm R2R-printed flexible modules.

This breakthrough has created new possibilities for automated experiments and optimization of printing parameters. Consequently, an automatic R2R fabrication and testing platform has been developed, enabling the fabrication of thousands of research cells per day, surpassing the previous typical production scale of tens of cells. The process parameters and device performance have been digitized, allowing for utilization with artificial intelligence

(AI) and machine learning (ML) techniques. This lecture will provide an overview of how these digital technologies can contribute to PV research, thereby revolutionizing the field.

Keyword: roll-to-roll, printed solar, printed PV, machine learning, lab automation

最终交流类型:

Tethered small molecular acceptors for stable polymer solar cells

张志国
Beijing University of Chemical Technology, China

During the last five years, polymer solar cells (PSCs) have witnessed a significant progress with an extensive investigations on donor-acceptor (D-A) type small molecular acceptors (SMA), enabling a significant leap forward to achieve over 18% power conversion efficiency (PCE). For the high-performance PSCs, active layers with nanoscale bicontinuous-interpenetrating network of polymer donors and SMAs are required to facilitate exciton dissociation and charge carrier transport. However, such deliberately tuned morphologies are usually in a state of thermodynamic instability, thus they are with an obvious tendency of burn-in degradation during long-term operations or at elevated temperatures. The degradation is due to the inevitable thermodynamic relaxation of the mixed domains in the blend from their initially trapped state to the binodal. On the other hand, the classical record-holding A-DA'D-A type SMAs have the disadvantages of excessive crystallinity and relatively high miscibility with polymer donors that could lead diffusion-induced deterioration of the morphology. Thus, how to balance the efficiency and stability, is still the current main focus on molecular engineering on SMAs for reaching the commercialization.

Recently, dimerization of SMAs emerges as a promising strategy to address the challenge. Here, flexible spacer tethered Y6-based SMAs were designed, and their photophysical properties was further regulated via the aromatic-core engineering. It shows that the tethered dimers processe a higher glass transition temperature, better crystallinity relative to its individual segment of Y6, and a larger Flory-Huggins interaction parameter with the polymer donor. As a result, tethered dimers delivered an efficiency over 18.0 %, which is much better than that of the Y6 based control device. Most importantly, the tethered dimers based PSC retained more than 80% of the initial PCE under long-term annealing at 80℃ for 1000 hours or at the maximum power point under continuous illumination for 700 hours. Our result suggests the tethered SMAs can achieve a high efficiency comparable to that of the state-of-the-art SMAs, while showing more advantages of operating stability.

Keyword: Tethered small molecule acceptor, molecular engineering, long-term stability, high efficiency

最终交流类型: Invited

Circularly Polarized Luminescence Switching driven by Precisely Tuned Supramolecular Interactions

田文晶
吉林大学

Circularly polarized luminescence (CPL) switching has attracted tremendous attention due to its potential applications in many fields, such as chiral sensing, information storage, and asymmetric catalysis. However, it remains highly challenging to achieve CPL switching based on precisely tuned supramolecular interactions and unveiling the mechanism of supramolecular chirality inversion. Herein, we demonstrated CPL switching based on two amphiphilic molecules, diethyl L-glutamate-9-Cyanophenanthrene (LGCP) and diethyl L-glutamate-Pyrene (LGP) via the precise regulation of supramolecular interactions. The LGCP assembly driven by hydrogen bonding showed r-CPL, while the LGP assembly driven by π-π interaction led to l-CPL. Remarkably, significant CPL switching was observed from the assemblies of LGCP/octafluoronaphthalene (OFN), while the assemblies of LGP/OFN exhibited minimum CPL variation. The successful CPL switching was attributed to the drastically strengthened molecular interactions, which altered the dominating interaction from weak hydrogen bonding to rather strong π-π interaction via the incorporation of arene-perfluoroarene (AP) interaction in LGCP/OFN system. Meanwhile, the dominating π-π interaction within the assembly of LGP/OFN illustrated quite limited variations upon AP interaction. This work provides a feasible strategy toward the efficient modulation of the chiroptical properties of multiple component supramolecular systems, meanwhile offering possibilities into the mechanism exploration of the chirality inversion of supramolecular assemblies.

Keyword: Circularly polarized luminescence switching, supramolecular interactions, chiroptical properties, mechanism exploration

最终交流类型: Invited

Refined Mesoporous Nanoarchitectures: Synthesis, Assembly and Application

振安 乔
Jilin University， China

Porous carbon spheres derived from polymer colloids with regular geometry, monodispersed morphology, well-controlled contents and structures play important roles in many areas of application, such as energy storage/conversion, gas adsorption/separation, catalysis, and chemo-photothermal therapy. Suitable polymerization reaction and synthetic strategy are both critical for the obtainment of stable polymer colloids as carbon precursors. Basic polymerization reactions are the cornerstones of synthetic strategies, which directly provides the direct molecular-based design of functionalized polymer/carbon spheres. Thus, this report mainly focuses on the summary of suitable polymerization reactions for colloidal polymer derived porous carbon spheres. Recent advances in the synthetic strategies and applications are also discussed, including their corresponding polymerization reactions.

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Keyword: Mesoporous materials; carbon nanomaterials; Porous carbon

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最终交流类型: Oral

Semitransparent organic solar cells constructed by ITO-free microcavity with homogeneous transmittance and colorful reflection

肖林格
National Center for Nanoscience and Technology

Semitransparent organic solar cells (ST-OSCs) exhibit promising application in building-integrated photovoltaics (BIPVs) such as smart-windows or domestic decoration which provides an excellent market opportunity to compete with silicon-based photovoltaics [1-2]. For example, the smart-windows with versatile or neutral chrominance are not only capable to harvesting incident light for electricity generation but also catering for the aesthetic and artistic value of the public, which are supposed to be building blocks for power-generation houses and domestic decorations [3-6]. Currently, ST-OSCs with neutral transmittance or versatile transmittance features with higher color purities have attracted tremendous attentions. Considering the neutral transmittance implementations, the transmittance CIE-1931 color coordinate is supposed to be as close as possible to the neutral color point (0.33,0.33) with an average visible transmittance (AVT) over 20% at the same time to satisfy the neutral color image of the original object [7,8]. While with respect to the colorful transmittance, the employment of general optical coupling methods such as one-dimensional photonic crystals [9-12] and microcavity-embedded top transparent electrodes [13-17] pursue the realization of monochromaticity of the transmittance spectrum for higher transmission color purity. However, plenty of the present researches only concentrate on the device transmission modulation while abandoning the reflection feature of ST-OSCs which can also be assigned to the practical value. On this basis, we simultaneously consider the transmittance and reflection behaviors of ST-OSCs as illustrated in Figure 1 and employ the ITO-free optical microcavity (MC) architectures, of which the transmittance and reflection properties can be modulated by adjusting the thicknesses of active layers, top and bottom electrodes and the anti-reflection layers. We discover that the transmittance chrominance of the ST-MC devices with different thicknesses possess little fluctuation and approach to the intrinsic transmission chrominance of the active layer materials, while the reflection color of the individual cell was obviously different. To conveniently and quantitatively describe the transmittance and reflection properties of ST-OSCs arranged together (here named as array), we firstly propose six parameters based on the AVT and CIE-1931 color coordinates. When comparing with ITO array, ST-MC array suggests more colorful reflection appearance and more homogeneous transmittance chrominance with slight deprivation of AVT and color neutrality. Further investigation of optical field modulations via electrode thicknesses demonstrates that suitable optical field coherent sharpness (OFCS) and thicker top electrodes facilitate better reflection performances while superfluous OFCS with excessively thick top and bottom electrode thicknesses cause more severe field contraction to the resonant wavelength which sacrifice both of AVT values and transmittance homogeneities as well as the electric performances of the subunits. To widely cover the reflection color gamut for the active layer materials with various of absorption features, optical simulations reveal that the reflection chrominance of the subunits can be regulated from red, orange, yellow to green and blue when adjusting the thicknesses of active layer and enlarging the anti-reflection coating thickness. This contribution provides a novel perspective for ST-OSC constructions and evaluations.

Keyword: Semitransparent organic photovoltaics, microcavity, building-integrated photovoltaics, ITO-free, optical evaluation

最终交流类型:

Design and Performance Electrode and Electrolyte Materials for Aqueous Batteries

黄燕
哈尔滨工业大学（深圳）

Aqueous batteries have received much attention in the field of electrochemical energy storage due to their use of water as electrolyte solvent, which can fundamentally solve safety issues caused by flammable organic electrolytes, reduce manufacturing costs and improve ionic conductivity. Aiming at the problem of zinc anode dendrite of aqueous zinc-ion batteries, the silver nanowire aerogel collector with zinc affinity was designed to increase the current density and surface capacity to 40 mA/cm2 and 20 mAh/cm2. On this basis, the zinc-free anode battery (DOD=100%) was further designed (Figure 1) [1]. Based on the inevitable problem of iodine entering the electrolyte and forming electrochemically inactive complexes at the zinc anode in aqueous zinc|| iodine batteries, the opposite approach is taken by introducing iodine into the electrolyte and developing a new type of aqueous iodine battery, greatly improving the cycling stability of the battery and other indicators (Figure 2) [2]. Based on the super water absorption characteristics of sodium polyacrylate hydrogel electrolyte, an aqueous aluminum-air battery capable of automatic snorkeling was designed to expand the application field of aqueous batteries (Figure 3) [3].

Keyword: Aqueous battery, Iodine electrode, Gel electrolyte, Cascade battery

最终交流类型:

Optical design for high-efficiency white perovskite LEDs

Hin Lap Yip
City University of Hong Kong

Metal halide perovskite light-emitting diodes (PeLEDs) show great potential to be the next-generation lighting technology, with external quantum efficiencies (EQEs) exceeding 20% for infrared, red and green LEDs. However, the efficiencies of blue and white devices severely lag behind. To improve the performance of blue PeLEDs, we employed an integrated strategy combining dimensional engineering of perovskite film and recombination zone modulation in the LED device to obtain an EQE of up to 5 %. While further incorporating the strategy of interfacial engineering, highly efficient blue PeLEDs with EQEs over 10% have been successfully realized in our group, establishing an excellent platform for white-light emission. In our latest work, we demonstrated efficient white PeLEDs by optically coupling a blue PeLED with a red-emitting perovskite nanocrystal layer in an advanced device structure, which allows extracting the trapped optical modes(waveguide and SPP modes) of blue photons in the device to the red perovskite layer via near-field effects. As a result, white PeLEDs with EQE over 12% are achieved, representing the state-of-the-art performance for white PeLEDs.

Keyword: Perovskite LEDs, Optical Engineering, White Light, Optical modes, Interface Engineering

最终交流类型:

Structural degree of freedom for energy storage materials

谷林
清华大学

The origin of functional materials is divided into two parts, multi-electronic system and single electronic system. Multi-electronic system is determined by various fields, while single electronic system is determined by local symmetry. From Noether’s vision, to every differentiable symmetry generated by local actions there corresponds a conserved flux. Materials with broken symmetry destroy the conserved quantities and therefore have functionality. Even the change under picometer scale in functional materials could break the symmetry. As a powerful characterization method, Spherical aberration corrected electron

microscopy could acquire information about atomic-scale structure and electronic structure, which could get rid of the constraint condition of periodic potential field, single electron approximation, and adiabatic approximation theories to obtain the structure-activity relationship in solid materials. In our recent work, we realized broken symmetry in functional material by electrochemical operation. For example, the interface regions, including surfaces and internal boundaries, may have a substantial impact on battery performance. Both the spatial inversion symmetry and translational symmetry are broken by the interfacial structure itself. This report will focus on physical mechanism of electrochemical energy storage materials to discuss the correlation between microstructure and electronic structure in the broken symmetric system.

Keyword: Energy storage materials; symmetry; degrees of freedom

最终交流类型: Invited

Material Design and Device Engineering for Efficient Organic Photovoltaic Cells

侯剑辉
中国科学院化学研究所

The developments on organic photovoltaic (OPV) materials and device engineering have contributed greatly to the rapid advances in photovoltaic performance of OPV cells. In the past years, we focused on the conjugated polymers based on benzothiophene units and developed a few polymer donors with superior photovoltaic performance, such as PBDB-T and PBDB-TF (also known as PM6). Based on these polymers and the non-fullerene acceptors developed by other research groups, we carried out a series of studies on material design and device engineering. In this presentation, I would like to introduce some interesting and useful strategies related to molecular design and device fabrication. What is more, our recent works including the single-junction cells with over 19% efficiency, the double-junction tandem cells with over 20% efficiency and the efficient OPV cells for indoor applications will be briefly introduced.

Keyword: Organic solar cell; conjugated polymer; material design; efficiency

最终交流类型: Invited

Development of organic photovoltaics with excellent device efficiency and stability

李宁
华南理工大学

As an important representative of emerging photovoltaic technologies, organic photovoltaics (OPV) can achieve excellent device performance and low-cost, continuous production and processing through solution printing technology, and are expected to make outstanding contributions to solar-driven multifunctional applications. In order to realize the industrialization and commercial application of OPV technology, research teams around the world have made a lot of efforts. In the past few years, through the synthesis of new materials, optimization of thin film micro-morphology, and development of advanced processing technologies, the power conversion efficiency of OPV devices has been continuously improved. However, factors such as the operational lifetime of OPV devices, large-area processing techniques, and processing costs are key issues that still restrict the industrialization of OPV technology. In this contribution, I will discuss the research key points and difficulties in the industrialization process of OPV technology, and propose some effective concepts to develop OPV devices with excellent performance and stability.

Keyword: organic photovoltaics; device stability; device performance

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最终交流类型: Keynote

Multifunctional Materials For Emerging Technologies

Federico Rosei
INRS

This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthesized via the bottom–up approach present an opportunity for future generation low cost manufacturing of devices. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices. [1-40].

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Keyword: multifunctional materials, nanomaterials, renewable energy

最终交流类型: Invited

Strategies for improving the performance of Sn-based perovskite solar cells

feng yan

The Hong Kong Polytechnic University

Tin-based perovskites are promising candidate materials for efficient lead-free perovskite solar cells (PSCs) due to their excellent optoelectronic properties and suitable bandgaps. However, it is challenging to prepare highly stable and efficient tin-based PSCs because Sn^{2+} in perovskites can be easily oxidized to Sn^{4+} upon air exposure. Many effective approaches have been developed to improve the device performance and a power conversion efficiency of over 14% has been achieved. In this talk, I will introduce the fabrication of air-stable $FASnI_3$ PSCs by adding hydroxybenzene sulfonic acid or gallic acid as antioxidant agents into the perovskite precursor solution along with excess $SnCl_2$. The interaction between the additives and $SnCl_2$ promote their homogenous dispersion in the perovskite film. Moreover, the strong antioxidant capacity of the additives enables enhanced oxidation stability of $FASnI_3$. The corresponding PSCs can maintain 80% of the efficiency over 1000 h upon air exposure without encapsulation, which is over ten times longer than the best result reported before. Our results suggest a novel strategy for the design of efficient and stable tin-based PSCs.

Keyword: perovskite solar cells; Sn-based perovskite; efficiency; Stability.

最终交流类型: Keynote

Printable Organic and Perovskite Solar Cells for Clean Energy

Kwan-Yue Alex Jen

City University of Hong Kong

Minimizing energy loss and increasing the field factor are key aspects to transcend the current limitations on the performance of organic photovoltaics (OPV). However, an inherent limit has set for an organic bulk-heterojunction (BHJ) blends from prominent non-geminate recombination through non-radiative charge transfer states. Our recent study on charge recombination in BHJ and Planar-Mixed Heterojunction (PMHJ) blends comprising a crystalline polymer donor with Se-containing Y6-derived non-fullerene acceptors has shown both high photovoltaic internal quantum efficiencies and high external electroluminescence quantum efficiencies. Crystallographic and spectroscopic studies reveal that the pseudo-2D, fused-ring molecular acceptors are not only intrinsically highly luminescent but also meets the criteria in achieving intrinsically radiative recombination within the blend, by promoting delocalized excitons with much longer luminescent lifetime and reduced exciton binding energies. These results provide the important demonstration of radiative non-geminate charge recombination in efficient OPV blends to achieve PCEs close to 20%. Moreover, a new "Dilution Effect" concept is introduced to explain the commonly observed composition-dependent Voc and reduced photovoltage loss in highly efficient ternary-based devices due to significantly reduced phonon-electron coupling. At the end, several novel interface/additive engineering approaches will be discussed to demonstrate high PCE (~25%) could be achieved in inverted perovskite solar cells and very efficient lead-capturing from decomposed perovskite devices. Their applications in various clean energy generation fields will also be discussed.

Keyword: organic solar cells, perovskite solar cells, solution processing

最终交流类型: Oral

Advancing Flexible Organic Lithium-ion Batteries: Redox Active Porous Polymers for Fast Charging and Extended Cyclic Life

Kamran Amin
Chinese Academy of Sciences

The quest for flexible and wearable electronics is driving the progress in the field of flexible Lithium Ion Batteries (LIBs). Redox active polymers are emerging as an important class of electrode materials for Flexible Lithium Ion Batteries (LIBs) due to their high capacity, structural diversity, ease of synthesis and functionalization, low cost and abundance.

Unfortunately, most of these polymers suffer from low electronic conductivity leading to poor performance. Conductive additives, binders and metal current collectors are frequently used to improve performance but their comparatively large amount in polymer-based batteries leads not only to low volumetric energy densities but also rigid non-flexible behavior. Also, maintaining the structural integrity of electrodes under applied force is quite challenging. Recently our group has reported several strategies to overcome these challenges [1]. CNTs were employed to synthesize a composite polymer with improved conductivity [2] and some very simple techniques were used to fabricate a free-standing binder and metal current collector free electrodes, [3] thereby reducing the dead electrode mass effectively and leading to the fabrication of flexible devices having enhanced performance under applied force.

In this talk we present an overview of the contribution of our group to the most recent progress in the field of polymer-based batteries, outlining the future challenges in this area. Also, some important characteristics of designing and assembling flexible organic batteries based on our research work will be discussed briefly.

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Keyword: Organic Lithium ion Batteries, Porous Polymers, Flexible Electrodes, CNTs

最终交流类型: Invited

Highly Efficient Organic Solar Cells

葛子义
中国科学院宁波材料技术与工程研究所

Organic solar cells have the advantages of low cost, light weight, flexibility and easy fabrication in large area. They have important application prospects in the fields of portable electronics, BIPV and military industry. We mainly introduce the progress in solution-processable flexible organic solar cells. Firstly, several solution processed non-conjugated small-molecule electrolytes were developed as cathode interfaces, leading to over 10%

efficiency for single-junction OSCs. Secondly, flexible OSCs with acid-treated PEDOT:PSS electrode was prepared with the efficiency over 10%. By further using the natural green acid treated electrode, FST-OSCs was fabricated with over 10% efficiency and 21% average visible light transmittance, that could utilize visible light for plant growth and infrared light for power generation. We successfully designed and synthesized a novel small molecular donors G19 to construct ternary organic solar cells with outstanding PCEs of 18.5% for rigid and 15.9% for flexible OSCs, which are among the highest efficiency reported. Recently, we utilized Isomerization strategy on a non-fullerene guest acceptor for stable organic solar cells with efficiency of 19.33% and flexible OSC with a record PCE over 18%.

Keyword: Organic solar cells, interfacial engineering, flexible, isomerization

最终交流类型: Invited

Monomicellar assembly to synthesize mesoporous materials

李伟
复旦大学

Mesoporous materials have large pore size (2-50 nm), high specific surface area, rich skeleton composition, adjustable geometric structure and unique nanoconfinement effect, and are a very important class of catalytic materials, which are widely used in petroleum refining, energy catalysis, fine chemical industry, environmental protection and other fields. However, the synthesis process still has problems such as insufficient efficiency and accuracy, relying on "trial and error method", and most of the prepared mesoporous materials are blocks, low utilization of active sites, and blocked diffusion mass transfer, resulting in poor catalytic performance. Starting from the construction of the basic structural units of mesoporous materials (single micellar units and functional monomers), we developed a directional assembly method with the self-assembly driving force - fine regulation of non-covalent bond interactions as the core, and created efficient mesoporous catalytic materials to solve the key scientific problems faced in their preparation and catalytic applications. Recent progresses will be also discussed briefly.

Keyword: Mesoporous materials, self-assembly, active sites design

最终交流类型: Invited

Lithium-rich layered oxides for high energy lithium-ions batteries

尉海军
北京工业大学

High-energy lithium-rich layered oxides (LLOs) are key positive electrode materials for achieving an energy density of 500Wh/Kg for lithium-ion batteries. However, there are lots of problems for these materials, especially poor long-term stability, which is a bottleneck restricting its further promotion and application. In the past 13 years, I have focused on a series of fundamental scientific and applied engineering issues related to LLOs. I have systematically conducted research on the crystal structure analysis, crystal structure evolution, electrochemical reaction mechanisms, material microstructure design and regulation, material interface design and optimization, and material compatibility in batteries. Recently, the industrial promotion of LLOs has also been achieved. This report will focus on the key issues of long cycle stability of LLOs materials and explore corresponding solutions.

Keyword: Lithium ion battery; lithium-rich layered oxides; cycle stablity; high energy

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最终交流类型: Invited

Advanced carbon materials for a green and sustainable energy future

Zhaojun Han
UNSW

Energy conversion and storage devices are critical for a sustainable energy future, yet their widespread application is hampered by the limited performance and high cost and/or scarcity of critical minerals. In this talk, I will report a range of carbon-based hybrid materials with controllable features and demonstrate their applications in multi-functional energy storage devices, green hydrogen production and electrochemical CO2 reduction reactions. I will also present future perspectives on the development of these materials, which may open new opportunities in the exciting field of low-cost carbon-based electrodes towards a green and sustainable energy future.

Keyword: catalysis, carbon, energy storage, CO2 reduction, hydrogen

最终交流类型: Invited

Breaking scaling relationships in alkynol semihydrogenation by manipulating interstitial atoms in Pd with d-electron gain

万颖
Shanghai Normal University

Semi-hydrogenation of alkynols to alkenols is one of the most widely studied industrially applicable catalytic processes in producing vitamins, medicines, fragrances, artificial fibers, etc. A palladium nanocatalyst supported on solid is a more preferred hydrogenation catalyst in the industry than homogeneous catalysts in terms of green chemistry and reusability of the catalysts, mainly taking advantage of the adsorption and dissociation of hydrogen molecules (H2) to form adsorbed H atoms (Had) over Pd surface[1]. However, due to the existence of scaling relationships of adsorption energies between the key adsorbed species, the increase in conversion is frequently accompanied by side reactions, thereby reducing the selectivity to alkenols[2].

We report that the simultaneous increase in alkenol selectivity and alkynol conversion is achieved by manipulating interstitial atoms including B, P, C, S and N in Pd catalysts[3]. A negative linear relationship is observed between the activation entropies of 2-methyl-3-butyn-2-ol (MBY) and 2-methyl-3-buten-2-ol (MBE) which is highly related to the filling of d-orbital of Pd catalysts by the modification of p-block elements. An increase in the d charge of Pd induces the rearrangement of MBE from an adsorption configuration through C=C bonds to one using the hydroxyl group (-OH) terminations which reduces the activation entropy. A catalyst co-modified by B and C atoms has the maximum d charge of Pd that achieves a 17-fold increase in the turn-over frequency values compared to the Lindlar catalysts in the semi-hydrogenation of 2-methyl-3-butyn-2-ol. When the conversion is close to 100%, the selectivity can be as high as 95%. The catalyst is stable and can be recycled 8 times with negligible loss both overall conversion and selectivity. Our work not only provides a green and industrially available synthesis route for interstitial Pd nanocatalysts but also guides the rational design of industrial Pd catalysts with unique chemoselectivity in organic reactions.

Keyword: d-electron gain, scaling relationship, Pd catalyst, interstitial atom, alkynol semihydrogenation

最终交流类型: Invited

Nanobubbles / droplets at the interface between electrode and electrolyte

Xiaoming SUN
Beijing University of Chemical Technology

In this report we want to provide some insightful fundamental understanding of the interfacial variations between electrode and electrolyte during GERs and GCRs. For example, visible bubbles emerge in GERs should have a high nucleation barrier and a rapid barrier-less growth process according to the traditional view, which, however, is contradicted by the experimental observation that a higher overpotential is required for enlarging the NBs to visible ones. We resolve this contradiction by observing the ‘‘pin-rise’’ growth mode of interfacial nanobubbles under electrolysis conditions with the combination of newly developed SPRi technology, atomic force microscopy, and molecular dynamics simulations. On the other hand, water management is crucial for the long-term performance of ion-exchange membrane-based fuel cells (FCs), while the lack of flooding pictures at the catalyst layer is seriously challenging for the further optimization of devices. A self-flooding phenomenon was observed at the bubble/electrode interface as the catalyst layer based on our built-up in situ model reaction system during ORR/HOR. The unexpected flooding phenomenon was attributed to the decrease in saturated vapor pressure driven by the generation of ions (H+ for acidic HOR and OH- for alkaline ORR), leading to the condensation of the water vapor at the bubble/electrode interfaces, which offers a novel perspective for water management in FCs. These works shed light on the behaviors at the three-phase boundaries and mechanisms thereof, which should be helpful for further optimization of various gas-involving electrochemical reaction-based devices.

Keyword: Bubbles, Catalysts, Diffusion, Electrodes, Surface interactions

最终交流类型: Invited

Refined Mesoporous Architectures: Synthesis, Assembly and Applications

振安 乔
Jilin University， China

Porous carbon spheres derived from polymer colloids with regular geometry, monodispersed morphology, well-controlled contents and structures play important roles in many areas of application, such as energy storage/conversion, gas adsorption/separation, catalysis, and chemo-photothermal therapy. Suitable polymerization reaction and synthetic strategy are both critical for the obtainment of stable polymer colloids as carbon precursors. Basic polymerization reactions are the cornerstones of synthetic strategies, which directly provides the direct molecular-based design of functionalized polymer/carbon spheres. Thus, this report mainly focuses on the summary of suitable polymerization reactions for colloidal polymer derived porous carbon spheres. Recent advances in the synthetic strategies and applications are also discussed, including their corresponding polymerization reactions.

Keyword: Nanomaterials, Mesoporous materials, Self-assembly

最终交流类型: Invited

Highly efficient organic solar cells based on electron acceptors with asymmetric terminals

陈红征
浙江大学

Organic solar cells (OSCs) show great promise in renewable development, with the power conversion efficiency (PCE) over 19% for single cells. However, the efficiency is still a shortcoming for the future industrialization of OSCs, compared with other solar cells. In this presentation, I will share our strategies to solve this issue. I will introduce new design strategies to access small molecule electron acceptors with asymmetric structures for high performance OSC applications. The asymmetric design of the acceptor allows the simultaneous achievement of enhanced charge generation and reduced energy loss. As a result, high efficiency is obtained in the binary OSCs by carefully designing asymmetric terminals for acceptors. Efficiency over 19% is also realized in the ternary OSCs with the asymmetric electron acceptor as the third component.

Keyword: organic solar cells, electron acceptor, asymmetrip terminals

最终交流类型: Invited

Nonfused Ring Acceptors for High Efficiency Organic Solar Cells

薄志山
Beijing Normal University, China

Organic solar cells (OSCs) have the advantages of light weight, flexibility, fabrication by printing or coating, and high power conversion efficiency (PCE) under weak light. In recent years, a big breakthrough has been made for OSCs based on fused ring acceptors (FREAs) with the PCE close to 20%. However, the preparation of most high-performance FREAs involves multi-step synthesis and low-yield ring closure reactions, which has become one of the bottlenecks in future practical applications. To lower the cost of acceptor materials, we have developed a series of low-cost simple nonfused ring electron acceptors (NFREAs), and the planar molecular backbone of NFREAs can be achieved by the aid of intramolecular noncovalent interactions such as F-H, S-O, and S-N. Through rational molecular design and intensive device optimization, the PCE of NFREAs has been further boosted to 19%, which can be comparable to the state of the art of FREAs.

Keyword: organic solar cells; nonfullerene acceptors; nonfused ring acceptors; power conversion efficiency; conjugated polymers

最终交流类型: Invited

Challenge and Opportunity of Emerging Thin-Film Solar Cells

孟庆波
中国科学院物理研究所

The application of renewable energy and photovoltaic technology is a major demand for our sustainable development. Thin-film solar cells have received extensive attention due to their significant advantages in lightness, flexibility, and multi-scenario applications. Research and development of thin-film solar cells with abundant constituent elements, higher performance, lower cost, and more environment-friendly is an important direction in the field of photovoltaics. Our team has been engaged in the research of key materials and technologies for thin-film solar cells for more than 20 years. This report will focus on our latest progress in perovskite, Kesterite copper-zinc-tin-sulfur-selenide solar cells, and photoelectric measurement and characterization of solar cells.

For perovskite solar cells, we have achieved advanced cell performance in perovskite cell modules, all-inorganic perovskite cells and flexible carbon electrode based solar cells. These achievements mainly benefit from our systematical research on working mechanism, interface regulation and defect passivation.

Kesterite copper-zinc-tin-sulfur (selenium) is another important material for thin-film solar cells, which has unique advantages such as abundant reserves of constituent elements, non-toxicity, high stability, and compatibility with existing thin-film photovoltaic technologies. In this regard, we have carried out systematic research on the regulation of crystal morphology and the regulation of multiphase evolution chemical reaction pathways, and achieved the world highest record efficiency of >14.5%.

The achievement of high performance in these devices mainly benefits from our precise measurement and physical mechanism understanding of the microscopic process of charge loss in solar cells. We have developed a modulated transient photoelectric measurement system and solar cell charge loss analysis technology, which have been widely used in the research of different types of solar cells, and have been used to provide technical support for a number of research groups overseas.

Keyword: Thin-film solar cells, perovskite, Kesterite, charge dynamics, interfaces

最终交流类型: Invited

Fused-ring electron acceptors for organic photovoltaics

占肖卫
北京大学

Organic photovoltaic cells (OPVs) possess some merits, such as facile fabrication, visual semitransparency, flexibility, low cost, high mass power density and short energy payback time. Fullerene derivatives showed higher power conversion efficiencies (PCEs) than other acceptor systems before 2015 and thus dominated as electron acceptor materials for 20 years. However, weak visible absorption of fullerenes and large energy loss in fullerene-based devices limit the theoretical PCE of fullerene-based OPVs to ~13%, and morphological instability of fullerenes leads to short device lifetime thus restricts the practical application of OPVs.

In 2015 we invented the milestone molecule ITIC, pioneered the conception of "fused-ring electron acceptor (FREA)", and then built up a FREA family. The FREAs present some advantages: 1) Their chemical structures are facile to tailor and synthesis is easy to scale up; 2) Their absorption and energy levels can be tuned and thus match with various high-performance electron donors; 3) Their crystallinity and film morphology can be regulated; 4) They exhibit strong and broad absorption, especially in the 700–1000 nm range, and can match with wide-bandgap donor materials to achieve panchromatic absorption; 5) They have high exciton diffusion coefficients and low exciton binding energy which are beneficial for exciton dissociation; 6) They show small energy losses in devices. Single-junction OPVs based on these FREAs exhibit power conversion efficiencies of >19%, which far surpass fullerene acceptor counterparts (~12%). Moreover, the FREA-based OPVs exhibit good morphology stability and long device lifetime. Now FREAs invented by Zhan group are commercial available from >10 companies. Around 350 research groups in >20 countries have utilized these FREAs to fabricate high-efficiency OPVs. The emergence of high-performance FREAs has begun to marginalize previously predominant fullerene acceptors, and is inaugurating nonfullerene era of the OPV field.

Keyword: organic photovoltaics, nonfullerene acceptor, fused-ring electron acceptor

最终交流类型: Invited

High Performance Organic Solar Cell Materials and Devices

彭强
四川大学

Bulk-heterojunction (BHJ) organic solar cells (OSCs), typically consisting of a polymer donor and a small molecular acceptor, have attracted extensive research attentions due to their unique features of low-cost large-area production, light weight, and mechanical flexibility. Recently, the PCEs of nonfullerene based OSCs have also increased beyond 19%. To further improve the performance of OSCs, the key materials including donor and acceptor materials along with the device structure and fabrication technology should be continuously researched.

In this presentation, we will report some advances in development of polymer donors and small molecular acceptors for efficient non-fullerene PSCs. The strategies include backbone design, side chain engineering, interface engineering. Also the new device structures and the new methods for optimizing the blend morphology will be presented. Based on these studies, PCEs more than 19% have been achieved in our group.

Keyword: Organic Solar Cells, Donor Materials, Acceptor Materials, Device Structure, Fabrication Technology

最终交流类型: Keynote

Nonfullerene Acceptors Based on Ladder-Type Heteroheptacenes without Sp3-Hybridized Carbons

Qingdong Zheng
苏州大学

Nanometer-sized colloidal metal halide perovskite semiconductors have emerged and brought unique opportunities for photovoltaic application due to the high defect tolerance of perovskite and many features that emerge at the nanoscale. Perovskite quantum dots (QDs) or more broadly, nanocrystals (NCs), show high photoluminescence (PL) quantum yields, spectrally tunable bandgap, flexible compositional control, and crystalline strain benefits. Metal halide perovskite nanocrystals are readily synthesized with exceptional optoelectronic quality opening a route for next generation light emitters, as well as exploring LHP physics at the nanoscale. $CsPbX_3$ (X=Cl-, Br-, I-, or mixed halide) QDs exhibit PL tunable from ultraviolet to near-infrared wavelengths by adjusting the halide composition and/or QD size.

Since the first report in 2016, $CsPbI_3$ QDs also became a point of interest in PV research. Currently $CsPbI_3$ holds the record efficiency for QD solar cells (16.6%) proving better than any previous QD material composition. This talk will highlight the unique potential of perovskite QD (PQD) solar cells, from synthesis to devices. We will discuss current state of the art and lay out many open opportunities in perovskite QD solar cells, and the related present and future pursuits in QD preparation and device architecture.

Keyword: Perovskite QDs, solar cells, surface chemistry

最终交流类型: Invited

Distinct Photovoltaic Performances of Polymers: A theoretical Simulation and AI Approach

林嘉平
华东理工大学

Polymer photovoltaic devices, which offer many advantages, have attracted increasing attention recently. It is noteworthy that block copolymer-based polymer solar cells, which are very promising, have exhibited low photoelectric conversion efficiency (PCE). Improving the photovoltaic performance of polymer solar cells presents a pressing challenge [1].

We applied a multi-scale approach by coupling dissipative particle dynamics method with a drift-diffusion model to elucidate the photovoltaic properties of multiblock copolymers consisting of alternating electron donor and acceptor blocks [2, 3]. A series of hierarchical lamellae-in-lamellar structures were obtained from the self-assembly of the multiblock copolymers. A distinct improvement in photovoltaic performance upon the morphology transformation from lamella to lamellae-in-lamella was observed. The hierarchical lamellae-in-lamellar structures significantly enhance exciton dissociation and charge carrier transport, thereby contributing to the improved photovoltaic performance. The hierarchical nanostructures can achieve much enhanced PCE, improved by around 25% compared with that of general ones. Our findings are supported by experimental evidence and provide guidance for designing advanced photovoltaic materials with hierarchical structures.

In addition, we also carried out an AI-assisted design of the donor-acceptor structure combinations of organic photovoltaic (OPV) materials. To obtain OPV materials with higher PCE, the trial-and-error research paradigm is usually utilized. However, this paradigm has long research cycles for discovering new structures [4, 5]. We build a database of the donor-acceptor structures and the corresponding PCE performance data. A robust prediction model for the PCE performance of OPV materials was established by developing a polymer fingerprints method for end-to-end graph neural network training. The well-trained model was utilized to predict the PCE of single-junction photovoltaic devices for 170,000 kinds of donor-acceptor combinations. A number of optimal combinations with potential to surpass the Y6 systems were screened. This AI-assisted design method can accelerate the design and high-throughput screening of the OPV structures with high PCE.

Keyword: Organic photovoltaics; Polymer structures; Theoretical simulations; Machine learning; Materials genome approach

最终交流类型: Invited

The theory, characterization and applications of noncovalent conformational locks

黄辉
University of Chinese Academy of Sciences, China

Noncovalent conformational locks (NoCLs) have become an important strategy to design high perfromance organic/polymeric semiconductors. Herein, we will present the recent progress of NoCLs, including theory, characterization and applications of noncovalent conformational locks.

Keyword: Noncovalent conformational locks, DFT calculations, organic/polymeric semiconductors

最终交流类型: Keynote

Tuning the optoelectronic properties of inorganic and carbon-based quantum dots for highly efficient luminescent solar concentrators

Alberto Vomiero
Luleå University of Technology, Sweden

Luminescent solar concentrators (LSCs) are an old class of devices based on semitransparent windows, in which luminophores are embedded in a transparent matrix.[1] The luminophores can absorb and re-emit solar light and are able to generate electric power by collecting the re-emitted light at the borders of the slab. In the past, lab-to-fab transition of such devices was impeded by intrinsic limitations of the luminophores in terms of low quantum yield, strong resorption due to small Stokes shift, low optical and photoconversion efficiency of the final device. In the last years, a renaissance of such devices has been driven by the development of new 0-dimensional nanostructures, with tunable optical properties, which can guarantee good performance of LSCs.[2,3] Specifically, high quantum yield can be obtained; resorption losses can be limited by modulating the Stokes shift; final color of the window can be tuned by tuning light absorption properties; UV and IR parts of solar spectrum can be exploited without affecting window transparency. We will give examples of different 0-dimensional systems, which have been developed toward high efficiency LSCs, among which inorganic quantum dots and carbon dots.[4,5] Several strategies will be illustrated to tune the optoelectronic properties of the luminophores, including doping, core-shell structuring, and surface treatments.

References

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Keyword: luminescent solar concentrators; quantum dots; carbon dots; optoelectronic properties.

最终交流类型: Invited

Vacancies boost nitrogen activation for ammonia synthesis

叶天南
上海交通大学

Ammonia synthesis is one of the most important catalytic processes in the chemical industry. While Fe and Ru are efficient for N≡N bond cleavage, low cost and earth abundant elements such as Ni and Co exhibit much poorer activity due to their weak nitrogen adsorption energy. Here, we report that Ni, Co-loaded rare-earth nitride works as stable and highly efficient catalyst for ammonia synthesis along with a new mechanism. A high density of nitride vacancies is formed with low formation energy, which enables N2 activation at the vacancy sites. Consequently, the reaction rate and turnover frequency (TOF) of the nitride catalysts are quite high at 400 °C and under ambient pressure, and even comparable to those of Ru-based catalysts. Kinetic analysis and isotope experiments combined with density functional theory (DFT) calculations indicate that the nitrogen vacancies generated play a dominant role in the reaction mechanism, and contribute to both the adsorption and activation of N2 molecules. These results indicate the potential role of vacancy sites in the reaction cycles, and provide a new catalyst design concept for earth-abundant catalysts in ammonia synthesis.

Keyword: Ammonia synthesis; rare-earth nitride; electron transfer; anionic vacancy

最终交流类型: Keynote

Research Progress of Photovoltaic Materials for Polymer Solar Cells

Yongfang Li
Institute of Chemistry, CAS, China

Polymer solar cells (PSCs) have attracted great attention in recent years, because of their advantages of simple device structure, light weight and capability to be fabricated into flexible and semitransparent devices. The key photovoltaic materials of PSCs are conjugated polymer donors and n-type organic semiconductor (n-OS) acceptors. Recently, the low bandgap n-OS acceptors (such as Y6) have promoted the research progress of the PSCs significantly. Here I will report our recent research progress on the photovoltaic materials of the polymer donors, new n-OS acceptors, polymer acceptors and giant molecule acceptors. We synthesized Y6 derivative acceptors m-TEH, o-TEH and T2EH with thiophene upper side chains, power conversion efficiency (PCE) of the PSCs based PBQ6 as donor and m-TEH as acceptor reached 18.51%. We developed a low cost medium bandgap D-A copolymer donor PTQ10 based on thiophene as D-unit and difluoroquinoxaline as A-unit. And the PSCs with PTQ10 as donor showed high PCEs of 18.55% for the binary device and 19.34% for the ternary device. We proposed the strategy of polymerized small molecule acceptor (PSMA) for the design and synthesis of high performance polymer acceptor, and PCE of the all polymer solar cells with new PSMA as polymer acceptor reached the level of 16~18%. Recently, we proposed the concept of giant molecule acceptor (GMA), and the PSCs based on GMA showed high PCE of over 18% and high stability.

Keyword: Photovoltaic Materials

最终交流类型: Invited

Alloy anodes as an alternative to alkali metal anodes

赵婕
复旦大学

Developing high-capacity anodes is a must to improve the energy density of lithium batteries for electric vehicle applications. Alloy anodes are one promising option, but without pre-stored lithium, the overall energy density is limited by the low-capacity lithium metal oxide cathodes. Recently, lithium metal has been revived as a high-capacity anode, but faces several challenges owing to its high reactivity and uncontrolled dendrite growth. Here, we show a series of Li-containing foils inheriting the desirable properties of alloy anodes and pure metal anodes. They consist of densely packed LixM (M = Si, Sn, or Al) nanoparticles encapsulated by large graphene sheets[1]. With the protection of graphene sheets, the large and freestanding LixM/graphene foils are stable in different air conditions. With fully expanded LixSi confined in the highly conductive and chemically stable graphene matrix, this LixSi/graphene foil maintains a stable structure and cyclability in half cells (400 cycles with 98% capacity retention). This foil is also paired with high-capacity sulfur cathodes to achieve stable full-cell cycling. Because of the higher chemical activity, sodium metal anodes are more problematic compared to lithium metal. We matched sodium-tin alloys with newly synthesized solid electrolytes. The NaSn|Na2BH4NH2|NaSn symmetric cell cycles at a current density of 0.1 mA cm−2 for 500 h. Moreover, the universality of NaSn and Na2BH4NH2 electrolyte is verified by TiS2 cathode, indicating the good compatibility with electrode material.

Reference

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Keyword: Li-ion batteries, prelithiated-alloy anodes, alkali metal anodes, solid electrolytes

最终交流类型: Invited

Low-temperature sodium/potassium-ion batteries

王华

Beihang University, China

Currently, lithium-ion batteries are the most widely used energy storage devices in commercial applications. However, their actual discharge capacity, rate and voltage platform are greatly reduced in low-temperature environment, which seriously degrades the energy density, power density and cycle life of the batteries, and restricts their practical production and application. Compared with conventional lithium-ion batteries, sodium/potassium ion batteries not only have the advantages of abundant resources and low cost, but also have more superiority in low-temperature application: (1) the desolvation energy of sodium/potassium ions is lower than that of lithium ions in the same solvent, enabling faster interfacial reaction kinetics; (2) the Stokes radius of sodium/potassium ions is smaller, and the conductivity of the sodium/potassium ion system is higher at the same electrolyte concentration. Herein, by rationally designing electrolyte components, optimizing electrode material structures, and regulating electrode/electrolyte interfaces, hard carbon anodes with high-rate reversible charging/discharging properties at low temperatures were achieved. Moreover, ultra-low temperature sodium and potassium-ion full batteries based on the hard carbon anodes were fabricated, and low-temperature high-energy sodium/potassium metal as well as anode-free batteries were developed. More interestingly, we achieved an Ah-level sodium-ion pouch battery with an energy density of 110 Wh/kg at -40°C (based on the weight of the entire battery) and a potassium-ion pouch battery with an energy density of 152 Wh/kg at -40°C (based on the weight of cathode and anode materials). This work demonstrates the great potential of sodium/potassium ion batteries for applications in low-temperature environments.

Keyword: low-temperature battery; sodium-ion battery; potassium-ion battery; hard carbon; alkali metal

最终交流类型: Invited

Nonfullerene acceptors based on ladder-type heteroheptacenes without sp3-hybridized carbons

郑庆东
南京大学

Control over the intermolecular interaction as well as the molecular orientation of organic semiconductors with respect to the substrate plays a critical role in determining the performance of polymer solar cells (PSCs). In this talk, we will focus on the development of novel electron-transporting materials based on ladder-type heteroheptacenes without sp^3-hybridized carbons for efficient PSCs. A series of ladder-type heteroheptacene-based small molecules with branched or unbranched side chains flanked in different positions of their conjugated backbone, or with varied electron withdrawing end groups flanked on the same conjugated backbone, were designed and synthesized to investigate the effect of side-chains and end group on the crystallinity, molecular orientation, charge transport and photovoltaic properties of these ladder-type heteroheptacene-based semiconductors. Furthermore, we report the effect of noncovalent intramolecular interactions on the photovoltaic performance of the nonfullerene acceptors. The removal of the sp^3-hybridized carbons leads to novel nonfullerene acceptors with efficient electron transport. As results, the best-performance nonfullerene acceptor with optimized molecular orientation affords an outstanding power conversion efficiency of ~18% which is the highest among all the A-D-A type nonfullerene acceptors reported to date.

Keyword: polymer solar cells, intermolecular interaction, nonfullerene acceptors, molecular orientation, power conversion efficiency

最终交流类型: Invited

Research Progress on Novel Dual-ion Batteries

唐永炳
Shenzhen Institute of Advanced Technology, CAS, China

The popularization of renewable energy creates more and more diversified usage scenario of energy storage technology. Besides good electrochemical performance, it is equally important to develop cost-effective energy storage technology which provides suitable performance with affordable cost. Dual-ion batteries (DIBs), a new type of energy storage device with working mechanism of cations/anions react with anode/cathode simultaneously, have received great attention in recent years owing to their merits of high voltage, low cost, and environmental friendliness. However, the limited performance of traditional graphite anode material and narrow electrochemical stable window of conventional electrolyte systems largely restrict the further development of DIBs. Our previous works demonstrated that an innovative integration design of alloying-type anode materials and current collector is capable of enhancing both the charge transfer efficiency and energy density of DIBs, and such novel battery configuration can be also successfully applied to other resource-abundant alkali/alkali earth metal (Na, K, Ca, etc) based DIBs, showing good application prospects. Moreover, multi-scale structural design of anode materials and rational design of electrolyte systems are proposed to realize the overall improvement of the

performances for novel DIBs. Practical application of novel dual-ion batteries was further explored and Ah-class dual-ion batteries was realized.

Keyword: Renewable energy, dual-ion batteries, integration design, multi-scale structural design, electrolyte optimization

最终交流类型: Keynote

Fused-Ring Electron Acceptors for Organic Photovoltaics

Xiaowei Zhan
华中科技大学

Metal halide perovskite solar cells (PSCs) currently attract enormous research interest because of their high power conversion efficiency (PCE) and low fabrication costs, but their practical development is hampered by difficulties in achieving high performance with long-term stability and scale-up manufacturing.

In his presentation, starting from the fundamental understanding of the device equivalent circuit, Prof. Li will firstly emphasize a vacuum flash–assisted solution processing method to prepare high-quality perovskite films with high electronic quality over large-area, as well as demonstrate a upscaling strategy of using full screen-printing fabrication technique coordinated with triple-layered device architecture, both of which has proved to be universally useful idea to fabricate large-area and efficient PSCs.1,2 Then he introduced a phosphonic acid–functionalized fullerene derivative in mixed-cation perovskites as a grain boundary modulator to consolidate the crystal structure, and also developed a redox-active radical polymer poly(oxoammonium salt) which can not only effectively p-dope the hole-transporting material by hole injection but also mitigate lithium ion diffusion, achieving a PCE of 21.4% for 17.1-square-centimeter minimodules. The PSCs retained 95.5% of their initial efficiencies after 3265 hours at maximum power point tracking under continuous 1-sun illumination at 70° ± 5°C.3 Thirdly, he will demonstrate a bifunctional molecule CBz-PAI with carbazole-triphenylamine and phenylammonium iodide units to passivate defects at the perovskite/HTL interface, benefiting to a favorable energy level alignment with the perovskite and constructing a hole shuttle between the perovskite layer and the HTL. This allows substantial enhancement in device performance and durability.

Finally, Prof. Li will present their recent research progress in the stabilization of 3D/2D perovskite heterostructures via inhibition of ion diffusion by cross-linked polymers (CLP) for scalable perovskite solar modules with high performance, where they incorporated a CLP on the top of a 3D perovskite layer and then deposit a 2D perovskite layer via a vapour-assisted two-step process to form a 3D/CLP/2D perovskite heterostructure, which achieved an efficiency of 19.6% for mini-modules and an stability of retaining 90% of initial performance after 4,390 hours operation under maximum power point tracking and one-sun illumination at elevated temperatures.5 These findings open a path to realize large scale robust PSCs of high performance and stability, enabling the timely commercialization of this state-of-the-art PV device.

Keyword: Perovskite Solar Cells

最终交流类型:

Advanced Materials for Rechargeable Zinc-Air Battery

Developing low-cost, high-energy, safe, and long-life energy storage systems is critical for the widespread commercialization of smart grid and electric vehicles. Rechargeable zinc-air battery has been considered as the most promising candidate as the energy storage system for transportation, smart grids, and stationary power. They can display a considerably several times higher specific energy and volumetric energy density than that of the Li-ion battery. Besides, zinc-air batteries also demonstrate other desirable characteristics, such as abundant raw materials, environmental friendliness, safety, and low cost. The current zinc-air battery is typically composed of four main components: an air electrode, an alkaline electrolyte, a separator, and a zinc electrode. Each main structural component faces challenges for the electrically rechargeable zinc-air battery. In this presentation, we will present our recent work on advanced energy materials development for next-generation rechargeable zinc-air batteries by focusing on the nanostructured bifunctional oxygen electro-catalysts and mechanical studies on their corresponding electrochemical behaviors during battery cycling. More specifically, we will discuss: 1) how the nanoengineered materials can enhance the catalytic activity and durability of oxygen electro-catalysts, 2) what are the structural evolution and actual species of oxygen electro-catalysts in the zinc-air batteries operate, 3) how the 3D air electrode architectures and mechanical understandings can advance the practical performance of the zinc-air batteries, as well as their extended applications include portable, flexible, and diversely shaped zinc-air batteries.

Keyword: Advanced Materials

最终交流类型: Keynote

Materials Design and Device Optimizations for Non-fullerene Organic Solar Cells

Yan He

Organic solar cells (OSCs) are flexible, semi-transparent and environmentally friendly devices which can be installed in areas where silicon panels are not suitable (such as glass windows on buildings). Conventional OSCs are based on fullerene acceptors as a key component. However, fullerene-based OSCs can only achieve modest efficiency of 12% at best, due to their large voltage loss (above 0.8V), and poor device stability.

Recently, there has been a major revolution in the OSC field, as researchers developed many high-performance non-fullerene acceptors that can overcome the limitation of traditional fullerene acceptors and open a new era for the OSC field. One of the unique features of non-emerging non-fullerene OSCs is the surprisingly small voltage losses of the devices (~ 0.5V). Since 2016, our team at HKUST has developed a range of non-fullerene systems that can simultaneously generate high photocurrent (near 100% yield) with small voltage losses (first published in Nature Energy). Moreover, we have recently achieved record-breaking OSCs based on a state-of-the-art non-fullerene acceptor, achieving an unprecedented efficiency of 16.7% in single-junction OSC device. Our work clearly indicate that OSCs have the potential to reach the high efficiency of inorganic solar cells.

Our results show that the key factor is the long charge transfer life-time that allows for efficient charge separation despite of a small energy offset. In the other aspect, we study structure-property relationship of high-performance donor and non-fullerene acceptor materials and reveal the key structure features that enable highly efficient non-fullerene organic solar cell devices with over 19% efficiency. With these understandings of mechanism and structure-property relationship, it is feasible to further increase the efficiency of organic solar cells beyond 20% in near future.

Keyword: Organic solar cells (OSCs)

最终交流类型: Keynote

先进热电制冷材料

赵立东
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摘要：热电制冷技术是一种利用半导体材料的帕尔帖效应直接将电能转换为热能的绿色制冷技术，热电制冷技术由于其控温精准、尺寸灵活、结构多样和局部冷却等众多优势，在微电子、传感器和5G光模块等关键领域具有比传统的机械压缩式制冷技术更强的竞争优势和应用潜力。目前，碲化铋（Bi2Te3）基材料仍为唯一的可广泛应用的热电制冷材料，然而Te元素的地壳稀缺程度等同于白金（全球产量仅可供应约2000万片制冷片，但光伏材料CdTe将抢走一半市场份额），且Bi2Te3及热电制冷器件存在可加工性能差、制冷性能不足和运行功耗过高等问题，因此，探索和开发新型热电制冷材料及器件至关重要。基于提出的“栅格化”策略，通过调控SnSe晶体中的本征缺陷，改善载流子迁移率，进一步优化室温热电性能，实现高效率电子制冷。

Keyword: 电子制冷

Topical Sessions =》 8. Nanophotonics and Optoelectronics

最终交流类型: Invited

Optical Studies of Single- and Mixed-Halide Perovskite Nanocrystals towards the Applications in Classical Optoelectronics and Quantum Technologies

王晓勇

Nanjing University, China

Semiconductor perovskite films are now being widely investigated as light harvesters in solar cells with ever-increasing power conversion efficiencies, which have motivated the fabrication of other optoelectronic devices such as light-emitting diodes, lasers and photodetectors. Their superior material and optical properties are shared by the counterpart colloidal nanocrystals (NCs), with the additional advantage of quantum confinement that can yield size-dependent optical emission ranging from the near-UV to -infrared wavelengths. So far, intensive research efforts have been devoted to the optical characterization of perovskite NC ensembles, revealing not only fundamental exciton relaxation and recombination dynamics but also low-threshold amplified spontaneous emission and novel superfluorescence effects. Meanwhile, the application of single-particle spectroscopy techniques to perovskite NCs has helped to resolve a variety of optical properties for which there are few equivalents in traditional colloidal NCs, mainly including nonblinking photoluminescence, suppressed spectral diffusion, stable exciton fine structures and coherent single-photon emission. While the main purpose of ensemble optical studies is to guide the smooth development of perovskite NCs in classical optoelectronic applications, the rich observations from single-particle optical studies mark the emergence of a potential platform that can be exploited for quantum information technologies.

In this talk, we will focus on single- and mix-halide perovskite NCs to demonstrate their novel optical properties obtained from our recent studies, with the purpose of promoting their potential applications in both classical optoelectronics and quantum technologies. First, we show that the surface stress can induce a permanent dipole moment in a single CsPbI3 NC, which can work with external electric fields to remove the exciton fine energy-level structures. Second, by means of resonant excitation of single CsPbI3 NCs, we have resolved a discrete acoustic-phonon mode that couples efficiently with the exciton via the piezoelectric potential. Third, we have employed a periodic heating method to completely suppress the phase-segregation effect in ensemble CsPbBrxI3-x NCs, thus paving the way towards their stable operation in various light-emitting and photovoltaic devices. Finally, we have deposited a single CsPbI3 NC on top of an individual CsPbBr3 microplate to create a single CsPbBrxI1.8 NC, whose ability to emit single photons mark the emergence of a novel heterostructure carrying both classical and quantum optical features.

Keywords:perovskite, nanocrystal, single-photon emission, phase segregation, classical optoelectronics, quantum technologies

最终交流类型: Invited

Spinoptronics in optical microcavities

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Fabry-Perrot (FP) microcavities with metal or DBR (distributed Bragg reflector)-coated mirrors provide an excellent platform for investigating the collective behavior of confined 2-dimensional photons and polaritons. The TE-TM mode splitting in such cavities acts as an effective magnetic field, leading to photonic spin-orbit (SO) coupling effect that the pseudospin of cavity photons changes anisotropically with their momenta [1]. Such mechanism has led to interesting observations including optical spin-Hall effect, magnetic-monopole-like half solitons, spinor condensate with half-quantum circulation, and polaritonic topological insulators [2].

We report the direct measurement of the Berry curvature and quantum metric of the photonic modes of a FP cavity containing an anisotropic organic microcrystal (Perylene). Photonic spin-orbit-coupling induced by the cavity together with the anisotropy of the material results in the action of an effective gauge field on photons, which includes an effect of emergent optical activity (OA). The photonic gauge field makes emerge geometrically non-trivial bands containing two gapped Dirac cones with opposite topological charges [3].

The same cavity structure with a DPAVBi microcrystal allows the observation of Voigt exceptional point at which the quantum metric is demonstrated to be divergent [4]. We also predict that in fully confined systems the eigenstates of the second excited manifold under TE-TM splitting are degenerate skyrmions which can be manipulated by the non-Hermitian properties[5].

Keywords: Microcavity, Optical activity, Berry curvature, quantum metric, spin-orbit coupling

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最终交流类型: Keynote

Microcavity-enhanced optical sensing

肖云峰

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Optical microcavities confine light to small volumes by resonant recirculation. Prominent examples are ultrahigh-Q whispering gallery microcavities which confine photons by means of continuous total internal reflection along a curved and smooth surface. The long photon lifetime and strong field confinement characteristics make them promising candidates for enhancing light-matter interactions, and have triggered intense research interest in both fundamental and applied photonics for decades. For example, in fundamental physics, benefitting from strongly enhanced light-matter interplays, ultrahigh-Q optical microcavities hold great potential for the studies of cavity quantum electrodynamics (photon-atom), cavity optomechanics (photon-phonon), nonlinear optics (photon-photon), etc. In applied photonics, microcavity-based sensors have attracted considerable interest in life and environment sciences for sensing, imaging and spectroscopy, due to their distinguished advantages such as high sensitivity, fast response, and miniature device sizes.

In recent years, we focus on ultrahigh-Q microcavity photonics, especially for optical whispering-gallery-mode (WGM) microcavities in both fundamental studies of modern physics and applications of integrated photonics. In the first part of this talk, I will introduce some representative fundamental studies of ultrahigh-Q microcavities on quantum and nonlinear optics, as well as chaos dynamic, including chaos-assisted broadband momentum transformation in asymmetric microresonators, symmetry-breaking-induced nonlinear optics at a microcavity surface and regulated photon transport in chaotic microcavities by tailoring phase space, etc.

In the second part of this talk, I will focus on microcavity sensing mechanisms and their practical applications in sensing, imaging and spectroscopy. In microcavity sensing, several novel sensing mechanisms will be presented, including single-nanoparticle detection with mode broadening and microcavity Raman laser, as well as single-molecule detection with interface whispering-gallery modes, dissipative acousto-optic interaction in optical microcavity for acoustic sensing. For microcavity-based imaging, microlaser particles and microcavity ultrasound detectors are developed for single-cell tracking and acoustic imaging. In microcavity-based spectroscopy, I will introduce microcavity-assisted broadband frequency microcombs and microcavity-enabled single-particle vibrational spectroscopy for biomechanical fingerprinting of biological cells.

Keywords:Microcavity sensing

最终交流类型: Keynote

New Functional Optoelectronic Chip based on Nanostructure

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A series of new physical mechanisms and unique optoelectronic properties in nanostructures provide the possibility to explore and study new optoelectronic chips.

Photons and phonons are important information carriers. Precise measurement of photons and phonons in micro-/nano- periodic structures allows the detection of multi-dimensional physical information and various physical quantities. Here, by manipulation of photons with metasurface units, a one-shot miniaturized ultraspectral camera fitting thousands of micro-spectrometers on a CMOS image sensor chip was proposed and applied to realize real-time on-chip spectral imaging. Micro-spectrometers with high center-wavelength accuracy of 0.1nm and spectral resolution of 0.8 nm were realized, and ultraspectral imaging results just under the lighting of a fluorescent lamp was obtained[1]. For phonons, optomechanical crystals were studied by dealing with the interaction between photons (light) and phonons (mechanical motion). A hetero optomechanical crystal was proposed and demonstrated by integrating two types of periodic structures into the system, and the optical and mechanical modes can be confined separately. This separate confinement gives rise to phonon lasing with a high mechanical frequency of 6.22 GHz[2][3]. Moreover, radiation-pressure-antidamping enhanced optomechanical spring sensing based on a silicon nanobeam optomechanical structure was proposed and demonstrated, which allows for a sensing resolution of δλ/λ0 ~ 10−7[4].

Some interesting phenomena and novel devices are arising by having free electrons interact with various nano-structures. We demonstrated the first on-chip integrated free electron light source by greatly decreasing the electron energy to 0.25~1.4keV for generating Cherenkov radiation (CR)[5]. In hexagonal boron nitride (hBN) with hyperbolic phonon polaritons, theoretical and simulation results revealed that CR can be generated using free electrons with an extremely low kinetic energy of 1 eV, which is about two-orders of magnitude lower than that in multilayer plasmonic hyperbolic metamaterial[6]. For generating Smith-Purcell radiation (SPR) in deep UV region, we had an electron beam pass through a grating with 30nm-wide slot and observed the SPR with shortest wavelength of ~230nm and the broadband SPR with wavelength covering 230~1100nm[7]. This work opens up the possibility of exploring high performance on-chip integrated free electron light source and optoelectronic devices, and provides a way for realizing integrated free electron laser.

Introduced by Allen in 1992, orbital angular momentum (OAM) was characterized as a new freedom of lightwave. Since then, it has been attracted much research interest and shown the potential on various applications. Compared with the bulk optics, photonic integrated devices are much more compact and, the most importantly, compatible with the matured CMOS fabrication process. We has proposed and demonstrated integrated OAM emitter, plasmonic vortex array, angular momentum beam splitter and sorter, the method to

identify the topological charge carried by OAM beam, etc. An integrated OAM emitter with a wide switching range of OAM modes was demonstrated. The independence of the micro-ring cavity and the gratings unit provides the flexibility to design the device and optimize the performance[8]. We also proposed an integratable method of generating vortex Smith-Purcell radiation by having free electrons pass on holographic gratings and numerical results indicated that the OAM wave with different topological charge could be obtained[9].

Photons are ideal flying qubits. Photonics provides an important way to develop quantum information technology. A quantum information system based on photonics includes functional units for quantum state generation, manipulation, and detection. How to integrate these functions on a photonic chip is a crucial technology for future quantum information applications. We have developed comprehensive solutions on integrated quantum light sources for various quantum entangled state generation at telecom band, based on spontaneous four wave mixing in silicon waveguides and micro-ring resonators. We also developed technologies of quantum state manipulation and detection on a silicon photonic chip[10]. Utilizing high-performance energy-time entangled photon pairs generated in silicon waveguides, we proposed and demonstrated a scheme of temporal ghost imaging based on the frequency correlation in the photon pairs, then developed a quantum secure ghost imaging scheme based on it[11]. Recently, we realized a fully connected quantum key distribution (QKD) network with 40 users and 780 QKD links based on a silicon photonic quantum light source [12]. It is the entanglement-based QKD network with the largest user number to the knowledge of authors.

In summary, the research achievements of our research group in the field of nanostructure optoelectronic chips are reviewed. Various nanostructures have been successfully developed to control the mechanism of photons, electrons, phonons, surface plasmon polariton and their interactions, and a series of new functional optoelectronic chips have been realized, such as free electron radiation, real-time spectral imaging, phonon sensing, optical orbital angular momentum radiation, quantum state generation and control. At present, some of the chips are being industrialized and expected to become practical in the near future.

Keywords:optoelectronics; nano-structure; photonic crystals; optomechanical crystals; free-electron radiation; optical orbital angular momentum; quantum state generation and control

最终交流类型: Oral

Strain engineering of 2D semiconductor materials and flexible optoelectronic devices

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Elastic strain engineering is a technique to regulate the electronic structure of materials by altering the relevant structure and mechanical properties of the materials. In the past decades, this technology has been widely applied in the semiconductor industry, in order to increase the electrical performance of the device by improving the carrier mobility of the silicon. However, the traditional semiconductor single crystal materials due to the limited strain that can be sustained, largely restricting the ability to regulate the electronic properties of semiconductor materials through elastic strain. Recently, two-dimensional layered materials have attracted considerable attention, which is characterized by a strong covalent bond within the plane, while the layers are only connected by very weak van der Waals force. Among the most remarkable two-dimensional (2D) materials are graphene, hexagonal boron nitride (h-BN), black phosphorus (BP) and transition metal dichalcogenides (TMDs) such as MoS2, WS2, WSe2, etc. These materials possess distinctive optical and electronic properties. More importantly, these 2D materials are generally able to endure greater elastic strain than bulk materials without damage. For example, most graphite materials will break when strained to 0.1%, but single-layer graphene can withstand 25% elastic strain. This makes 2D materials a promising field to explore in elastic strain engineering. Therefore, the strain engineering of 2D materials has a wide range of research prospects and potentials. In this report, I will report some recent research progress in strain engineering of 2D semiconductor materials and flexible optoelectronic devices to the teachers. These include: experimental evidence of nanoscale local strain modulation induced ferromagnetism in 2D ReSe2; strain engineering of band, excitonic properties of 2D GaSe and PbI2, realization of wide-spectrum light absorption and enhancement of light absorption efficiency by designing nanoscale wrinkled morphology, providing theoretical and experimental basis for the construction of high-performance solar cell devices; modulation of WSe2/WS2 heterojunction coupling properties and excitonic emission characteristics by applying strain on flexible substrates; Preparation of strain sensors based on two-dimensional GaSe and SnSSe, realizing characteristics of resistive, repeatable, and high strain sensitivity.

Keywords:2D semiconductor materials, Strain engineering, Wrinkle strain structures, flexible optoelectronic devices

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最终交流类型: Invited

Quantum light sources based on III-V Quantum Dots

刘峰

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Single-photon sources play a key role in photonic quantum technologies. Semiconductor quantum dots (QDs) can emit indistinguishable single photons under resonant excitation.

However, the resonance fluorescence technique typically requires cross-polarization filtering, which causes a loss of the unpolarized quantum dot emission by 50%. In this talk, we will present a method for generating indistinguishable single photons with optically controlled polarization by two laser pulses off-resonant with neutral exciton states. This scheme is realized by exciting the quantum dot to the biexciton state and subsequently driving the quantum dot to an exciton eigenstate. By combining with a magnetic field, we demonstrated the generation of photons with optically controlled polarization (the degree of polarization is 101(2)%), laser-neutral exciton detuning up to 0.81 meV, high single-photon purity (99.6(1)%), and indistinguishability (85(4)%). Laser pulses can be blocked using polarization and spectral filtering. Our work makes an important step toward indistinguishable single-photon sources with near-unity collection efficiency.

In addition to generating single photons, semiconductor QDs can also generate entangled photon pairs deterministically with high entanglement fidelity. In this talk, we will present wavelength-tunable on-demand entangled photon sources based on droplet-etched GaAs quantum dots. Such wavelength-tunable entangled photon sources are crucial for constructing large-scale quantum internet and integrated quantum optical circuits.

Finally, we will present an all-optical method to control high-orbital states of a hole. To date, coherent manipulation of single charge carriers in quantum dots is limited mainly to their lowest orbital states. Ultrafast coherent control of high-orbital states is obstructed by the demand for tunable terahertz pulses. In this talk, we will present a method to control high-orbital states of a hole via stimulated Auger process. The coherent nature of the Auger process is proved by Rabi oscillation and Ramsey interference with a fidelity of 95.9%. Harnessing this coherence further enables the investigation of single-hole relaxation mechanism. A hole relaxation time of 161 ps is observed and attributed to the phonon bottleneck effect. Our work opens new possibilities for understanding the fundamental properties of high-orbital states in quantum emitters and developing new types of orbital-based quantum photonic devices.

Keywords:quantum dot, single photon source, entangled photon source, photonic crystal cavity

最终交流类型: Keynote

Sub-nanometer Resolved Single-Molecule Optical Imaging

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Aspirations for reaching atomic resolution with light have been a major force in shaping nano-optics, whereby a central challenge is to achieve highly localized optical fields. The plasmonic nanocavity defined by the coinage-metal tip and substrate in a scanning tunneling microscope (STM) can provide highly confined and dramatically enhanced electromagnetic fields upon proper tuning of plasmonic resonance, which can modify both the excitation and emission of a single molecule inside the nanocavity and produce intriguing new optoelectronic phenomena. In this talk, I shall demonstrate two recent STM-based phenomena related to single-molecule optical spectroscopy. The first is single-molecule Raman scattering [1]. The spatial resolution of tip enhanced Raman spectroscopy (TERS) has been further driven down to the Angstrom scale at the single-bond level [2,3]. Such a capability not only yields a new methodology called scanning Raman picoscopy for structural reconstruction [3] and tracking bond breaking and forming of surface reactions [4,5], but also enables to clarify the chemical enhancement mechanism in TERS through well-controlled local contact environments [6,7]. The second phenomenon is single-molecule electroluminescence. Through managements over molecular quenching and energy level alignment, we demonstrate clear single-molecule electroluminescence and even single-photon emission [8]. Furthermore, by precisely controlling intermolecular distances, we can not only demonstrate coherent dipole-dipole coupling in homodimers [9], but also reveal intriguing transitions from incoherent hopping-like Forster energy transfer to coherent wavelike electronic energy transfer in donor-acceptor heterodimers [10]. In addition, the wavelike quantum-coherent transfer channel is found three times more efficient than the incoherent channel in a one-step transfer process, highlighting the advantage of coherent channels in electronic energy transfer processes in large molecular networks. Our results provide new routes to optical imaging, spectroscopy and engineering of light–matter interactions and intermolecular coupling at the sub-nanometer scale.

Keywords: Optical imaging, Nano-imaging, Single molecules, Nano-photonics and optoelectronics

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最终交流类型: Invited

Confined-enhanced Raman spectroscopy

Jixiang Fang

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The discoveries of surface-enhanced Raman spectroscopy (SERS) have ever rekindled broad interests of the scientific community owing to its enormous potential in many fields, like food science, environment, public safety, etc. However, regretfully, these techniques have not been successfully commercialized and used for practical applications yet. The molecule-nanostructure interactions should be proposed to be intensively studied since the adsorption and desorption behaviors of target molecules on the surface of nanostructures are crucial to the SERS property. Here, we report a strategy, which we name confined-enhanced Raman spectroscopy, in which the overall Raman properties can be remarkably improved with in situ formed active nanoshells on gold nanoparticles. The in situ-formed packaged active nanoshell can confine and anchor molecules onto the surface of plasmonic nanoparticles, and avoid desorption from hot spots so that the blinking effect can be eliminated in the time-resolved SERS spectra. It is the first time to realize the single-molecule detection of analytes with super sensitivity, high stability, and high signal reproducibility based on gold nanoparticles. In addition, in practical application, we can design packaged nanoshells with different components to make this strategy suitable for SERS detection in diverse molecule systems, including biomedical diagnosis and catalytic reaction.

Keywords:single-molecule SERS，confined-enhanced Raman spectroscopy，in situ-packaged shell

最终交流类型: Oral

Co-deposition of hole-selective contact and absorber for improving the processability of perovskite solar cells

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中国科学院大学

Simplifying the manufacturing processes of renewable energy technologies is crucial to lowering the barriers to commercialization. In this context, to improve the manufacturability of PSCs, we have developed a one-step solution-coating procedure in which the hole-selective contact and perovskite light absorber spontaneously form, resulting in efficient inverted PSCs. We observed that phosphonic or carboxylic acids, incorporated into perovskite precursor solutions, self-assemble on the indium tin oxide substrate during perovskite film processing. They form a robust self-assembled monolayer as an excellent hole-selective contact while the perovskite crystallizes. Our approach solves wettability issues and simplifies device fabrication, advancing the manufacturability of PSCs. Our PSC devices with positive–intrinsic–negative (p-i-n) geometry show a power conversion efficiency of 24.5% and retain >90% of their initial efficiency after 1,200 h of operating at the maximum power point under continuous illumination. The approach shows good generality as it is compatible with different self-assembled monolayer molecular systems, perovskites, solvents and processing methods.

Keywords:Perovskite, Solar cells, Co-deposition, SAM, manufacturability

最终交流类型: Invited

Nonlinear optical studies on low dimensional structures

刘韡韬

复旦大学

Two-dimensional (2D) materials with honeycomb lattices have been of great interest in recent years for their peculiar optical and electronic properties, and optical second-harmonic generation (SHG) has become widely used as a powerful in situ, noninvasive tool to characterize these 2D systems, providing both spectroscopic and structural information about material properties. On the other hand, most previous studies remained qualitative, and it is desirable if we could further extract quantitative, microscopic information about various TMD lattices from SHG responses. We provide an analytical method for extracting detailed structural information about 2D honeycomb lattices from SHG anisotropy patterns based on the molecular bond additivity model. We applied the method to both strained TMD layers and multiwalled WS2 nanotubes on a single-tube level. As it is highly sensitive to the crystallographic symmetry, SHG microscopy unveiled multiple structural domains within a single WS2 nanotube, which are otherwise hidden under conventional white-light optical microscopy. Moreover, the polarization-resolved SHG anisotropy patterns revealed that different domains on the same tube can be of different chirality. In addition, we observed the excitonic states of individual WS2 nanotubes via SHG excitation spectroscopy, which were otherwise difficult to acquire due to the indirect band gap of the material.

Indium selenide (InSe), a layered semiconductor with direct band gap and high carrier mobility, holds promising applications in bendable electronics and ultrafast optoelectronics. Yet its crystal structure exhibits polytypism with four different stacking orders that are nearly-degenerate in energy but are predicted to have contrasting electronic structures for versatile applications. We found the unambiguous discrimination of different InSe polytypes using symmetry-sensitive oblique incident optical second harmonic generation (SHG) is demonstrated. These results would help promoting the precise application of InSe crystal for piezoelectric transducer and strain sensing, as well as showing the oblique incident SHG to be a powerful structural analytical tool for van der Waals layered materials. Overall, our method will help quantitative studies of 2D materials with SHG and is readily applied to more general cases.

Keywords:SHG; 2D honeycomb lattice; bond additivity model

最终交流类型: Invited

Confined-Enhanced Raman Spectroscopy

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Recently, infrared selective thermal emitters have been proposed to act as cost-efficient infrared sources, providing a new platform for plenty of infrared applications in biochemical sensing, [thermal imaging, thermophotovoltaics, radiative cooling, super-Planckian near-field thermal radiation and spectroscopy characterization. Based on a variety of optical designs, such as grating, FP cavity, Tamm plasmon polaritons (TPPs), photonic crystals, metamaterials, metallic and dielectric metasurfaces, flexibly controllable thermal emitters have been proposed.

With the rapid development of infrared applications, there is an increasing demand for micro-molecular sensors with multiple characteristic wavelengths in LWIR (long-wave infrared range). It is of great significance to study the multiband thermal emitters which can cover the LWIR as much as possible. The research of thermal emitters with high spatial resolution is also crucial for the applications of infrared micro-molecular sensing and imaging. Although plasmonic metasurfaces based multiband thermal emitters have been proposed, exposed dielectric middle spacers with infrared emission in these structures would increase the background thermal emission and then subsequently weaken the contrast between desirable thermal emission signal and background noise in thermal imaging. Higher thermal imaging contrast is beneficial for achieving higher spatial resolution. A microchip which simultaneously possesses multiband thermal emission peaks in LWIR and highly improved thermal imaging contrast is rarely reported up to now.

In this work, based on a micro-meta-cavity array that combines metasurfaces and FP cavity, we propose a thermal emission microchip with high spatial resolution. Various meta-cavities can be designed for desired resonant wavelengths. We have designed a 3×3 meta-cavity array to realize multiband thermal emission by varying the length and period of the nanohole unit cell, covering two LWIR domainsand . The coupling between metasurfaces and FP cavity is manipulated to realize narrower thermal emission peak than that of a sole metasurface or FP cavity. Through designed meta-cavity patterns, we experimentally demonstrate polarization, wavelength and spatial multiplexing thermal emission with a high spatial resolution near wavelength scale. The high spatial resolution obtained is attributed to the large thermal imaging contrast between the meta-cavity and the surrounding planar gold layer. This meta-cavity design opens up a new avenue for micro-thermal imaging and micro-molecular sensing.

Keywords:metasurfaces, meta-cavity, thermal emission, optical absorption

最终交流类型: Invited

Exploring nanopolaritons and local-strains in low-dimensional materials with SNOM

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Polaritons in two-dimensional (2D) materials, such as plasmon polaritons in graphene and phonon polaritons in hBN, have shown their unique capabilities to concentrate light into deep subwavelength scales. Precise control of the excitation and propagation of 2D polaritons has remained a central challenge for future on-chip nanophotonic devices and circuits. To solve this issue, we exploit Cherenkov radiation, a classic physical phenomenon that occurs when a charged particle moves at a velocity greater than the phase velocity of light in that medium, in low-dimensional material heterostructures. Here, we report an experimental observation of Cherenkov phonon polariton wakes emitted by superluminal one-dimensional plasmon polaritons in a silver nanowire and hexagonal boron nitride heterostructure using near-field infrared nanoscopy. The observed Cherenkov radiation direction and radiation rate exhibit large tunability through varying the excitation frequency. Such tunable Cherenkov phonon polaritons provide opportunities for novel deep subwavelength-scale manipulation of light and nanoscale control of energy flow in low-dimensional material heterostructures.

Strain plays an important role in condensed matter physics and materials science because it can strongly modify the mechanical, electrical, and optical properties of a material and even induce a structural phase transition. Strain effects are especially interesting in atomically thin two-dimensional (2D) materials, where unusually large strain can be achieved without breaking them. Measuring the strain distribution in 2D materials at the nanometer

scale is therefore greatly important but is extremely challenging experimentally. Scanning near-field optical microscopy (SNOM), is a microscopy technique for nanostructure investigation that breaks the far field optical resolution limit by exploiting strongly confined evanescent waves.

In this talk, I will first briefly introduce the SNOM technique, and then talk about a few examples of exploring novel polaritons and local-strains in low-dimensional materials with SNOM, including detection of local strains in hBN and bilayer graphene, Cherenkov radiation of phonon polaritons in silver-nanowire/hBN heterostructures.

Keywords:SNOM，polaritons, local strain, low-dimensional materials

最终交流类型: Invited

Metasurface Enabled Photothermoelectric Photoresponse of Semimetal Cd3As2

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The three-dimensional Dirac semimetal Cd3As2, a bulk analog of graphene, has attracted widespread attention because of its ultrahigh carrier mobility and gapless Dirac band structure. Similar to graphene, Cd3As2 can be used in broadband photodetectors with a detection spectrum ranging from ultraviolet to long-wave infrared. In contrast to monolayer graphene, which has an absorption coefficient of ~2.3%, the bulk characteristics of Cd3As2 endow it with a strong absorption capability and consequently better photoresponsivity. In addition, similar to graphene, the Cd3As2 photodetector exhibits an ultrafast response up to the picosecond scale, as revealed by previous femtosecond pump-probe measurements. Meanwhile, the oxidation layer on the surface of Cd3As2 provides good stability through isolation from the external environment. Therefore, Cd3As2 is a promising material for high-performance photodetectors.

Owing to the metallic nature, external bias can lead to high dark currents in photodetectors based on semimetals. Therefore, such photodetectors usually operate without external bias, which limits the charge separation of photoexcited carriers and subsequent photoresponsivity. In an unbiased photodetector, the nonzero photoresponse depends on the generation and subsequent separation of electron-hole (e–h) pairs. The charge separation mechanism of the Cd3As2 photodetector primarily includes the photovoltaic (PV), photo-Dember (PD), and photothermoelectric (PTE) effects. Among these, the PV effect uses the built-in electric field induced by the work function difference between Cd3As2 and metal electrodes to separate the photoexcited e–h pairs, resulting in photovoltage. The PD effect arises from the asymmetric diffusivity of photoexcited electrons and holes, which creates a transient spatial charge distribution and hence a voltage buildup. However, the photoresponses of Cd3As2 photodetectors based on the PV or PD effect are adjacent to the metal electrode, which restricts the response area and potential applications of the photodetector. The PTE effect generated by the temperature gradient-induced electron diffusion rate difference also plays a critical role in the generation of the photoresponse of the Cd3As2 photodetector, as revealed by terahertz emission investigations. The PTE effect enables the efficient harvesting of energy, high-efficiency photoelectric energy conversion, and photodetection.20-21 Recent progress in the discovery of topologically enhanced shift current response as an efficient charge separation mechanism has significantly boosted the development of photodetectors based on semimetallic materials, particularly in the mid-infrared range. But such charge separation mechanism is limited to inversion symmetry broken Weyl semimetals and does not apply to Dirac semimetals with inversion symmetry. Alternatively, the excellent thermoelectric properties of Dirac semimetal Cd3As2 and the flexible engineering of metasurfaces can induce efficient charge separation through the PTE effect, which can serve as an efficient charge separation mechanism for semimetal-based photodetectors.

In this study, we designed and fabricated a metasurface onto a Cd3As2 photodetector to artificially engineer its photoresponse. The absorption enhancement of the Cd3As2 by the metasurface results in temperature gradient distributions near the boundaries and generates thermoelectric photoresponses through the PTE effect. Power-dependent photocurrent measurements show that the Cd3As2 metasurface device has a linearly dependent photoresponse as a second-order effect. Moreover, wavelength-dependent photocurrent measurements illustrate that the metasurface can enhance the photoresponses over a broadband range from 488 nm to 4 μm. Particularly for 650-nm (1.91 eV) and 720-nm (1.72 eV) excitation, the photocurrent responsivities at the metasurface boundaries increased by one order of magnitude compared with those near the electrode junctions. The Cd3As2 metasurface device exhibited a responsivity of approximately 1 mA/W. Although Cd3As2 has a nearly isotropic photoresponse because of its centrosymmetric lattice, the metasurface provides a linear polarization-dependent photoresponse with a ratio of anisotropy of ~2.1.

The metasurface makes it possible to develop polarization-sensitive photodetection for other non-centrosymmetric topological semimetals. The measurements of photoemission electron microscopy (PEEM) showed higher photoemission on the Cd3As2 metasurface due to the higher electric field resulting from the interference of incident light and quasi-cylindrical waves (QCW). Finite-difference time-domain (FDTD) simulations also show the absorption enhancement diagram of the Cd3As2 metasurface. These findings demonstrate the considerable potential of designing metasurfaces for artificially controllable PTE photoresponse of photodetectors.

Keywords:metasurface, photothermoelectric effect, photodetector, semimetal nanoplate

最终交流类型: Invited

All-dielectric metasurfaces for vortex generation

肖淑敏

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Optical vortex beam carrying orbital angular momentum (OAM) has been intensively explored due to its promising potential in high-capacity optical communications and quantum optics. A series of techniques have been developed for creating optical vortices including spiral phase plate, hologram, spatial light modulator, and modulated microcavities. Metasurface is one prominent example. The flat-profile of metasurface is essential to minimize and integrate the OAM beam generator. Its sub-wavelength unit size can greatly increase the resolution, crucial for high quality vortices. Recently, vortex beam with topological charge up to l = 100 and multiplexed vortex beam array have been successfully produced with metasurface J-plate and vortex metalenses, respectively. Despite of these progresses, the typical metasurfaces only consider the phase modulation of eilf. Under the illumination of Gaussian beams, the modulated outputs are not the eigenmodes in quadratic index media and shall spread to other radial orders, resulting in relatively low purity and restricting practical applications in communications, quantum random walk, as well as the high-precision interferometric experiment.

We introduce a new paradigm for generating high-purity vortex beams with metasurfaces. By applying optical neural networks to a system of cascaded phase-only metasurfaces, we demonstrate the efficient generation of high-quality Laguerre-Gaussian (LG) vortex modes. Our approach is based on two metasurfaces where one metasurface redistributes the intensity profile of light in accord with Rayleigh-Sommerfeld diffraction rules, and then the second metasurface matches the required phases for the vortex beams. Consequently, we generate high-purity LGp, l optical modes with record-high Laguerre polynomial orders p=10 and l=200, and with the purity in p, l and relative conversion efficiency as 96.71%, 85.47%, and 70.48%, respectively. Our engineered cascaded metasurfaces suppress greatly the backward reflection with a ratio exceeding -17 dB. Such higher-order optical vortices with multiple orthogonal states can revolutionize next-generation optical information processing.

Keywords:metasurface,vortex light

最终交流类型: Invited

Exciton Polaritons Enabled Low-threshold lasing of Halide Perovskite Single-Crystal Microstructures

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Exploring exciton-polariton in emergent micro/nano-sized semiconductors with large oscillation strength, such as halide perovskites, is important for the development of low-consumption nonlinear light sources, e.g. lasers. In this talk, I will introduce some recent results on the exciton polaritons and low-threshold lasing of metal halide perovskite (CsPbBr3) single-crystal microstructures grown by chemical vapor deposition and anti-solvent methods. These microstructures exhibit great optical quality and can form active optical microcavities with the side-facets serving as reflectors, and the semiconductors as gain media. Main results include: 1) probing the light slowing effect in the perovskite microstructures with strong exciton-photon coupling, and showing that the light slowing effect is stronger in the microstructures with the smaller volumes; 2) realizing the continuous-wave optically pumped lasing from the perovskite microstructures, and revealing that the exciton polaritons increases the group index, modal confinement and thus reducing the lasing threshold; 3) developing a continuous-wave optically pumped laser with the device area smaller than 1 mm2, and uncovering an abnormal scaling law of lasing threshold and cavity sizes in strong exciton-photon coupling regime. These findings suggest that halide perovskite

family provide an idea platform to study strong light-matter interaction and develop exciton polariton devices with great potentials in next-generation all-solid state quantum technologies.

Keywords:exciton polaritons, strong light-matter interaction, perovskite, microlaser, nanolaser

最终交流类型: Invited

On the Metastability of the Optoelectronic CsPbI3 Perovskite Phase and How to Tame It

Julian Steele

The University of Queensland

A new generation of semiconducting materials based on metal halide perovskites has been launched into the scientific spotlight, exhibiting outstanding optoelectronic properties and providing promise for the development of efficient optical devices [1]. As a vivid example, solar cells made from these materials have quickly reached conversion efficiencies on par with well-established technologies, like silicon. Their widespread success is due, in part, to a unique ability to retain high-quality optoelectronic performance while being easily solution-processed into thin films. However, the interesting photophysics of metal halide perovskites come with a catch; their soft ionic structure promotes complex thermal-induced phase transitions and a variety of dynamic structural behaviors. Such properties have ultimately made understanding several important structure–property relationships ambiguous and obstructed a clear technological path due to inherent phase instability [2].

Our aim in this contribution is to highlight the fundamental aspects of metal halide perovskites that dictate a stable crystal structure, through the lens of thermodynamic preference and phase formation energies [3]. Taking the all-inorganic CsPbI3 system as a suitable case study, we focus on several ways in which its thermodynamically unstable perovskite structure can be maintained at room temperature and elucidate the restructuring pathways taken during destabilization. In addition, we will discuss the origin and mechanisms of phase decay within real-world devices, with emphasis made toward direct visualization using advanced in situ techniques and arriving at quantitative results. For several notable features of halide perovskites dealt with in this contribution, e.g., strain [4,5] and compositional stabilization [6], environmental phase change triggers [7], the non-perovskite phase restructuring pathway [3], and lattice anchoring [8], we attempt to rationalize them using state-of-the-art materials modelling techniques.

It is within this spirit that we not only modify the phase stability of metal halide perovskites, but regulate it for enhanced functionality.

Key Words Perovskite, polymorphic, condensed matter

最终交流类型: Invited

Exceptional point induced mode switching in non-Hermitian waveguide systems

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Degeneracy points of eigenvalues in the parameter space of non-Hermitian systems are known as exceptional points (EPs). Differing from degeneracy points in Hermitian systems, the corresponding eigenvectors also degenerate at EPs, which leads to various novel physical properties and fascinating phenomena. In particular, the distribution of eigenvalues in the vicinity of EPs of non-Hermitian systems represents as typical Riemann surfaces with multiple branches. As a result, dynamically encircling the EPs in the parameter space gives rise to the transfer from one eigenmode to another. Under the situation that the parameters evolve slowly along a closed trajectory encircling the EP, the mode switching is only related to the evolution direction of the parameters rather than the initial state due to the effect of nonadiabatic transition. The asymmetric mode switching possesses great potential for developing non-reciprocal optical devices such as optical isolators and beam splitters.

Keywords: Non-Hermitian system, Exceptional point, Nanophotonics, Waveguide, Mode switching

最终交流类型: Keynote

Advancing nanolasers based on photonic topological cavities

Hong-Gyu Park

Korea University

Nanolasers are key elements in the implementation of optical integrated circuits owing to their low lasing thresholds, high energy efficiencies, and high modulation speeds. With the development of semiconductor wafer growth and nanofabrication techniques, various types of wavelength-scale and subwavelength-scale nanolasers have been proposed. For example, photonic crystal lasers and plasmonic lasers based on the feedback mechanisms of photonic band gap and surface plasmon polaritons, respectively, have been successfully demonstrated. In addition, nanolasers employing new mechanisms of light confinement, including bound states in the continuum (BIC) lasers and photonic topological insulator (TI) lasers and, have been developed. In particular, vortex nanolasers with orbital angular momenta were recently demonstrated based on topological disclination states. In this talk, I outline the operational mechanisms, optical characterizations, and practical applications of these nanolasers based on recent results in my research group. Their scientific and engineering challenges will be discussed.

Key Words nanolasers, photonic crystal laser, plasmonic laser, BIC laser, photonic topological cavity

最终交流类型: Keynote

Meta-couplers for linking propagating waves and surface waves

周磊

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Metasurfaces are ultra-thin metamaterials composed by artificial planar meta-atoms arranged in some specific macroscopic orders, which exhibit extraordinary capabilities to control light waves [1]. In particular, gradient metasurfaces can serve as an ideal bridge to link propagating waves and surface waves [1]. In this talk, I will review our ten-years' efforts in designing high-efficiency meta-couplers to convert propagating light to surface waves with controllable wave-fronts [1-4]. Specifically, I will introduce our latest efforts of using a meta-coupler to efficiently squeeze incident light to on-chip photonic devices with subwavelength openings [4].

Keywords:Metasurfaces, surface plasmons, on-chip photonics

Reference:

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最终交流类型: Oral

Phase-Dependent the Optical Properties in Colloidal Semiconductor Nanocrystals

宁甲甲

吉林大学

In the past decades, semiconductor nanocrystals (NCs) have attracted scientists' attention due to their quantum confinement effect, showing the potential for solar cell, light-emitting diodes, optoelectronic devices and biomedical target. Crystal structure, as one of the intrinsic properties, gives the periodicity of atoms' arrangement in materials, which can influence most of the properties in materials.

We developed the synthetic routes for one-dimensional ZnSe nanorods (NRs) with cubic ZB and hexagonal WZ structure.1-3 The nuclei dependent the dimension was proposed to explain the formation mechanism of ZnSe NRs with cubic ZB structure. The further ZnS shell growth on ZnSe NRs also showed the different growth procedure for the different phased NRs.4 ZnS shell preferred to grow at sides of ZnSe NRs with cubic ZB structure, the aspect ratio of ZnSe NRs with become smaller, even to dot-shaped. However, the island-growth can be observed on WZ ZnSe NRs after the growth of a few monolayers ZnS shell. After the ZnS shell growth, the photoluminescence quantum yield is greatly improved to 40% for ZnSe NRs.

Compared to ZnSe NRs with WZ structure, ZB phased ZnSe NRs exhibited the much faster photoluminescence emission lifetime, meaning the potential of ZnSe with ZB structure for light-emitting diodes device. Polarized emission is a special optical property in anisotropic nanostructures, ZnSe NRs with the blue region emission also exhibited polarized emission. Unusually, the shorter ZnSe NRs with ZB phase gave the bigger emission anisotropy than the longer NRs with WZ structure. The stronger pilar moment induced by the anisotropic structure in the cubic crystal structure was proposed to explain the difference in emission anisotropy between ZB and WZ ZnSe NRs.

Keywords:crystal structure, optical properties, semiconductor nanocrystals

最终交流类型: Invited

Twisted Lattice Nanocavity with Quality Factor Exceeding 200 Billion

Renmin Ma

Peking University, China

Simultaneous localization of light to extreme spatial and spectral scales is of high importance for testing fundamental physics and various applications. However, there is a long-standing trade-off between localizing light field in space and in frequency. Here we discover a new class of twisted lattice nanocavities based on mode locking in momentum space. The twisted lattice nanocavity hosts a strongly localized light field in a 0.048 lambda^3 mode volume with a quality factor exceeding 2.9×10^11 (~250 ms photon lifetime), which presents a record high figure of merit of light localization among all reported optical cavities. Based on the discovery, we have demonstrated silicon based twisted lattice nanocavities with quality factor over 1 million. Our result provides a powerful platform to study light-matter interaction in extreme condition for tests of fundamental physics and applications in nanolasing, ultrasensing, nonlinear optics, optomechanics and quantum-optical devices.

Keywords:Twisted Lattice Nanocavity, light mater interaction, Purcell factor, Quality factor, mode volume

最终交流类型: Oral

Eco-friendly indium phosphide quantum dot light-emitting diodes regulated by shell engineering

赵家龙

广西大学

Semiconductors quantum dots (QDs) have derived considerable attention in display due to their tunable wavelength, high emission efficiency and extraordinary color purity, stability, and solution processability, which make their display devices such as quantum dot light emitting diodes (QLEDs) more competitive compared to the liquid crystal display. However, though Cd-based QLEDs on three primary colors have already approached extraordinary external quantum efficiency with excellent stability and high color purity, the intrinsic toxicity of heavy metal element Cd might induce adverse repercussions no matter on humanity health or environment. Therefore, it is significant to find eco-friendly QDs with less toxicity.

First the synthesis of InP QDs is generally based on a kind of expensive liquid inflammable phosphorus, tris(trimethylsilyl)phosphine which can spontaneously ignite in air and explode at high thermal energy. Therefore, we find a less expensive, harmless, and more environmentally friendly phosphorus to promote the applications of InP QDs. We have successfully synthesized various InP QDs covered the whole visible photoluminescence spectra and fabricate QLEDs on primary colors to demonstrate those QD emitters' possibility on practical applications.

Further although the red-emitting InP QDs and QLEDs have already made great achievements, the study on green InP-based QLEDs still lagged behind. As the most sensitive color of human eyes, it is of particular importance to improve the performance of green InP-based QLEDs for better application in display. Meanwhile, the color purity of InP QDs suffers from a broad size distribution and generously exhibits a broad linewidth. Thus, we meticulously design and regulate the inner shell component to balance the lattice stress, diminish interface defects and facilitate the homogenous growth of outer shell. As a consequence, the regulated green InP/ZnSeS/ZnS QDs exhibit the narrowest FWHM (~35 nm) photoluminescence and excellent efficiency (~97%). Remarkably, the pure green-emitting InP QLEDs with EQE (15.2%) were obtained.

Keywords: Keywords: Quantum dots, Quantum dot light emitting diodes, Indium phosphide, Photoluminescence, Electroluminescence

最终交流类型: Oral

Topological Single Photon Emission from Quantum Emitter Chains

Yubin Wang

Tsinghua University

We propose a scheme for generating highly indistinguishable single photons from an active quantum Su-Schrieffer-Heeger chain composed of a collection of noisy quantum emitters. Strikingly, the single photon emission spectrum of the active quantum chain is exceedingly narrow relative to that of a single emitter or a topologically trivial chain. Furthermore, this effect is amplified dramatically in proximity to the non-trivial-to-trivial phase transition point. Exploiting this effect, we demonstrate that the single photon linewidth of a long topological quantum chain can be arbitrarily reduced, rendering it an ideal source of indistinguishable single photons. Finally, by analyzing the most critical parameters concerning experimental realization and providing a microscopic and quantitative analysis of our model, we take concrete examples of actual quantum emitters to establish the viability of our proposal.

Keywords: Su-Schrieffer-Heeger model, Single photon emission, Topological transition

最终交流类型: Oral

Polarization-Sensitive Photodetectors Enhanced by Ferroelectric Field

Yan Chen

The Chinese University of Hong Kong (Shenzhen)

Stacking two or more periodic structures to generate moiré patterns has attracted interest and enabled unusual phenomena in electronic and photonic materials. Previous reports of moiré lattices are either patterned in the same plane or formed by closely stacked bilayer lattices. Long-range coupled moiré lattices are desired but have not been possible because the amplitudes of resonant modes typically decay rapidly with spatial separation of the lattices. This talk describes an ultralong-range coupling of photonic lattices in bilayer and multilayer moiré architectures mediated by dark surface lattice resonances. Using dipole emitters as a probe, we demonstrate that plasmonic nanoparticle lattices exhibit moiré phenomena even when the different layers are spatially separated by hundreds of micrometers (three orders of magnitude larger than lattice spacing). Our studies of remote moiré coupling offer a design strategy to realize reconfigurable photonic devices and engineered light-matter interactions.

Keywords:Plasmonic nanoparticle lattices, moiré photonics, lasing, light-matter interactions

最终交流类型: Oral

Core-Shell Plasmonic Metasurface and Devices

邓诗凯

中科院上海微系统所

Plasmonic nanostructures can squeeze light into subwavelength volumes with enhanced local electromagnetic fields important for light–matter interactions in nanophotonics, photochemistry, biosensing, and nonlinear physics. Compared to dielectric resonators that confine optical fields within their high-refractive-index materials, plasmonic nanostructures confine light at nanoscale volumes at their metal-dielectric interfaces. Structural design at the plasmonic nanoparticle surface, which can lead to unparalleled scientific and technological advances, is not readily feasible through conventional processing and metrology techniques. This seminar will highlight how the design and fabrication of core-shell plasmonic nanoparticle lattices can result in fundamental insights and novel applications in plasmonic and photonic devices, including: (1) annealing treatment and chemical vapor deposition process of plasmonic nanoparticle lattices for ultranarrow resonances, (2) interfacial engineering of nanoparticle lattices for nanolasing, and (3) plasmonic photoelectrocatalysis in copper–platinum core-shell nanoparticle lattices.

Keywords:Nanophotonic, plasmonics, nanoparticle lattices, graphene, copper plasmonics

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最终交流类型: Oral

Coherent Optical Spin Hall Transport for Spin-optronics at Room Temperature

石莹

Tsinghua University

Spin degrees of freedom in condensed matter have been proposed as efficient information carriers towards next-generation spintronics. It is crucial to develop effective strategies to generate and control spin currents, e.g., by exploiting the spin Hall or valley Hall effects. However, the scattering, and rapid dephasing of electrons pose major challenges to achieve macroscopic coherent spin currents and realistic spintronic devices, specifically at room temperature, where strong thermal fluctuations could further obscure the spin flow. Exciton polaritons in semiconductor microcavities being the quantum superposition of excitons and photons, are believed to be promising platforms for spin-optronic devices. Long-range spin current flows of exciton polaritons may be controlled through the optical spin Hall effect. However, this effect could neither be unequivocally observed at room temperature nor be exploited for realistic polariton spintronic devices due to the presence of strong thermal fluctuations or large linear spin splitting. Here, we report the observation of room temperature optical spin Hall effect of exciton polaritons with the spin current flow over a distance as large as 60 um in a hybrid organic-inorganic $FAPbBr_3$ perovskite microcavity. We show direct evidence of the long-range coherence at room temperature in the flow of exciton polaritons, and the spin current carried by them. By harnessing the long-range spin-Hall transport of exciton polaritons, we have demonstrated two novel room temperature polaritonic devices, namely the NOT gate and the spin-polarized beam splitter, advancing the frontier of room-temperature polaritonic device in perovskite microcavities.

Keywords:Optical spin Hall effect; Room temperature; Exciton polariton coherent propagation; Polaritonic devices

最终交流类型: Oral

Machine Learning Enables Nanoparticle Rotation Tracking with Optical Microscopy

胡竞天

哈尔滨工业大学（深圳）

Single-particle tracking techniques are crucial for studying biological transport processes such as endocytosis and membrane signaling. In particular, rotational dynamics of nanoscale optical probes can provide information on cellular activities such as protein diffusion and cytoskeleton formation. However, tracking rotational dynamics of these optical probes is challenging due to optical diffraction limitations. In addition, analysis methods that can extract particle orientations reliably from their microscopy images are lacking. Imaging techniques have enabled orientation sensing of rod-shaped nanoparticles based on their polarization-dependent optical responses but are restricted to in-plane rotations due to the symmetry of the probe. A computational particle-tracking platform that combines advances in

imaging technique, probe design, and computational analysis method is needed to realize 3D rotation tracking of single nanoparticles.

This presentation reports an imaging platform based on deep-learning algorithms and differential interference contrast (DIC) microscopy for tracking the 3D rotations of nanoparticle optical probes. To establish the deep-learning models, we constructed large image datasets of anisotropic nanoparticles with labeled orientations. In all imaging environments, the optimized models could predict the particle orientations from their DIC images with an accuracy limited only by instrumental approach. Lastly, we demonstrated that the deep-learning model could achieve 3D orientation tracking with in-plane and out-of-plane rotations determined simultaneously.

Keywords:Machine learning, convolutional neural networks, differential interference contrast microscopy, imaging probe

最终交流类型: Oral

Ultrafast Coherent Dynamics of Exciton Polariton Propagation at Room Temperature

陈俞忠

北京量子信息科学研究院

Exciton polaritons are widely considered as promising platforms for developing room temperature polaritonic devices, owing to the high-speed propagation and nonlinear interactions.[1] However, it remains challenging to explore the dynamics of exciton polariton propagation specifically at room temperature where the lifetime could be as small as few picoseconds. In this highly nonequilibrium systems, the prevailing time-averaged measurement methods cannot give access to the true nature of the exciton polariton condensates. Herein, by using the time-resolved photoluminescence spectroscopy approach, we have successfully traced the ultrafast coherent dynamics of a moving exciton polariton condensate in a one-dimensional formamidinium-based (FA-based) hybrid perovskites $FAPbBr_3$ microwire microcavity. The propagation speed of the room temperature exciton polariton condensate is directly measured to be ~ 12.2 um/ps, which is in excellent agreement with the value indirectly extracted by fitting the polariton dispersion with a theoretical model.

Moreover, we have developed a time-resolved Michelson interferometer to quantify the time-dependent phase coherence of the moving condensate, which reveals that the actual coherence time of exciton polaritons could be much longer (nearly 100%) than what was believed before. Our work sheds new light on the ultrafast coherent propagation of exciton polaritons at room temperature.

Keywords: Exciton Polariton, Ultrafast Propagation, Dynamics

最终交流类型: Invited

Ultrafast near-field spectroscopy in low-dimensional materials

Juanmei Duan

Carl von Ossietzky University of Oldenburg

Probing light-matter interactions with ultrafast spectroscopy in low dimensional material gives the possibility to observe novel physical phenomena in condensed matter systems. Especially, near-field microscopy without the optical diffraction limitation can be used to investigate the local optical properties of a sample at nanoscale. A broadband, interferometric scattering-type scanning near-field optical spectroscopy (s-SNOM) technique in our group is applied to reconstruct the complex response function of a single nanostructure in the time domain and with nanometer-spatial resolution. The unwanted background signal in the near-field measurement can be efficiently suppressed by demodulating the optical signal at higher harmonics. In addition, the near-field signal to background ratio can be amplified by employing a homodyne mixing technique, i.e. a Michelson interferometer. Therefore, the amplitude and phase of the local optical near-field from samples with high spatial and spectral resolution can be achieved with our s-SNOM technique. Thus, this unique technique is highly promising in investigating the complex behavior of the strong light-matter interactions in localized quantum emitters with nanoscale. Moreover, strong optical near-fields can couple with wavepackets of free, 100 eV electrons with < 50 fs temporal resolution in an ultrafast point-projection microscope. Phase matching between electrons and near field is achieved due to strong spatial confinement of the near field from the nanometer-sized Yagi-Uda antenna. Phase modulation of the electron by transverse-field components results in a transient electron deflection, which allows us to direct mapping of different vectorial components of highly localized optical near fields. This brings the vast capabilities of in use of photon-induced near field electron microscopy to probe optical fields, to shape electron wave functions.

Keywords： ultrafast optics, near-field optics, SNOM, low dimensional materials

最终交流类型: Invited

Interaction between surface plasmons and excitons

魏红

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When the interaction between an optical cavity and quantum emitters is strong enough to reach the strong coupling regime, exciton polaritons are produced. The exciton polaritons inherit the properties of both light and matter, and show great potentials for applications in physical and chemical sciences and related technologies. Metal nanostructures can confine electromagnetic field into tiny spaces of deep subwavelength scale due to the excitation of surface plasmons and result in a very small mode volume, which leads to a large plasmon–exciton coupling strength. Therefore, plasmonic nanocavities are favorable for realizing strong coupling at room temperature. In recent years, the strong coupling of plasmonic nanostructures and excitons has attracted intense interest.

In this presentation, I will talk about our research on the strong coupling of single plasmonic nanogap structures and nanowires with monolayer transition metal dichalcogenides. We achieved the strong coupling of monolayer WSe_2 and lithographically defined single gold nanobowties, and the intermediate coupling of two exciton states in monolayer MoS_2 and the nanogap structure of silver nanowire on gold film. In the coupling system of single silver nanowires and monolayer WSe_2, we found that the photoluminescence and scattering light share the same spectral profiles resulting from strong coupling, which unifies the photoluminescence and scattering spectra in the plasmon–exciton strong coupling systems and sheds new light on understanding the rich spectral phenomena in the strong coupling regime.

Keywords:surface plasmons, excitons, strong coupling, Rabi splitting, multimode coupling

最终交流类型: Invited

Lateral optical superlattice constructed by heterostructure and modulated homostructure

王琛

清华大学

Layered semiconductor optical materials, represent a material system that is setting for breakthroughs in fundamental research and transformative technologies, with few surface dangling bonds, atomic level uniformity, rich optical structure selection and optics physics, exhibiting excellent optical/electronic properties that are difficult to achieve in other candidates. To make functional optical devices, materials integration to create optical structure is a must-have. For layered optical semiconductor, van der Waals (vdW) integrations is straightforward as it’s 2D essence. Another possibility is lateral integration for lateral optical heterostructure or even lateral optical superlattice. Here we reported lateral integrated optical superlattice by heterostructure, but this solution is limited by lattice mismatch. Thus it’s also necessary to develop a new strategy to create lateral optical superlattice by modulated homostructure, serving as a new solution to create complex optical superlattice for high performance optical devices and photonics.

Keywords:lateral optical superlattice, heterostructure, modulated homostructure

最终交流类型: Oral

Ultracompact Perovskite Lasers: mechanisms, optical designs, integration

Sergey Makarov

Harbin Engineering University

Abstract — Recently, the study of halide perovskites has attracted enormous attention due to their exceptional optical and electrical properties. As a result, this family of materials can provide a prospective platform for modern nanophotonics [1] and metaphotonics [2,3], allowing us to overcome many obstacles associated with the use of conventional semiconductor materials. Resonant halide perovskite micro- and nanocrystals is a rapidly developing research area driven by its potential applications for lasers, nanophotonics, and optoelectronic devices. Here, we overview the recent progress in the field of halide

perovskite microlasers starting from record-small single-particle light-emitting microcrystals supporting lasing generation [4] to the larger designs where the perovskite microlasers [5, 6] are coupled with waveguiding systems [7,8,9].

Keywords:Perovskite, nanolaser, nanoparticle, polariton.

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最终交流类型: Invited

Universal integration of layered semiconductor for high performance nanoelectronics

王琛

清华大学

As scaling of Moore's law slowing down at sub 10nm node, it's necessary even urgent to develop emerging chip materials, novel devices structure, new integration process, special system architecture for post Moore's era. Layered semiconductor materials, represent a material system that is setting for breakthroughs in fundamental research and transformative technologies. Van der Waals (vdW) integrations is straightforward as it’s 2D essence, however, the vdw gap will limit the electron transportation dynamics. Another possible solution is lateral integration, however, it’s hard to integrate material with lattice mismatch 5% or larger. Thus it’s necessary to develop a universal strategy to integrate emerging layered semiconductor in both vdw and lateral dimension, together with 3D integration technology for heterostructure optoelectronics applications, serving as fundamental solution for post Moore era materials hybrid integration for functional and novel devices.

Keywords:vdw integration, lateral integration, hyper mismatch, post Moore's era

最终交流类型: Invited

Natural hyperbolic plasmon polaritons in 2D materials

晏湖根

复旦大学

In-plane hyperbolic plasmon polaritons naturally exist in some 2D materials, which promise applications in on-chip photonics. In this talk, I'll show our investigation of such plasmons in WTe2 thin films through far-field infrared spectroscopy. We have realized tunable hyperbolic plasmons in Mo-doped WTe2 and have shown that stacked bilayers of WTe2 offer us a versatile platform for hyperbolic plasmons.

Keywords:hyperbolic plasmon, WTe2, anisotropy

最终交流类型: Invited

Microcavity exciton polaritons for quantum simulation and computation

Sanjib Ghosh

Beijing Academy of Quantum Information Sciences

Microcavity exciton polariton are hybrid quasi-particles that emerge from the quantum superposition of photons and excitons[1]. Due to their composite nature, exciton polaritons show a variety of rich physical phenomena, such as optical spin-Hall effect [2], higher-order topological lasing [3], and room temperature Bose-Einstein condensate [4]. Motivating from these wide range of physical phenomena, we explore the remarkable promise for harnessing quantum nature of exciton polaritons in semiconductor microcavities for quantum simulation and quantum computation. Previously, it was shown that a graph of exciton polariton condensates can be used for simulating spin Hamiltonians, which in turn solves certain computational tasks [5,6]. We show that a randomly arranged graph of exciton polaritons can be used as a neural network to perform complex pattern recognition[7,8] and can be extended in the

domain of quantum neural network [9,10]. Beyond the quantum simulator regime, we show that semiconductor microcavities can be used for realizing qubits and quantum gates for universal quantum computing[11]. However, there are certain technical limitations in the presently available experimental systems [11]. Finally, we present the idea of a quantum Su–Schrieffer–Heeger system for generating high-quality single photons from a set of noisy emitters [12].

Keywords:Microcavity Exciton Polaritons, Quantum Simulators, Quantum Computing

最终交流类型: Invited

Two-dimensional semiconductors: in-situ characterization and potential optoelectronic application

于霆

武汉大学

Two-dimensional (2D) semiconductors, typically 2D transition metal dichalcogenides (TMDs) exhibit rich fundamental physics and promising optoelectronic applications. In this talk, I will report our works on probing physical properties of 2D semiconductors by some in-situ techniques. The potential optoelectronic applications, in particularly of WS2 will be also discussed.

Keywords:2D， TMD，in-situ， optoelectronics

最终交流类型: Keynote

Roles of phase in manipulation, measurement and reconstruction of light fields

Jianlin Zhao

西北工业大学

As an important parameter of light field, phase plays a very important role in both the propagation and superposition of light fields. The manipulation for the spatial structures of light fields, including the amplitude, phase, polarization and their spatial distributions, can be attributed to the manipulation of their phase distributions in many cases. In addition, the measurement and reconstruction of a complex light field often depend on the measurement and reconstruction of the phase distribution of the light field. This report mainly discusses the relationship between the phase distributions of light fields and their spatial structures, the important and special roles of phase in the efficient generation and multi-dimensional modulation of light fields with special spatial structures, as well as the measurement and reconstruction methods of complex light fields and applications.

Keywords: Roles of phase

最终交流类型: Keynote

Light Trapping and Amplification using Photonic Bound States in the Continuum

Son Tung Ha

Institute of Materials Research and Engineering

The field of nanophotonics has witnessed remarkable progress in the manipulation of light at the nanoscale, leading to unprecedented control over its propagation and interaction with matter [1]. A fascinating phenomenon arising recently is the concept of photonic bound states in the continuum (BICs), which enables the confinement and enhancement of light within a specific region of the electromagnetic spectrum. These advancements hold great promise for applications in various fields, including sensing, energy harvesting, and optical communications. In this talk, I will show that, by leveraging the unique properties of these resonant states, we can develop advanced strategies for enhancing light-matter interactions and harnessing their potential for various optoelectronic applications. The talk will briefly cover the theoretical foundations of photonic BICs, including their origin, characteristics, and underlying physical mechanisms. The design and fabrication of nanostructured systems capable of supporting BICs will also be discussed, highlighting our most recent experimental results in the field. Specifically, the amplification of light through the interaction with gain media will be presented, showcasing the potential for low-threshold lasers [2-5] and strong light-matter interaction [6-7]. The talk concludes with a discussion on the future prospects and challenges in the field. By harnessing the capabilities of photonic BICs, we can pave the way for the development of highly efficient and compact nanophotonic devices, opening new avenues for applications in optical communication, sensing, and quantum technology.

Keywords:nanophotonics, light trapping, strong coupling, nanolasers, bound states in continuum.

最终交流类型: Keynote

Single molecule detection and imaging via nanoscale optical-field and light-matter interaction control

李志远

华南理工大学

In this talk we report our route toward single-molecule detection and imaging, one of the ultimate goals of molecular sciences and optical sciences, via nanoscale optical-field and light-matter interaction control.

Raman scattering carries many key characteristic information in molecular structure, but its weak signal intensity hinders Raman scattering for practical spectroscopic applications. Based on a simple additive concept, we built an optical nanocavity composed of gold nanoparticles sitting on silicon wafers coated with gold film and covered with a 2 nm layer of SO2, screened rhodamine B and the two-dimensional material WS2 as matched molecule and adsorbed surfaces. Due to the synergistic electromagnetic and chemical enhancement mechanisms, Raman spectroscopy can be observed at a minimum concentration of 10-18 M rhodamine B (12 molecules, 5 mm × 5 mm) and with a maximum Raman signal enhancement factor reaching 16 orders of magnitude, thus enabling to detect and localize unambiguously the Raman signal of single molecule.

Microscopy is a kind of technology to observe molecules more visually. Scanning near-field optical microscopy (SNOM) offers a way to break down the diffraction limit of conventional optical microscopy and reach a fine spatial resolution down to ~10 nm, but suffers from low transmission efficiency of optical signal power. We designed and 3D printed a polymer-core/gold-shell spiral-grating conical nanostructured tip on the end facet of single-mode optical fiber. Numerical simulations and optical measurements for this deliberately designed and fabricated high-resolution, high throughput, and high contrast SNOM tip show it has 10% transmission efficiency, ~5 nm spatial resolution of optical imaging, 20 dB signal-to-noise ratio, 7000 pixels per second fast scanning speed, and 50 nm bandwidth around 785 nm. This tip thus enables to transport Ti:Sapphire femtosecond signal and offers the prospect to build a high temporal-spatial resolution optical microscopy and spectroscopy instrument.

Keywords: Single molecule, SERS, SNOM

最终交流类型: Oral

Tailoring polaritons with soliton angle in 2D moiré materials

Zhiqiang Li

Sichuan University

Spatially tailoring polaritons with subwavelength resolution may enable many novel phenomena and applications. In this work, we demonstrate a new pathway for spatial engineering of polaritons using networks of solitons—localized structural deformations—in moiré materials formed by 2D atomic crystals. A key enabling parameter for such control is the soliton angle that characterizes the local strain direction. By visualizing polaritons in minimally twisted bilayer graphene on boron nitride, we demonstrate on–off switching and continuous modulation of polariton-soliton interactions by varying the soliton angle. These behaviors arise from continuous tuning of the local band structure and optical conductivity by soliton angle. Spatial variations of soliton angle profile can be exploited for subwavelength-scale spatial control of the wavefront, propagation direction and phase of polaritons, enabling generation and dynamic manipulation of directional polaritons. These functionalities are enabled by the unique physics of moiré soliton networks, which are unachievable using other techniques. Our findings provide a versatile route for spatial engineering of light–matter interactions at subwavelength scales in diverse moiré systems, opening up opportunities for realizing previously unattainable nanophotonic functionalities.

Keywords:polaritons, spatial engineering, 2D materials, solitons

最终交流类型: Invited

Universal Integration of Layered Semiconductor for High Performance Nanoelectronics

Chen Wang

Hong Kong Polytechnic University

As an emerging class of light-responsive semiconductors, hybrid organo-metal perovskites seamlessly marry the characteristics of organic and inorganic materials, offering a

new fertile playground to explore light-matter interactions. Furthermore, forming heterostructures with judiciously chosen semiconductor materials offers the promise of going beyond the limit of individual perovskite materials in terms of performance and stability. Here, I will show that mixed-halide hybrid perovskites themselves already form heterostructures composed of coexisting multiple crystallographic phases over a wide temperature range, which is correlated with the glassy behavior of organic cations. In addition, band/structure engineering in nano-heterostructures was developed to improve the performance and stability of perovskite devices, via coupling with low-dimensional materials such as 0D quantum dots, 1D carbon nanotubes and 2D metal dichalcogenides.

Keywords:Perovskite; Heterostructure; Optoelectronics

最终交流类型: Invited

All-optical control of semiconductor plasmons

陈佳宁

中国科学院物理研究所

Plasmonics has been widely employed in many application fields, but most use metals or metal-dielectric hybrid structures. To endow semiconductors with similar metallic plasmonic properties was a long-time pursuit by the scientific community owing to the promising perspective of controlling light with an electric method. Pioneer's works demonstrated that light scattering of semiconductor gratings is subjective to the electric gating, and electrical tunable graphene plasmons modes can be visualized in real space. However, bestowing plasmonic properties to the vast category of semiconductors remains unexplored and challenging due to the obstacles in achieving high carrier density by the electric gating method. We successfully achieved optical excitation and manipulation of non-equilibrium plasmons in semiconductors. Non-equilibrium plasmons offer new manipulating methods due to the tunable transient dielectric properties related to the pumping level. Band structures of materials also play a vital role in their transient plasmonic properties. The practical excitation and manipulation of non-equilibrium plasmons introduce the category of semiconductors to the well-established plasmonic field and bring the mid-infrared to Terahertz bands to the adequate plasmonic working bandwidth, which was, as we have known, primarily used in the visible to near-infrared frequency bands. Non-equilibrium

plasmons possess several exotic features over conventional metallic plasmons, such as the anisotropic dispersion that not only differs from metal but is also topologically tunable upon optoelectronic tuning, the fast-triggering time, and the long lifetime, which are all shown in our work.

Keywords:plasmon; small-gap semiconductor; pump probe

最终交流类型: Invited

Cathodoluminescence spectroscopy for nanophotonics

方哲宇

北京大学物理学院

Cathodoluminescence (CL) spectroscopy is proved to be a powerful tool to explore nanoscale optical properties, whereby free electron beams achieve a spatial resolution far beyond the diffraction limit of light. With new methods for the control of electron beams and the collection of light, the dimension of information that CL can access has been expanded to include polarization, momentum, and time, holding the promise to provide invaluable insights into the study of materials and optical near-field dynamics. With a focus on the burgeoning field of CL spectroscopy, this speech outlines the recent advance and applications of this technique, as illustrated by our experimental works.

Keywords:Cathodoluminescence, ultrafast electron microscopy, nanophotonic

最终交流类型: Invited

Geometric Phase and Nonlinear Photonic Metasurfaces

李贵新

南方科技大学

Compared to the conventional optical elements, two dimensional photonic metasurfaces, consisting of arrays of antennas with subwavelength thickness, enable the manipulation of light-matter interaction on a more compact platform. Using metasurfaces, the polarization, phase and amplitude of light can be controlled by spatially variant meta-atoms at the subwavelength scale. Many exotic phenomena in linear optics such as imaging with ultrathin

flat lenses, optical spin Hall Effect, highly efficient holography etc., have been successfully demonstrated. However, growing demand for integrating more functionalities into an optoelectronic circuit also relies on the availability of tailored nonlinear optical properties of metasurfaces. In this talk, I will share the latest progress in nonlinear photonic metasurfaces. The concept of nonlinear geometric phase and its application in nonlinear wavefront engineering will be discussed.

Keywords: Plasmonic metasurface, geometric phase, nonlinear optics

最终交流类型: Invited

Electromagnetic asymmetry and optical magnetism for enhanced second-harmonic generation

雷党愿

City University of Hong Kong, Hong Kong, China

Symmetric plasmonic nanocavities, such as two close-spaced metal nanospheres of the same size and constituting material, usually support only bright plasmon modes (with a net dipole moment) under light illumination. Breaking the cavity symmetry introduces mode hybridization between its bright and dark modes, leading to new fascinating plasmon modes like Fano resonance and bound states in the continuum (BICs). In this talk, I will discuss four “dark” aspects of symmetry-broken plasmonic nanocavities and their implications in second-harmonic generation (SHG), namely 1) light-induced electromagnetic asymmetry (Nature Communications 2021, 12, 4326), 2) plasmon-induced optical magnetism as a new second-order optical nonlinearity (Laser & Photonics Reviews 2021, 14, 2453), 3) molecular conductivity triggered SHG (Nano Letters 2023, 23(12), 5851-5858), and 4) optical magnetism driven multiphoton luminescence (Nano Letters 2021, 21(6), 2453-2460).

Keywords:electromagnetic asymmetry, optical magnetism, second-harmonic generation, plasmonic nanocavity, quantum conductivity

最终交流类型: Keynote

Manipulation of Polaritons in Van der Waals Materials

戴庆

National Center for Nanoscience and Technology, China

Polaritons are interface electromagnetic waves formed by the coupling of light with charges in materials. Polaritons in Van der Waals materials have significant development potential in fields such as molecular sensing, on-chip information processing, and super-resolution imaging, owing to their broad frequency response, high confinement, long lifetime, and ease of control. In this presentation, I will introduce our recent studies on the manipulation of polaritons in Van der Waals materials, including the long-range transmission of plasmons using suspended graphene, topological hybridization of plasmons and hyperbolic phonon polaritons through graphene and molybdenum oxide heterostructures, and advancements in nanoscale negative refractive devices.

Keywords: Polaritons, Plasmons, Van der Waals materials, Graphene, Negative Refractions, Topological Hybridization

最终交流类型: Oral

Polarization-sensitive photodetectors enhanced by ferroelectric field

陈艳

复旦大学

With the further miniaturization and integration of multi-dimensional optical information detection devices, polarization-sensitive photodetectors based on anisotropic low-dimension materials have attractive potential applications. However, the performance of these devices is restricted by intrinsic property of materials leading to a small polarization ratio of the detectors.

we design a ferroelectric-tuned van der Waals heterojunction device structure by integrating a GeSe/MoS2 VHJ and poly (vinylidene fluoride-trifluoroethylene)-based ferroelectric polymer. An ultrahigh electric field derived from the ferroelectric polarization can effectively modulate the band alignment of the GeSe/MoS2 heterojunction. Band alignment transition of the heterojunction from type II to type I is demonstrated. The combination of anisotropic GeSe with MoS2 realizes a high-performance polarization-sensitive photodetector exhibiting low dark current of approximately 1.5 pA, quick response of 14 μs, and high detectivity of 4.7 × 1012 Jones. Dichroism ratios are also enhanced by ferroelectric polarization in a broad spectrum from visible to near-infrared. The ferroelectric-tuned GeSe/MoS2 van der Waals heterojunction has great potential for multifunctional detection applications in sophisticated light information sensing. More profoundly, the ferroelectric-tuned van der Waals heterojunction structure provides a valid band-engineering approach to creating versatile devices.

To analyze the mechanisms of the polarization-enhancement of the ferroelctric field, we further construct a black phosphorus (BP) homojunction photodetector defined by ferroelectric domains with ultra-sensitive polarization photoresponse. With the modulation of ferroelectric field, the BP exhibits anisotropic dispersion changes, leading an increased photothermalelectric (PTE) current in the armchair (AC) direction. As a result, the BP photodetector demonstrates an ultrahigh polarization ratio (PR) of 288 at 1450 nm incident light, a large photoresponsivity of 1.06 A/W, and a high detectivity of 1.27 × 1011 cmHz1/2W−1 at room temperature.

In summary, we used this single device to obtain the intensity and polarization information of light. The photodetectors enhanced by ferroelectric field is a promising device for integrated optoelectronics.

Keywords:Photodetectors, Ferroelectrics, polarization-sensitive, 2D materials

最终交流类型: Keynote

High Efficiency Sn Perovskite LEDs

王建浦

Changzhou University, China

Tin (Sn)-based perovskites are important for fabricating lead-free perovskite optoelectronic devices, yet achieving high efficiency devices remains a significant challenge due to the presence of high density of defects in Sn perovskites. The formation of defects in Sn perovskites, especially how exactly the defects form, is still not well understood. In this talk, we reveal that major defects in Sn perovskites instantly form during the fast aggregation of clusters at the initial growth process (~15 s from the starting of spin-coating process), and ~80% of the luminescence intensity is quenched within 6 s. We further find that additives which form strong chemical interactions with tin (II) iodide in precursor solutions, can effectively prevent the fast aggregation of clusters and avoid the formation of luminescence quenchers. With this approach, efficient near-infrared lead-free perovskite light-emitting diodes are demonstrated.

Keywords:Perovskite light-emitting diode，Sn-based perovskite

最终交流类型: Keynote

Laser field with extreme spatial confinement

童利民

Zhejiang University, China

Laser field with tighter optical confinement is always desired for lower-dimensional light-matter interaction in wide applications. Generally, limited by optical diffraction, a photonic laser cavity is unable to confine a lasing field much better than half the vacuum wavelength l0. The emerging plasmonic nanocavity opens a route towards deep-sub-diffraction lasing field with optical confinement down to l0/30. However, due to the trade-off between optical confinement and plasmon loss of oscillating free electrons, scaling down the cavity size of a plasmon nanolaser is a great challenge due to the insufficient gain and thermal issues.

Here we introduce a photonic approach to a lasing mode supported by low-loss oscillation of polarized bound electrons in an active nano-slit-waveguide cavity, which circumvents the confinement-loss trade-off of nanoplasmonics, and offers a laser field with confinement down to sub-1-nm level. Moreover, using a waveguiding scheme, we show that, an extremely confined laser field can be generated with great flexibilities for broadband and/or ultrafast pulsed operation, as well as linear combination of multiple sub-nm optical fields with engineerable spatial, spectral, and time sequence in a single output. Extremely confined laser fields introduced here may pave a way towards new regions for light-matter interaction, and developing novel optical technologies ranging from superresolution nanoscopy to ultra-sensitivity detection.

Keywords:Laser field, optical confinement, sub-nanometer scale, nanolaser, waveguide

最终交流类型: Keynote

Organic Microlaser Materials and Devices

赵永生

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Organic Microlaser Materials and Devices

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Exploring a universal technique for the manufacture of reproducible organic material geometries in large quantities, just as photo-lithography is to the traditional silicon-based electronics and photonics, is essential for the upcoming flexible integrated photonics. We developed a solution printing strategy for the function-directed controllable and rapid fabrication of high-quality organic microlaser arrays, which was subsequently applied as the building blocks of the panels of organic laser displays and as the elements if photonic integrated circuits. The printed soft photonic systems show competitive performances with their nowadays silicon-based counterparts; and moreover, they even take advantages of mild processing, flexible doping, active/responsive characteristics, etc.

Keywords: Organic optoelectronics; organic laser; laser display; photonic skin

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最终交流类型: Invited

The direct observation of spin-state excitation as the physical origin of metal-insulator transition in FeSb2

苗霖
东南大学

To open an insulating gap in metal is the core question within the quantum material research as it always relates to many-body interaction, and is of essence to advance information technology. The opening of a gap can be naively described as the localization of free electrons, which could be driven by correlation from charge, orbital, spin, and even the intertwined degrees of freedom. Among the materials with a transition from metal to insulator, FeSb2 is featured with exotic properties, e.g. the colossal thermoelectric effect at low temperatures and the puzzling gap-opening mechanism [1-4]. The resistivity of FeSb2 ramps up to nearly tens of orders of magnitude when the temperature cools down to two Kelvin, along with the crossover from paramagnetism to diamagnetism. Various theoretical approaches have been proposed with the different microscopic basis of the degrees of freedom to interpret MIT. Unfortunately, the macroscopic response of insulating FeSb2 to the electric and magnetic field is not characteristic enough. And all these theoretical schemes of totally different microscopic basis can not exclusively address the problem of MIT just from the aspects of the transport and magnetic susceptibility measurements. Because of lacking the explicit and directional spectroscopic evidence, it is extremely difficult to distinguish those proposals and the physical origin of MIT still remains an open question.

In this talk, we will present a systematic X-ray absorption spectroscopic study on FeSb2 and its doped compounds. Together with the atomic multiplet simulations, FeSb2 is found to host the ground state mixed by high-spin and low-spin. Furthermore, the nature of the gap tuned by either temperature or substitution is featured with a high-spin state populated from a low-spin state. Thus the spin-state excitation is directly observed, constituting the most explicit evidence to support that the MIT of FeSb2 is driven by the spin-state excitation, in the framework of energy hierarchy in the vicinity of the Fermi level.

Keyword: X-ray spectroscopy, correlated semiconductor, spin-state excitation, metal-insulator transition

最终交流类型: Keynote

Nanomaterials at High Pressure

邹勃
Jilin University, China

Pressure, as a unique thermodynamic variable, provides a powerful means to study the structural and electronic behaviors of nanomaterials。

High-pressure studies offer a potential strategy to the synthesis of nanocrystals with new phases, and provide new insights into the phase stability in metastable Nanocrystals.

Our findings represent a significant step forward in a deeper understanding of the high-pressure phase diagram of nanomaterials and even provide a promising strategy to prepare desired nanomaterials with new structures that do not exist in their bulk counterparts, thus greatly increasing the choice of materials for a variety of applications.

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Keyword: High Pressure, Phase Transition, Pressure-Induced Emission

最终交流类型: Invited

Manipulation of Van der Waals Exciton Polaritons

张龙
Xiamen University, China

Manipulating cavity exciton polaritons has led to new concepts in fundamental physics and better optoelectronic devices. In this talk, I will discuss two different ways to manipulate cavity exciton polaritons in the Van der Waals material system. Harnessing the doping dependence of the two dimensional (2D) semiconductors, the Rabi splitting, dispersion, and nonlinearity of exciton polaritons can be electrically controlled. This result represents an important step to combine the correlation physics in Van der Waals materials and cavity photonics. On the other hand, the flexibility of integrating 2D materials with various types of cavities allows us to investigate the Rabi splitting dependence of the polariton linewidth. This work can reach a general conclusion on the coupled oscillator system: the impact of inhomogeneous broadening of an oscillator on its coupled state can be suppressed by raising the Rabi splitting.

Keyword: Van der Waals Semiconductor, Exciton Polaritons, Rabi Splitting

最终交流类型: Invited

In-operando visualization of polymer electrolyte|electrode interface evolution in solid state lithium batteries

陈琪
Suzhou Institute of Nano-Tech and Nano-Bionics, CAS, China

Solid-state lithium metal batteries (LMBs), in which a liquid electrolyte is replaced by a solid-state electrolyte, have shown great promise in achieving high safety and high energy density simultaneously. Among the various kinds of solid-state electrolytes, polymer electrolytes (PE) with high flexibility and elasticity favors formation of intimate physical contact with lithium metal anode and composite cathode, which is a prerequisite to realize long-cycling stability. However, complex electrical-chemical-mechanical coupling evolution at PE|electrode interfaces during cycling makes it challenging to realize a long cycle life.[1] Therefore, visualization of interfacial dynamic evolution, especially under practical charging and discharging process, can provide a guideline to improve cycle stability.

In this talk, we will introduce the investigation of interfacial dynamic evolution during cycling of PE based LMBs via in-operando cross-sectional scanning probe microscopy.[2-3] The PE consisted of ionic liquid with a low transference number (tLi+) exhibited significant back and forth migration during charging and discharging process, which was attributed to the electrostatic attraction between large amount migrated anions and ionic liquid cations in mainchain segment. The significant interfacial morphology evolution may expose the uncoated electrode materials and bring unrestricted interfacial side reaction. The complexed interfacial electrical-mechanical-chemical coupling escalated interface impedance, which can be alleviated by increasing tLi+. Based on the understanding, the constitutes of PE has been tuned deliberately, which achieved not only a high conductivity and tLi+, but also a high mechanical strength and wide electrochemical stability window. As a result, the assembled Li|PE|LiNi0.5Co0.2Mn0.3O2 cell with a cutoff voltage of 4.5 V delivered a high discharge specific capacity of ~164.19mAh g−1 at 0.5 C and stable cycling performance with a discharge capacity of 146.96 mAh g−1 even after 200 cycles. To the best of our knowledge, this is one of the fewest polymer electrolytes with self-supporting properties for 4.5 V class LMBs with a high capacity retention of ~90% after 200 cycles.

Keyword: atomic force microscopy; in-operando characterization, polymer electrolyte, transference number, lithium metal batteries

最终交流类型: Keynote

Electrical Characterization of Nanoscale 2D Materials-Based Field-Effect Transistors

Won Jong Yoo
Sungkyunkwan University

Nanoscale two-dimensional (2D) materials including graphene, hexagonal boron-nitride (h-BN), black phosphorus (BP), transition metal dichalcogenides (TMDs) and others have recently been investigated intensively, holding great promise as semiconducting materials for future nano-electronics, nano-optoelectronics, and quantum information device technologies that can overcome serious limitations in nano-device performance and power dissipation of currently used silicon-based semiconductor devices, as they can be effectively applied to realize ultra-thin body with efficient electrostatic control. While the ultra-thinness of 2D materials gives rise to novel electrical and quantum properties, accurate characterization of those properties is very questionable when judging from the experimental results reported from various published papers. Particularly, the characterization of key parameters used in semiconductor devices such as conductivity, carrier density, mobility, Schottky barrier height, contact resistance, interface trap density is very important for the development of future nanoscale devices, since conventional characterization methods used for bulk semiconductor materials often fail in the limit of ultra-thin 2D materials. Furthermore, formidable challenges are presented in 2D device processing originated from the out-of-plane van der Waals (vdW) structure of ultrathin 2D materials. As a serious challenge, untunable Schottky barrier height (SBH) and corresponding strong Fermi level pinning (FLP) at metal interfaces are observed with 2D vdW materials, giving rise to unmodulated semiconductor polarity, high contact resistance, and lowered device mobility. We understand that the observed FLP is very likely attributed to inefficient doping into 2D materials and hybridized compounds formed under contacting metals. In this talk, I would like to review key electrical characterization techniques required for nanoscale FET devices and the related issues arising from adapting the techniques, and further to review the FLP occurring in 2D semiconductor devices, focusing on the effects on device performances and the methods for improving metallic contact.

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Keyword: Nanoscale, characterization, two-dimensional, standardization, field-effect transistor

最终交流类型: Keynote

Novel Photophysics of Halide Perovskite Nanostructures

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Nanyang Technological University, Singapore

Halide Perovskites have demonstrated outstanding performances for both light harvesting and light emission applications, with record power conversion efficiencies (PCE) >25% in solar cells and external quantum efficiencies (EQE) >20% in LEDs. Their spectacular development pace bears testimony of their potential for true technological disruptions. The perovskite field has since exploded beyond these domains to lasing, radiation detectors, bioimaging, neuromorphic and spintronics applications. An exciting range of frontier phenomena in optical gain, hot-carriers, photon recycling, spin, nonlinear

and ferroelectric properties etc. in perovskite nanostructures have since been uncovered. Recently, further efficiency improvements have decreased significantly. For any new efficiency breakthroughs, fresh perspectives and approaches must be developed. Recent discoveries of slow hot carrier cooling phenomenon in halide perovskites [1-3] revealed that such perovskites are highly promising hot-carrier absorber materials capable of unlocking disruptive high-efficiency hot-carrier photovoltaics to overcome the Shockley-Queisser limit. In this talk, I will trace the developments on the slow hot carrier cooling properties of halide perovskites beginning with the discovery of slow hot hole cooling in 2013. [1] Our group further uncovered that hot electron cooling is slow as well and is relatively balanced with the hot holes. [4] I will also focus on our group's efforts: (i) to further retard the hot carrier cooling using perovskite nanoparticles; (ii) to achieve efficient extraction of the hot carriers; [3] and (iii) to understand origins and mechanisms of slow hot-carrier cooling in halide perovskites [5]. I will distil some of these exciting photophysical phenomena and highlight our group's latest works in some of these areas [6 - 8]. A succinct overview of the state-of-the-art as well as the prospective outlook will also be presented.

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Keyword: Ultrafast Spectroscopy, Halide Perovskite, Photophysics, Carrier Dynamics

最终交流类型：Keynote

Characterizing and Manipulating Single Defects inside Semiconductors

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The comprehensive characterization and engineering of single defects in semiconductor is of great interest, both from a scientific and technological point of view. In this talk, we try to discuss the ways to characterize and manipulating the structural and electronic properties of single defects inside semiconductors. We would report some experimental results using tip-enhanced Raman and photoluminescence spectroscopy, which unambiguously characterize the structural, electronic and optical of sub-surface defects in some two-dimensional semiconductors. These observations of single defects in semiconductors may open up a certain new way towards the atomic-scale design and fabrication of new semiconductor and quantum devices.

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Keyword: Single Defects, Doping in Semiconductor, STM, Raman, Photoluminescence

最终交流类型: Invited

Probing the Three Dimensional Nature of Two Dimensional Materials

田学增
中科院物理所

Two-dimensional (2D) layered materials have a thickness of several atomic layers, which exhibit strong quantum confinement effects and weakened Coulomb shielding effects, and many unique physical properties, providing a very good research platform for understanding complex quantum effects, such as strong correlation effect, unconventional superconductivity, etc. Recent studies have shown that although the van der Waals force is weaker than the Coulomb force, the moiré superlattice in the two-dimensional van der Waals heterojunction also undergoes relaxation reconstruction of the lattice structure due to the van der Waals force. However, due to the intrinsic three-dimensional structure of lattice relaxation, currently there is no studies to reveal the three-dimensional sub-angstrom scale characteristics of two-dimensional materials, which leads to theoretical research in this field can only be based on certain assumptions. The lack of microscopic physical images greatly limits the in-depth understanding of 2D materials [1].

In this talk, I will firstly briefly introduce the recently-developed scanning atomic electron tomography (sAET) dedicated for the study of layered materials. sAET is capable to localize the 3D atomic coordinates in 2D layered materials with picometer precision [2] [3] [4]. Then, I will give three examples of application of sAET into layered materials, including a Re-doped MoS2 monolayer, a MoS2-WSe2 lateral heterogeneous monolayer, and an multilayer PtTe2 semi-metal material. I will show the correlated study of 2D materials structures and band engineering properties at the atomic level. We identified many fundamental 3D atomic structures associated with the sample, such as dopants, vacancies and atomic-scale ripples and measured the 3D atomic displacement and the full strain tensor of the 2D material. Furthermore, the experimental 3D atomic coordinates were used as direct input to DFT to correlate crystal defects with the electronic band structure at the single-atom level. We anticipate sAET will be generally applicable to the determination of the 3D atomic coordinates of 2D layered materials, heterostructures and thin films.

Keyword: atomic structure; 2d materials

最终交流类型: Invited

Bright phosphorescence arising from optomagnetic effect in a plasmonic cavity

张杨

University of Science and Technology of China, China

Most organic optoelectronic processes in nature follow the well-known spin selection rule of optical transitions between molecular electronic levels. Such a spin selection rule in conventional optics is obtained within the framework of the electric light−matter interaction, since the magnetic counterpart is usually neglected due to the weak response of a material to the magnetic field at optical frequencies. On the other hand, plasmonic structures are predicted to squeeze the plasmon mode volume and generate pronounced oscillating magnetic fields at optical frequencies, which can trigger evident novel optical processes, in particular, the spin forbidden singlet−triplet transition. Yet, the experimental demonstration of such a direct transition between electronic states with different spin multiplicities due to plasmon-induced optomagnetic effect remains elusive so far.

Scanning tunneling microscopy (STM)-induced luminescence (STML) technique exploits confined plasmonic field defined by the metallic noble tip and substrate, which, together with the highly localized electron excitations, can enable not only to tailor the interaction between the molecule and the cavity at the atomic scale but also to study optoelectronic phenomena occurring at the single-molecule level. For example, it can reveal molecular photon emission statistics, vibronic coupling, intermolecular dipole-dipole coupling and wavelike energy transfer through fluorescence measurements. Despite the advances in STML studies on molecular fluoresence, there is no clear demonstration on the spin forbidden singlet−triplet transition (i.e., phosphorescence) at the individual molecule level until now, because phosphorescence is a weak and spin-forbidden transition that can be easily masked by other optical transitions with similar energies.

In this talk, I shall address such an issue with STML technique and demonstrate bright electro-phosphorescence from an individual molecule due to optomagnetic effect in a plasmonic cavity. The results not only enable new opportunities to study the optical phenomena on the direct transitions between states with different spin multiplicities at the atomic scale, but also provide new insights into the design and fabrication of strong phosphorescence sources.

Keyword: Scanning tunneling microscope induced luminescence; Plasmonic cavity; Phosphorescence; Magnetic light−matter interaction;

最终交流类型: Keynote

Applications of 4D-EELS

高鹏
北京大学

Phonon plays an essential role in mechanical, electrical, optical, and thermal properties of materials. In heterostructures, the breakdown of translational symmetry at the interface leads to the emergence of new localized phonon modes. These modes have an essential role in thermal and electrical transport properties in devices, especially in miniature ones wherein the interface may dominate the entire response of the device. However, the phonons at the crystal interface have been largely unexplored in experiments because the conventional spectroscopies, nano-optics, or scanning probe-based microscopies lack the combined spatial, momentum and spectral resolutions to measure the phonon dispersion at nanoscale. Recently, we propose a four-dimensional electron energy loss spectroscopy (4D-EELS) technique based on the inelastic scattering in scanning transmission electron microscope. By scanning the electron beam in real space of sample while monitoring both the energy loss and the momentum transfer, we are able to reveal position- and momentum- dependent lattice vibrations at nanometer scale with high efficiency. The space, momentum and energy resolutions can be delicately balanced by carefully adjusting experimental parameters, and thus widely tuned to optimize the data acquirements for specific samples under study.

In this talk, we show the principle of 4D-EELS and some application examples, including the local phonon dispersion relation for the heterostructure interface and the single nanostructure [1,2]. We also try to correlate the measured local phonons with the local thermal properties for heterointerfaces and dislocations [3,4]. At last, we extend this to probe the phonon polaritons with far-infrared frequencies and large momentum, which cannot be measured by the current scanning near field optical microscopy [5].

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Keyword: 4D-EELS, interface, local phonon

最终交流类型: Invited

Synthesis of Porous Graphene Nanoribbon on Metal Surfaces

朱俊发
University of Science and Technology of China

The low-dimensional porous graphene nanomaterials might have intriguing electronic properties and open exciting possibilities in the field of functional materials. By using rationally designed precursor molecules, on-surface synthesis (OSS) approach has emerged as a powerful platform for the synthesis of porous low-dimensional graphene-based nanostructures with atomic precision. In this presentation, we report our recent work on the synthesis of porous graphene nanoribbon and nanosheet on different metal surfaces. We have successfully synthesized the one-dimensional graphene nanoribbons (GNRs) containing periodic [14]annulene pores on Ag(111) and the two-dimensional graphene nanosheets containing periodic [30]annulene pores on Au(111), originating from a same precursor. Two

distinct reaction pathways on the two surfaces are regulated by different thermodynamic and kinetic mechanisms. With the combination of the scanning tunneling microscopy (STM), synchrotron radiation photoemission spectroscopy (SRPES) and density functional theory (DFT) calculations, we identified the reaction products, intermediates precisely, and obtained insights into the reaction mechanism. On Ag(111), the formation of porous GNR is a thermodynamically favored pathway, by going through a flexible and reversible organometallic intermediate state. In contrast, on Au(111), because the debromination process is the rate-limiting step for the covalent coupling reaction and the generated covalent structures are irreversible, giving rise to the hierarchical formation of covalent chains and 2D porous nanosheet. The reaction mechanisms were confirmed by a series of control experiments, and the appropriate thermodynamic and kinetic parameters for optimizing the reaction pathways were proposed. Furthermore, DFT calculations revealed the influence of surface confinement on the band structures of these two nonplanar pores embed carbon materials, which enhances the conjugation of π-electrons thus shrinking the band gap.

Keyword: on-surface synthesis, graphene nanoribbons, scanning tunneling microscopy (STM), synchrotron radiation photoemission spectroscopy (SRPES)

最终交流类型: Oral

Electric-field induced 2D polymerization/depolymerization of boroxine-linked single-layer COFs at the solid/liquid interface

Zhinan Fu
KU Leuven

Single-layer covalent organic frameworks (sCOFs) are single-molecule thick, sheet-like macromolecules. Surface-supported sCOFs enable their nanoscale characterization, which constitutes one of the most important challenges within the COF field as the nanoscale structure often determines the function of these materials.[1] On-surface synthesis of sCOFs is intensively studied, and our group[2,3] showed in cases of boronic acids control of the reversible phase conversion between self-assembled molecular networks (SAMNs) and covalent organic frameworks (sCOFs) by changing the orientation of the electric field (EF) between the tip and the surface. However, little is known regarding the impact of external variables on the mechanism and dynamics of the EF-triggered polymerization/ depolymerization at the solid/liquid interface.

Herein, we explore the impact of boronic acid concentration and the kind of solvent. At low concentration, by changing the bias from positive to negative, molecules are desorb from the surface. By changing the bias from negative to positive, molecules are observed to adsorb to the surface. In the high-concentration regime, by changing the bias from positive to negative, formation of sCOFs takes place rather than desorption processes. As for the solvent effect, the surface-confined boronic acid condensation reaction [4] was observed at the solution/solid interface in both protic solvents (octanoic acid (OA) and heptanoic acid (HA)) and aprotic solvents (methyl octanoate (MO) and 1,2,4-trichlorobenzene (TCB)). However, preliminary results also show differences. At the OA/HOPG interface, positive bias-induced depolymerization results in an “amorphous” structure, while at the HA/HOPG or MO/HOPG interface, the compact self-assembled networks (SAMNs) form. At the TCB/HOPG interface, sCOF formation was only observed at negative bias. In contrast, no sCOFs are observed at the phenyloctane/HOPG interface, revealing the important role of solvent in the EF-triggered polymerization/depolymerization.

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Keyword: scanning tunneling microscopy, covalent organic frameworks, boroxine, concentration, solvent

最终交流类型: Invited

Linking atomic-scale investigations in 2D materials with macroscopic-scale devices via gate-tunable STM/AFM

Jiong Lv
National University of Singapore

Recently, engineering vdW heterostructures promotes itself as a versatile tool to create unconventional electronic and magnetic structures of various 2D materials including insulators, semiconductors, metals, superconductors, ferromagnets. The ability to engineer these materials with atomic precision, to understand and eventually control their physical properties has profound impact in developing next-generation technologies. In this talk, I will discuss our recent progress on atomic-scale investigation of defects and atomic arrangements in the emergent 2D materials, including inorganic 2D semiconductors, 2D magnets, and 2D organic-inorganic hybrid perovskites using joint scanning tunneling microscopy (STM) and atomic-force microscopy (AFM). Additionally, I will describe how the application of vdW technologies to the gate-tunable STM can dramatically expand its capabilities, allowing us to probe electronic and magnetic properties, and ultimately control electronic correlation and excitonic effects in these low-dimensional materials. Additionally, precise tuning of the spin-correlated flat-band states and bandgap in 2D magnets via electrostatic modulation of Coulomb interactions not only provides new strategies for optimizing the spin transport channels but also may exert a crucial influence on the exchange energy and spin-wave gap, which could raise the critical temperature for magnetic order. The atomic-scale insights obtained through this platform pave the way for further improving macroscopic-scale device performances.

Keyword: gate-tunable STM/AFM, atomic-scale investigations, 2D materials, devices,

最终交流类型: Invited

he progress of new project IEC standard “ graphene thin film -carrier mobility and sheet resistance: Hall measurement”

王浩敏
Shanghai Institute of Microsystem and Information Technology，CAS, China

The paradigm for technological advancements for emerging electronics is moving toward user-friendly solutions that includes ease of use, wearing sensation, portability, and human sensibility. The application potential of wearable and soft devices, electronic and e-skins has been, thus, of great interest during the past decades.Graphene is composed of a single layer of carbon atoms arranged in hexagons resembling a honeycomb structure. Since the material’s discovery, scientists have shown that different configurations of graphene layers can give rise to a variety of important properties. Graphene has extremely high carrier mobility and has important application potentials in the field of electronics. At present, there are many methods for synthesis of graphene film, and the methods for measuring electrical properties are different. It is difficult to compare product performance, and then it limits the promotion and application of the material. Hall measurement method usually delivers accurate results, so it is recognized by almost all of the researchers, but the measurement method has not formed a unified standard and normative operation in the industry. Therefore, the speaker proposes a measurement method for the electrical properties of graphene that can be widely applicable, and intends to reach a consensus with the industry to form national and international standards.

Keyword: Graphene thin film, Hall measurement, carrier mobility and sheet resistance

最终交流类型: Invited

Robust quantum Hall phase in graphene by interfacial charge coupling

韩拯
Shanxi University, China

Quantum Hall edge states are known to be an ingredient for realizing quantum excitation states such as Majorana fermions when coupled to superconductivity – a route toward quantum computation. However, quantum Hall often requires extreme experimental conditions of very low temperature and high magnetic fields, which hold it back from practical applications.

In this talk, we will introduce a van der Waal hybrid system in which an unusually robust quantum Hall phase is realized, due to the coupling between graphene and an interfacial charge order in CrOCl.[1] Our theoretical considerations suggest that, due to e-e interactions, the electrons filled (charge transferred from graphene with the help of vertical electrical field) in the surface state (from the Cr-3d orbital, which is about 0.7 nm below graphene) of CrOCl can spontaneously form a long wavelength order, i.e., it undergoes a Wigner crystallization. Graphene on top of such a long-range charge order can then also have enhanced e-e interaction, leading to a gap opening at the CNP, and an enhanced Fermi velocity.[2]

Our findings suggest that the paradigm of charge transfer can play key roles in the engineering of quantum electronic states, when the e-e interactions are taking effects. And, according to theory, such a quantum superlattice may be a universal phenomenon in many layered materials [2, 3], and enriched physical phenomena are yet to be discovered.

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Keyword: Quantum Hall, Coulomb interaction, graphene, heterostructure, interfacial coupling

最终交流类型: Invited

The progress of new project IEC standard “ graphene thin film -carrier mobility and sheet resistance: Hall measurement”

孔自强
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The paradigm for technological advancements for emerging electronics is moving toward user-friendly solutions that includes ease of use, wearing sensation, portability, and human sensibility. The application potential of wearable and soft devices, electronic and e-skins has been, thus, of great interest during the past decades.Graphene is composed of a single layer of carbon atoms arranged in hexagons resembling a honeycomb structure. Since the material’s discovery, scientists have shown that different configurations of graphene layers can give rise to a variety of important properties. Graphene has extremely high carrier mobility and has important application potentials in the field of electronics. At present, there are many methods for synthesis of graphene film, and the methods for measuring electrical properties are different. It is difficult to compare product performance, and then it limits the promotion and application of the material. Hall measurement method usually delivers accurate results, so it is recognized by almost all of the researchers, but the measurement method has not formed a unified standard and normative operation in the industry. Therefore, the speaker proposes a measurement method for the electrical properties of graphene that can be widely applicable, and intends to reach a consensus with the industry to form national and international standards.

Keyword: Resistance standard；Graphene thin film；Carrier mobility and sheet resistance；Hall measurement

最终交流类型: Invited

Chiral Charge Density Wave in Monolayer 1T-TiTe2

宋灿立
清华大学

Chirality is a ubiquitous phenomenon in nature and has been broadly recognized at multiple hierarchical levels ranging from subatomic and molecular to galactic scales, yet the emergent chiral electronic states in condensed matter systems have been hugely constrained to materials exhibiting magnetism or spin-orbital coupling. Recently, chiral charge density

waves (CDW) emerge from some low-dimensional achiral materials that have attracted increasing attention, but their origin and physical consequences are still to be explored. In this talk, we report direct visualization of a chiral 2 × 2 CDW that stems from a helical stacking of the triple-q CDW components, in the monolayer limit of 1T-TiTe2 by scanning tunneling microscopy. By layer-dependent quasiparticle interference (QPI) imaging and density functional theory calculations, we reveal that the backscattering of electronic states can be significantly suppressed by the chirality-driven orbital texture on the Fermi surface of monolayer TiTe2. Our results establish monolayer TiTe2 as a promising playground for manipulating the chiral ground states, as well as extending the functionalities of CDW materials in chirality-based electronic devices.

Keyword: Chirality, Charge density waves, TiTe2, backscattering, scanning tunneling microscopy

最终交流类型: Keynote

Interaction between plasmonic nanocavity and two-dimensional excitons at low exciton number

许秀来
Peking University

Plasmonic nanocavity with mode volume beyond the diffraction limit can greatly enhance the interaction of light and matter. At the same time, two-dimensional transition-metal dichalcogenides have attracted wide attention in the field of nanophotonics and quantum optics because of their excellent physical properties. It is of great significance to realize the interaction of such cavity and excitons and reduce the number of excitons involved in coupling to the level of few excitons or even single exciton for future research in cavity quantum electrodynamics and the development of practical photonics devices. We fabricated a compact bowtie nanocavity and successfully realized a strong coupling of MoS2 excitons and bowtie nanocavity with high robustness by using gold-assisted mechanical exfoliation and nondestructive wet transfer techniques. The number of excitons involved in the coupling is reduced to about 40-48, which is the lowest for this type of work so far. In order to realize the interaction between excitons and nanocavity at the level of single exciton, we investigated the coupling of single localized defect excitons in a two-dimensional layer with chiral plasmonic nanocavity. By designing a chiral plasmon mode with high quality factor and coupling it with a WSe2 monolayer, we have successfully achieved cavity-dependent photon

output from a single quantum emitter. The solution of the dynamics model of this coupled system shows that the chiral photon output mainly comes from the spontaneous emission of the quantum emitter which is strongly modified by the chiral plasmonic nanocavity. This proves that the valley-dependent optical selection rules are absent in such quantum emitters. The research in this part not only deepens the understanding of the physical properties of quantum emitters in two-dimensional semiconductors, but also provides a platform for future research of practical quantum optical devices.

Keyword: plasmonic nanocavity; two-dimensional semiconductor exciton; strong coupling; quantum emitter; chiral single photon output

最终交流类型: Invited

Probing Electron-Phonon Interactions in Perovskites Using Ultrafast Spectroscopy

吴波
华南师范大学

Halide perovskites have recently garnered great attention because of their promising applications in diverse optoelectronic devices such as solar cells, LEDs and photodetectors. Despite being solution-processed, these materials exhibit remarkable characteristics such as long carrier lifetime and excellent carrier mobility. Electron-phonon interaction plays a key role in carrier transport which is nevertheless complicated by the soft and hybrid lattice. Therefore, understanding the electron-phonon interaction is of significance for further optimizing the performance of optoelectronic devices based on them.

In this talk, we will present our recent studies on elucidating the correlation between electron-phonon interactions and carrier transport in a few representative perovskites using ultrafast spectroscopy including transient absorption, time-resolved THz transmission, exciton-diffusion mapping etc. The materials include 3D Pb-based and Sb-based perovskites for photovoltaic applications, 2D perovskites for light-emission and photon upconversion. We reveal depending the type and strength of electron-phonon interaction, the carrier transport can be significantly different which exerts great impact on their optoelectronic performance.

Keyword: Ultrafast spectroscopy, perovskite, electron-phonon interaction

最终交流类型: Oral

on-surface investigation of alkane transformation via chemical bond imaging

李雪超
苏州大学

The soaring demand of modern society for materials with extreme physical and chemical properties has inspired the design and synthesis of artificial carbon-based nanostructures. On-surface synthesis, which surmounts the limitation of solubility in solution synthesis, has become a respected modern method to construct molecular nanostructures with novel π-conjugation modes on metal surfaces. In this presentation, I will discuss our recent efforts in selective on-surface reactions of alkanes investigated by chemical bond imaging techniques, including :(1) stereospecificity in the deep dehydrogenation of n-alkanes on Cu(110); (2) strategies to achieve generalized on-surface alkane transformation beyond Cu surfaces; and (3) the possibility to direct transform ethyl groups into ethynyl groups in on-surface synthesized polymers.

Keyword: Carbon nanostructure, On-surface synthesis, C-H activation, alkane transformation, scanning probe microscopy

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最终交流类型: Oral

Single-particle Spectroscopic and Photoelectronic Characterizations on Plasmonic Chiral Nanostructures

Weihai Ni
Soochow University

Tens of years has witnessed the development of single-particle characterization as an important method for the investigation of physical and chemical properties of nanostructures. The capability in solving inhomogeneous broadening in ensemble measurements, resolving individual differences, and building correlation between structures and properties has evidenced single-particle characterization to be significantly advantageous over normal ensemble measurements. By excluding average effects, single-particle characterization has been extensively used in mechanism studies in chemistry, physics, biology, material, energy, environment sciences. In this report, we mainly discuss single-particle characterizations on plasmonic chiral nanostructures for the correlation of microscopic morphological structures to their optical activity,[1] optical activity enhancement of molecules,[2] and circular polarized differential hot electron generation.[3] This report aims to provide new thoughts for developing powerful characterization approaches for the investigation of the chiroptical properties of nanostructures.

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Keyword: Single-particle characterization; Chirality; Localized surface plasmon resonance; Hot electron; Circularly differential scattering.

最终交流类型: Invited

Identifying a critical ice nucleus on hydrophilic and hydrophobic metal surfaces

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Water/solid interfaces are ubiquitous and are important to an incredible range of everyday phenomena and technological developments including wetting, corrosion, heterogeneous catalysis, environmental and atmospheric chemistry, biological science, and astrophysics. One of the most fundamental issues of water science is the development of the basic physics principles which enable a fully prediction of the structure and dynamics of water/solid interfaces. Ideally, the key step to attack this problem is the identification of water structures on various surfaces, especially common stable water clusters regardless of the substrates. However, recent molecular-level studies have shown that a tremendous variety of surface water structures can form on surfaces and these structures vary from substrate to substrate. Here we demonstrate the presence of common water clusters found on hydrophilic (Pt(111), Cu(110)) and hydrophobic (Cu(111)) metal surfaces using scanning tunneling microscopy and noncontact atomic force microscopy. Water molecules self-assemble into a structure with a central flat-lying hexagon and three fused pentagonal rings on Cu(111) and

Pt(111) surfaces, forming a cluster consisting of 15 individual water molecules. The cluster serves as a critical ice nucleus during the ice nucleation: ice growth beyond this cluster bifurcates to form two-dimensional (three-dimensional) layers on hydrophilic (hydrophobic) metal surfaces. The structure motif of 15-mer was also observed on several other hydrophilic surfaces in previous studies. In addition, similar water clusters with two-fold symmetry are also observed on Cu(110) surface. The presence of 15-mer motif and its derivatives on metal substrates with broad parameters of lattice and water-metal interaction indicates that this kind of structure may exist on more metal substrates to assist in ice nucleation. This study reveals the inherent similarity and distinction at the initial stage of ice growth on hydrophilic and hydrophobic metal surfaces, which is a key step towards a general model for water-substrate interaction.

Keyword: Water, hydrophilic surface, hydrophobic surface, nc-AFM, STM

最终交流类型: Invited

Quantum interference between dark-excitons and zone-edged acoustic phonons in few-layer WS2

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Fano resonance which describes a quantum interference between continuum and discrete states, provides a unique method for studying strongly interacting physics. Here, we report a Fano resonance between dark excitons and zone-edged acoustic phonons in few-layer WS2 by using the resonant Raman technique. The discrete phonons with large momentum at the M-point of the Brillouin zone and the continuum dark exciton states related to the optically forbidden transition at K and Q valleys are coupled by the exciton-phonon interactions. We observe rich Fano resonance behaviors across layers and modes defined by an asymmetry-parameter q: including constructive interference with two mirrored asymmetry Fano peaks (weak coupling, $q > 1$ and $q < -1$), and destructive interference with Fano dip (strong coupling, $|q| << 1$). Our results provide new insight into the exciton-phonon quantum interference in two-dimensional semiconductors, where such interferences play a key role in their transport, optical, and thermodynamic properties.

Keyword: Fano resonance, dark exciton, acoustic phonon, WS2

最终交流类型: Invited

Mechano-Raman spectroscopy

徐伟高
Nanjing University, China

Based on nanomaterial units of different structures and properties, the concept of bottom-up stacking and construction of complex functional structures provides a rich space for people to design and assemble new materials. In such new materials, the total performance is critically related with interfacial coupling structure. Herein, we will pay special attention to the mechanical coupling between layered materials and plasmonic metals. Shear phonons are collective atomic-layer motions in layered materials that carry critical information about mechanical, thermal and optoelectronic properties. Phonon branches with co-directional atomic-layer motions carry unique information about the global structure and hidden interfaces in layered crystals and heterostructures, but they are not detectable due to the very limited electron–phonon coupling. Here we utilize the propagating feature and mechanical coupling between shear phonons and localized plasmonic cavities to successfully realize direct characterization of ground-state shear phonons down to 4 cm^{-1} in energy by introducing mechano-Raman spectroscopy (MRS). MRS has the ability to characterize the global crystal structure with more than 10^8-fold enhancement and to accurately measure sub-picometre displacements under ambient conditions with a thermal-noise-free feature. The propagating behavior and the capacity of MRS to detect optically hidden interfaces are demonstrated. The broad tunability of plasmons makes the MRS technique a robust tool for extensive applications, including global crystal flaw detection, mechanical sensing and the mechanical modulation of light.

Keyword: Raman scattering; localized surface plasmon; shear phonons; layered materials

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最终交流类型: Invited

Observation and manipulation of spin coherence in colloidal quantum dots

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Coherent manipulation of solid-state spins is important for quantum information processing. Current solid-state spin systems either operate at very low temperatures or are

difficult to scale-up. Colloidal quantum dots (QDs), by contrast, can be synthesized in large quantity in solution at low cost, yet with high finesse in size and shape control. Further, they are usually strongly quantum-confined, thus their carriers well isolated from the phonon bath, which could enable long-lived spin coherence at room temperature. We studied coherent spin dynamics in solution-grown perovskite QDs using transient magneto-optical spectroscopy. We observed ensemble-level quantum beats resulting from an exciton fine-structure gap and quantitatively controlled the gap energy using temperature-programmable lattice distortion. This unique mechanism has important implications for the application of perovskite QDs in quantum light-sources and coherent exciton control. Further, by dissociating excitons using ultrafast interfacial electron transfer, we achieved room-temperature all-optical initialization, manipulation and readout of hole spins in CsPbBr3 QDs. This represents a milestone towards a scalable and sustainable future of spin-based quantum information processing.

Keyword: quantum dots; spin coherence; coherent manipulation; lead halide perovskites; ultrafast spectroscopy

最终交流类型: Invited

Hyperbolic phonon polaritons in biaxial van der Waals α-MoO3 crystal

Huanjun Chen
Sun Yat-sen University, China

Polaritons, the hybrid quasiparticles associated with strong coupling of electromagnetic waves with electric or magnetic dipoles in the materials, enable efficient subwavelength light trapping and manipulation. Such a capability has opened up new avenues for enhancing various light−matter interactions at the nanoscale. In recent years, two-dimensional (2D) atomic crystals are demonstrated to support a variety of polaritons, which can greatly benefit the fundamental research and optoelectronic applications in the mid-infrared to terahertz regions. In this talk, I will discuss our recent studies on the hyperbolic phonon polaritons (HPhPs) in the mid-infrared regions (9.8~11.0 μm) in van der Waals (2D) α-MoO3 crystal.

Due to its low-symmetry crystalline structure, the polar α-MoO3 exhibits rich phonon modes. As a result, the α-MoO3 supports strong HPhPs in the mid-infrared range, giving rise to ultrahigh electromagnetic field confinements. The electromagnetic confinements can reach ~ λ0/120, which can be tailored by altering the thicknesses of the α-MoO3 2D flakes and by

metal ion intercalation. In addition, their PhP characteristics can also be tuned by nanostructuring of the 2D flakes, as well as stacking two layers of α-MoO3 with different twisted angles. These results have unveiled excellent electromagnetic field localization performances of the natural two-dimensional atomic oxides, which may have great potentials in nanophotonic devices operating in the mid-infrared region.

Keyword: phonon polaritons, hyperbolic, van der Waals crystals, α-MoO3, mid-infrared

最终交流类型: Invited

Bottom interface engineering for high performance perovskite optoelectronic devices

Shi CHEN
University of Macau

Halide perovskite optoelectronic devices have attracted great research interests in recent years. Among various improvement strategies, interfacial engineering appears as the one which still has many potentials in device performance optimization. The upper interface has been extensively engineered to passivate interfacial defects, provoke charge transfer, and enhance moisture resistance. However, the bottom interface is less studied due to the multiple requirement in perovskite film formation, interfacial energy level alignment and dual functional passivation. In our recent studies, we attempted to use three methods: dual ion passivation, graphene coverage, and substrate modification to successfully achieve effective bottom interfacial engineering, and improved device performance in photovoltaics, LEDs, and photodectors.

Keyword: halide perovskite, bottom interface engineering, optoelectronic device

最终交流类型: Invited

Visualizing local electronic structures of quantum materials by micro-ARPES

杨乐仙
Tsinghua University

Recently, with the swift development of the study of mesoscopic and low-dimensional materials, the need for understanding fine electronic structures of quantum materials with precise spatial information has quickly emerged. Thanks to the coherent property of synchrotron radiation and laser sources, it is possible to focus the light beam down to micro-or nanoscale (typically several hundreds of nanometers) to realize angle-resolved photoemission spectroscopy (ARPES) measurements with spatial resolution. Spatial-resolved ARPES promises great potential in investigating a series of scientific frontiers, such as local electronic structures of mesoscopic materials, quantum materials with phase separation, and low-dimensional electronic structures of topological quantum materials. I will show our recent progress in the development of laser-based micro-ARPES instrument and the application of spatial-resolved ARPES in the study of different materials such as type-II iron-based superconductor and higher-order topological insulator Bi4Br4.

Keyword: laser-arpes, micro-ARPES, electronic structure, quantum materials

最终交流类型: Invited

Photonic Spin-Orbital Coupling in the Optical Microcavities filled with Organic microcrystals

廖清
首都师范大学

Organic semiconductor materials have shown important applications in the fields of organic solid-state lasers and molecular photonics due to their high optical gain, molecular tailoring, easy tuning of optical properties, and flexible integration. Influenced by the formation of potential wells in microcavities, excitons and photons are subjected to strong interactions to form a new quasiparticle, the exciton polaritons. We have designed the optical microcavities filled with organic microcrystalline, such as double-layer metal thin film structure. In the microcavity, the coexistence of three different kinds of effects: the TE-TM splitting, linear birefringence and optical activity.1-3 When these effects combine, we demonstrate helical polariton lasing from topological valleys in an organic anisotropic microcrystalline cavity.

Keyword: Photonic Spin-Orbital Coupling, Organic microcrystals, Optical Microcavities

最终交流类型: Invited

Charge Transport in Single Carbon Nanorings and Nanobelts

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Carbon nanorings cycloparaphenylenes (CPPs) and carbon nanobelts (CNBs) are typical hoop-shaped nanocarbons that have unique radially oriented π-systems. Here, we study the electronic transport performance of a series of CPPs and CNBs by incorporating them into molecular devices using the scanning tunneling microscope break junction technique1-3. We show that, compared with traditional linear molecules, the hoop-shaped CPPs and CNBs have significantly higher conductance. DFT-based calculations further elucidate the crucial role of the structural distortion played in facilitating the radial π-electron delocalization and charge transport across these belt-shaped carbon skeletons. Furthermore, we demonstrate the cleavage of non-polar C–C bonds in CPPs via electric field-catalyzed electrophilic aromatic substitution, which produces long linear oligophenylene wires terminated with covalent Au-C bonds. These findings show the potential of using hoop-shaped nanocarbons to achieve unprecedented electronic performance, and may stimulate future design of nanoscale devices based on more curved π-conjugated molecules.

Keyword: Single molecule, charge transport, carbon nanorings, carbon nanobelts

最终交流类型: Oral

The utilization of vorticity in nanoscale superfluid helium

Hao Sha
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The quantization of circulation in superfluids and superconductors is an extraordinary demonstration of quantum mechanics at a macroscopic level. In superfluid, the circulation and angular momentum are maintained by quantum vortices, which are topological line defects. However, detecting these vortices experimentally in superfluids has historically been extremely challenging. Recently, advancements have been made in visualizing quantum vortices in bulk liquid helium[1] and superfluid helium droplets[2]. These droplets, akin to bulk superfluids on a nanoscale, provide a self-contained and undisturbed environment for sustaining quantum circulation.

In this study, we introduce an innovative technique that allows the creation of quantum vortices in helium droplets for the first time. This is achieved through controlled energy collisions between the droplets and ions. During the collision, the linear momentum of the ions is transferred to the angular momentum of the helium droplets, leading to the formation of quantum vortices. Subsequently, noble metal atoms are introduced into the post-collision droplets, resulting in the formation of nanoparticles within the vortices. These nanoparticles can then be deposited onto a surface, enabling the visualization of vortex patterns using transmission electron microscopy (TEM). This comprehensive depiction of vorticity provides valuable insights into the behavior of quantum fluids across a wide range of angular momentum, thus enhancing our understanding of superfluidity. Overall, this approach introduces exciting possibilities for harnessing the vorticity of superfluid helium and exploring the dynamics of quantum fluids with varying angular momentum. It represents a significant step forward in the study of quantum vortices and their role in superfluid and superconductor systems.

Keyword: Helium droplet, vortex, nanoparticle, transmission electron microscopy

最终交流类型: Oral

Molecular-Level Insights on Reactive Arrangement in On-Surface Photocatalytic Coupling Reactions Using Tip-Enhanced Raman Spectroscopy

蔡镇锋
四川大学

Plasmon-enhanced photocatalytic coupling reactions have been used as model systems in surface-enhanced Raman spectroscopy and tip-enhanced Raman spectroscopy (TERS) research for decades[1-2]. However, the role of the reactive arrangement on the efficiency of these model reactions has remained largely unknown to date, often leading to conflicting interpretations of experimental results.

In this presentation, we use nanoscale TERS imaging in combination with molecular-resolution ambient scanning tunnelling microscopy (STM) and density functional theory (DFT) modelling to investigate the role of the reactive arrangement in photocatalytic coupling of 4-nitrobenzenethiol (4-NTP) to p,p′-dimercaptoazobisbenzene on single-crystal and polycrystalline Au surfaces (Figure 1a). TERS imaging with 3 nm resolution clearly revealed a significantly higher catalytic efficiency inside a kinetically driven disordered phase of the 4-NTP adlayer on Au compared to the thermodynamically stable ordered phase (Figure 1b, 1c).[3] Furthermore, molecular-level details of the self-assembled structures in the disordered and ordered phases obtained using ambient high-resolution STM enabled an unambiguous structure−reactivity correlation of photocatalytic coupling (Figure 1d, 1e). Finally, quantitative mechanistic insights obtained from DFT modelling based on the accurate parameters determined from STM imaging confirmed that a combination of steric hindrance effect and energetic barrier leads to a lower reaction efficiency in the ordered phase of the 4-NTP adlayer.

Keyword: coupling reaction, nanoscale, structure-reactivity relationship, scanning tunneling microscopy, tip-enhanced Raman spectroscopy

最终交流类型: Invited

Ultrafast photo-induced carrier dynamics in thin films solar cells characterized by THz spectroscopy

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In the research of novel optoelectronic materials, the characterization of non-equilibrium carrier transportation during the photoelectric conversion is of great significance in guiding the design of high-efficiency devices. The combination of transient absorption spectroscopy, time-resolved terahertz spectroscopy and time-resolved terahertz emission spectroscopy based on ultrashort pulsed lasers can be used to distinguish several physical processes during the optical electronic conversion such as the hot-electron extraction, polaron and exciton formation, positive-negative charge separation and transportation, and energy and charge transfer processes from multiple dimensions. These research could provide guidance for the synthesis and design of novel optoelectronic materials and devices from the characterization of non-equilibrium states and intermediate processes.

Keyword: perovkite solar cell; terahertz spectroscopy; ultrafast dynamics of optoelectronics

最终交流类型: Keynote

Visualized Atomic-scale Fabrication

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With the rapid development of semiconductor technology, the 5 nm feature size of fabrication is already achieved. It is thus quite essential to explore more precise manufacturing and characterization method to evaluate the shape/structure stability and possible new properties of sub-5nm material components, especially under external stimuli such as strain, electric, or thermal fields. Along with the reduction of dimensions, the surface-to-volume ratio of the materials increases. Surface atoms are preferably reconstructed for

adapting their geometrical and electronic structure to the environment. Thus, the surface structure begins to dominate material properties ranging from electronic and structural aspects when the characteristic dimension is reduced to sub-5 nm. With the development of in situ techniques inside transmission electron microscope (TEM), external fields and probes can be applied to individual nanostrucutures, which extends the capability of TEM and may give new insights into the fabrication, and the relationship between atomic structure and unique properties. Here we review our progress in atomic resolution fabrication and dynamic characterization of individual nanostructures and nanodevices based on the idea of "setting up a nanolab inside the TEM". The electron beam inside the TEM can be used as a tool not only to image but also to stimulate the structural evolution. Additional probes from a special-designed holder provide the possibility to further manipulate and measure the electric/mechanical/ photoelectric properties of the nanostructures in the small specimen chamber of a TEM. Besides, the development of liquid cell TEM technique provides an opportunity to dynamically observe the nucleation and growth of nanocrystals in liquid environment, which enrich the coverage of investigation inside the “multifunctional nanolab”. All phenomena from the in-situ experiments can be recorded in real time with atomic resolution.

Keyword: in-situ TEM, atomic-scale fabrication, electron beam irradiation

最终交流类型: Invited

Defect-related optical properties and optoelectronic applications of 2D materials

吕俊鹏
Southeast University, China

Two dimensional transition metal dichalcogenides exhibit semiconducting properties and their electronic structure is adjustable with the number of layers. As the number of layers decreases from multiple layers to monolayers, their band structure changes from indirect band gap to direct band gap, so photoluminescence can be achieved. Most of the band gaps of two-dimensional transition metal dichalcogenides are in the visible spectral range, which lays a foundation for their applications in the fields of display, lighting, visible light communication and so forth. In this presentation, we will report the progress of fluorescence pattering in two-dimensional transition metal dichalcogenides, explore the originations of the fluorescence pattering from the boundary state, spatial distribution of defects,

physical/chemical adsorption and other aspects, and improve the fluorescence quantum yield by defect engineering.

Keyword: 2D materials

最终交流类型:

The gain performance of perovskite micro/nanostructures

杜文娜
国家纳米科学中心

Perovskite micro/nanostructures have recently emerged as a highly attractive gain material for nanolasers. To explore their applications and further improve performance, it is essential to understand the opitcal gain properties. Firstly, we obtained high quality $CsPbBr_3$ microplatelets (MP) with anisotropic orthorhombic phase. Optical gain of $CsPbBr_3$ single crystal MP in and out of the plane were investigated respectively via micro-scale variable stripe-length measurement and transient absorption spectra. For in-plane direction, a polarization-dependent optical gain was observed and the gain along [002] is larger than that of [1-10]. The behavior was attributed to the lowest energy transition dipole moment of [002] induced by the smaller deviation of Br-Pb-Br bond from the perfect lattice. Along the [002] direction, we obtained the optical gain value up to 5077 cm^{-1}, which is the record value ever reported. In addition, the exact gain in out-of-plane direction is obtained by the modified TA method. Our results provide new perceptions in the design of novel functional anistropic devices based on perovskite micro/nanostructures.

Keyword: gain, perovskite, micro/nanostructures

最终交流类型:

The importance of initial stats to the pathways of on-surface reactions

李青
陕西师范大学

On-surface synthesis is a powerful tool to prepare low dimensional organic matierials on surfaces. Moreover, since on-surface reactions take place under ultra-high vacuum, it provides ideal model system to investigate the reaction mechanism.

For a specific reaction, the precursor molecule initially adsorb on the surfaces. In this presentation, by combining scanning tunneling microscopy, SR-XPS and first principle

calculations, we demonstrate: 1, How the substrate-molecule interaction in the initial state influences the reaction barrier and selectivities [1,2]. 2, How the specific adsorption configuration of the precursor molecules in the initial state influences the reaction barrier [3].

Refs:

[1], JACS 138, 2809 (2016);
[2], JACS 141, 168 (2019)
[3], JACS 144, 21596 (2022)

Keyword: initial stats

最终交流类型: Invited

Modeling Of Artificial Flagellated Micro-Swimmers Propelled by External Actuation

阮海辉
The Hong Kong Polytechnic University

In this work, we proposed a bar-joint model based on the corrected resistive force theory (CRFT) for studying artificial flagellated micro-swimmers (AFMSs) propelled by acoustic waves in a two-dimensional (2D) flow field or with a rectangular cross-section. An artificial micro-swimmer normally refers to an object synthesized at the microscopic scale [1] and capable of interacting with a fluidic environment to achieve locomotion. People have proposed these tiny untethered robots [2] to kill bacteria and implement targeted therapy in vivo. It is noted that the inertia of flagella and surrounding fluids can be ignored because the Reynolds number is sufficiently low at the microscale [3]. In a low Reynolds number (LRN) regime, it has been proved that whipping the flagellum of a micro-swimmer can propel itself forward because the interaction between the flagellum and its surrounding fluid can generate propulsion [4]. To simplify the swimming problem, as described by Liu et al. [3], the effect of actuation (e.g., an acoustic power) is simplified to actuation forces and torques on the head of a flagellated micro-swimmer, which leads to flagellum wiggling and propulsion. Under the LRN and assuming slender body, an asymptotic expression in terms of the slenderness can be obtained, known as the slender body theory (SBT). If omitting these interactions and only considering the drags, the SBT is simplified into the resistive-force theory (RFT) [5].

The models of the AFMS based on the RFT are usually one-dimensional (1D), which confines the swimmer's motion to a straight line. Considering the need for manipulation or steering in applications, establishing at least a 2D AFMS model to address plane motion is therefore indispensable. Inspired by Purcell's three-link swimmer, a flexible flagellum has been modeled by using multiple rigid bars linked by flexible joints (aka. the bar-joint models) [6], which intrinsically fulfills the inextensible constraints of a flexible flagellum. Note that the most prevailing AFMS fabrication is based on layer-by-layer photocuring (i.e., 3D printing) [7], which leads to flagella with rectangular cross-sections and thus, the need to modify the SBT and RFT. The SBT for arbitrary cross-section has been developed by adding a dimensionless coefficient tensor K [8] depending on a cross-sectional geometry and the

fluid velocity field. However, such a geometry-dependent K is insufficient to predict the locomotion of an AFMS because of the complexities。

To deal with arbitrary flagellum cross-sections or 2D problems (i.e., with rectangular cross-sections), we assume that the relative fluid velocity field can be expressed as: U(s) = C(s).S(s), where U(s) represents the relative velocity of the fluid with respect to the flagellum part at point s, C(s) the unknown resistive tensor and S(s) the distribution of Stokeslets based on the SBT [5]. For non-circular ones, it is assumed that the relative fluid velocity for the non-circular case is: U = (C+K).S. Note that fluid-structure interaction (FSI) simulations are required to determine K because the dynamics of a solid body (e.g., the wiggling profile of a flagellum), which affects U and K, cannot be determined a priori for general situations. Hence, we assume that K = [Kij] (I, j = 1, 2 for 2D problems) is the only correction tensor to determine. Based on the RFT, the fluid forces Ff is the integra of S along a slender body and is assumed to be proportional to the local velocity of the body. Thus, the substitution of Ff with the second order approximation of S will reach the expressions of the resistive coefficients c. Note that c will be the function of K if we assume the correction factor K = K11 = –K22 due to the property of zero divergence of the tensor K for a LRN regime. For the bar-joint model, the flagellum is simplified into rigid bars with a constant length, which are connected with linear torsion springs at joints except that the first bar is assumed to be rigidly connected to the head. With the bar-joint model and the CRFT, one can obtain the equilibrium equations of external forces, the moment equilibrium equations of bars, and constraint equations for inextensibility conditions. The correction factor K is determined by comparisons of swimmer's trajectories (or errors of time-averaged terminal velocities) between the CRFT-based bar-joint model and the FSI simulation, i.e., K is determined to minimize this error. Note that the classical RFT for 3D cylindrical flagellum leads to over 90% deviation in terminal velocity from those of 2D FSI simulations, while the proposed CRFT bar-joint model can reduce the deviation to below 5%; hence, it enables a reliable prediction of the 2D locomotion of an acoustically actuated AFMS with a rectangular cross-section.

Keyword: artificial micro-swimmer, acoustic actuation, resistive force theory, propulsion

最终交流类型: Invited

Etching Free Ultrafast Fabrication of 2D Metallic Nanomaterials: From Numerical Simulations to Experiments

杨勇
香港城市大学

In recent years, self-rolling of thin films and atomically thin layers (2D materials), such as graphene and WSe2, is considered as a novel method --even being termed as the “roll-up” technology in the literature--for the development of important micro- and nano-devices, such as microgripper, micromotors, resonators, micro-inductors and etc. On the other hand, the rise of nanotechnology has been propelled by low dimensional metals. Albeit the long-perceived importance, synthesis of freestanding metallic nanomembranes, or the so-called 2D metallic nanomaterials, has been restricted to elemental metals with a very limited in-plane size (< 10 mm). Moreover, the traditional chemical etching based “roll-up” technologies suffer from a low fabrication efficiency and generally produce only scroll-like structures. In this talk, we first demonstrate a low-cost method to synthesize 2D metallic nanomaterials through polymer surface buckling enabled exfoliation. The 2D metallic nanomaterials so obtained could be as chemically complex as high entropy alloys while possessing in-plane dimensions at the scale of bulk metals (> 1 cm). With our approach, we successfully synthesized a variety of 2D metallic nanomaterials, including elemental metals, complex alloys, metallic glasses and even metallic-ceramic composites. In addition, we also develop a versatile, ultrafast and etching free method to synthesize self-rolled nanosheets with controllable morphologies through polymer surface buckling enabled exfoliation. It is intriguing that, by controlling the geometry of the 2D metallic nanomaterials, we are able to control their morphology such that these 2D metallic nanomaterials can transition from scrolls to helices. From the perspective of thermodynamics and kinetics, our extensive finite element simulations reveal that the seemingly complex configurational transition (scroll-helix-scroll) is a kinetic process, which nonetheless could be intervened by geometric self-locking and can be correlated with the dimensionless geometric factor that can be easily derived from the shape of a nanosheet. Our current findings could be useful for the future design of low dimensional devices.

Keyword: Roll-up technology; 2D metals; Nanosheets; Configurational transition; Finite element simulations

最终交流类型：Oral

Self-Assembly of star-polyelectrolytes in various solvent conditions

李斌
中山大学

Star-polyelectrolytes do not only have a more extending conformation and higher local charge density, but also have more flexibility for tuning different conformations, such as arm numbers and lengths, by comparing with linear polyelectrolytes. The property of star-polyelectrolytes provides larger probability for controlling self-assembly behavior in solvent to obtain plentiful morphologies. In order to reveal the underlying mechanism of charge-driven self-assembly of star-polyelectrolytes, we study the self-assembly of star-polyelectrolytes with different numbers of arms in solvent at varied ionic strengths and temperatures using coarse-grained molecular dynamics simulations. We obtain various morphologies with a sequence of unassembled, loosely aggregates, disordered aggregates, sheet aggregates and cross-linked aggregates, as the decrease of ionic strengths, which is due to stronger electrostatic interaction between the polyelectrolyte ion pairs. The self-assembled structures are more ordered by following the aforementioned morphological sequence, which is attributed to the synergistic effect of the exclusion volume effects and electrostatic interactions. The tendency of the structural transition also exhibits by increasing the arm numbers or decreasing the temperatures, as the electrostatic coupling is enhanced between polyelectrolyte ion pairs. However, the ionic strength is the main factor for affecting the self-assembly structures. In addition, the dissociation and reaggregation of polyelectrolyte from aggregate is observed under higher temperature, especially in the star-polyelectrolyte with low arm numbers. The amphiphilic star-polyelectrolytes self-assembles into worm-like micelles, as well as amorphous aggregates, under different arm numbers and ionic strengths. We also investigated the free energy profile of opposite polyelectrolyte pair association, and found that the star-polyelectrolytes with more arms experience stronger Coulomb attraction, and the conformation of star-polyelectrolytes shows non-monotonic processes during the process of pulling a pair of opposite star-polyelectrolytes. Our simulation results help to understand the self-assembly mechanism of star-polyelectrolytes in various solvent conditions and provide theoretical guides for designing star-polyelectrolytes with different functional groups.

Keyword: star-polyelectrolytes, Debye length, coarse-grained simulation, polyelectrolyte coacervation, self-assembly

最终交流类型: Invited

Transport mechanisms of water molecules in nano channels

朱重钦
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Water transport through membranes incorporating carbon nanotubes (CNTs) or nanoporous graphene has attracted considerable interest over the past two decades. It is known that the diffusion and transport behavior of water through a nanotube can be fundamentally different from those of bulk water through a macroscopic tube. We systematically studied the transport of water through zero-dimensional (0D) nanopores, and found water flow rate exhibits unexpected nonlinear dependence on the pore size. This counter-intuitive behavior is attributed to the quantized nature of water flow at the nanoscale. In addition, considering the presence of dangling bonds, we investigate water flow of hydrogen-functionalized nanoporous graphene membranes. The charge values on hydrogen atoms (qH) and carbon atoms at the pore rim are systematically adjusted. For qH > 0, the flow rate decreases as qH increases, whereas for qH < 0, the flow rate tends to increase first and then decrease with increasing qH, yielding a peak at ~ –0.2 e. Further, we explored the nanotube length-dependent water physical transport behavior of water. Different from wide (8,8) CNTs, we show that the flow rate of water through 0.83-nm-diameter (6,6) and 0.96-nm-diameter (7,7) CNTs exhibits anomalous transport behavior, whereby the flow rate increases markedly first and then either slowly decreases or changes slightly as the CNT length l increases. The critical range of l for the flow-rate transition is 0.37 to 0.5 nm. Calculations show that the free energy barrier for a single water molecule to pass though a (6,6) or (7,7) CNT is extremely low and essentially independent of length. Therefore, the variation of the free energy barrier with the length cannot explain the anomalous flow rate of water through the narrow-diameter CNTs. Indeed, this anomalous water transport behavior is attributed to the l-dependent mechanical stability of the transient hydrogen-bonding chain that connects water molecules inside and outside the CNTs and bypasses the CNT orifice.

Keyword: nanotube, nanopore, MD simulation, water transport, hydrogen bond

最终交流类型：Invited

Cooperation of different types of nanoparticles in endocytosis

杨恺
苏州大学

Cell entry is one of the common prerequisites for nanomaterial applications. While it has been extensively studied for a homogenous group of nanoparticles (NPs), fewer studies have been performed when two or more types of NPs were administered together. We previously described a synergistic cell entry process for two heterogenous groups of NPs, where NPs functionalized with TAT peptide (T-NPs) stimulate the cellular uptake of co-administered unfunctionalized NPs (bystander NPs, B-NPs). Here, we established a simulation system to recapitulate this so-called bystander uptake process. The simulation also allowed us to take one step further and investigate the synergy between any two NPs, whether coupled to TAT or not. Our simulation revealed that when placed apart from each other initially, two NPs first move towards each other instead of initiating cell entry separately. Only T-NP can invoke an inward bending of membrane mimicking endocytosis upon contact with the membrane, which attracts the nearby T-NP or B-NP into the same “vesicle”. A two-phase decline of free energy for the entire system occurred as two NPs get closer until contact, which is likely the thermodynamic driver of bystander uptake, and the synergy between cell entry of any two NPs. Experimentally, we found that T-NPs increase the apparent affinity of B-NPs to the plasma membrane, suggesting that T-NPs indeed help B-NPs “trapped” in the endocytic vesicles. Next, we varied the sizes of B-NPs and found that 50 nm is the optimal diameter for bystander uptake. In the simulation, we also found that the size of B-NPs influences the free energy decline, and thus the tendency and dynamics of NP co-entry. Overall, our study revealed a synergy during NP cell entry driven by free energy decline and described the NP size dependence of this process. These efforts provide a useful system to further understand the synergistic cell entry among individual NPs or multiple NP types on a biophysical basis, and provide insights on future design of nanostructures for intracellular delivery.

Keyword: endocytosis; nanoparticles; cell membranes; computer simulations

最终交流类型：Invited

A Multiscale Theory of Cellular and Tissue Plasticity

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Tissues, organs and organisms achieve complicated three-dimensional geometries through morphogenesis, where a large number of cells deform and move in a highly coordinated and programmed manner. Interestingly, accumulating evidence has demonstrated that the capability of cells to undergo irreversible deformations (often referred to as cell plasticity) is critical for tissues to form and maintain the desired shapes, as manifested in processes such as embryo development, collective cell migration, skin pattern shaping and synaptogenesis. However, the fundamental question of how plasticity is initiated in individual cells and then propagates within the tissue remains elusive. Here we develop a mechanism-based theory of cellular and tissue plasticity that accounts for all key processes involved, including the activation and development of active contraction at different scales as well as the formation of endocytic vesicles on cell junctions, and achieves quantitative agreement with all existing experiments. Specifically, it is shown that, in response to optical or mechanical stimuli, the myosin contraction and thermal fluctuation-assisted formation and pinching of endocytic vesicles could lead to permanent shortening of cell junctions, and that such plastic constriction can stretch neighboring cells and trigger their active contraction through mechanochemical feedbacks and eventually their plastic deformations as well. Our theory predicts that endocytic vesicles with a size around 1-2 μm will most likely be formed and a higher irreversible shortening of cell junctions could be achieved if a long stimulation is split into multiple short ones, all in quantitative agreement with experiments. Our analysis also shows that constriction of cells in tissue can undergo elastic/un-ratcheted to plastic/ratcheted transition as the magnitude and duration of active contraction increases, ultimately resulting in the propagation of plastic deformation waves within the monolayer with a constant speed which again is consistent with experimental observations. By elucidating the mechanisms by which mechanical plasticity is triggered and transmitted in cells, our work provides insights for finding ways to direct processes such as embryo development and tissue formation in the future.

Keyword: Cell and tissue mechanics, plasticity, active contraction, endocytosis

最终交流类型: Invited

Dynamic behavior of water droplets on nanostructured surfaces

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Dynamic behavior of water droplets on rough surfaces has important implications to diverse areas. On a rough surface, two wetting states commonly observed are either the Wenzel state (droplets contact the bottom of the roughness and show no air pockets beneath the droplets) or the Cassie state (water droplets contact these surfaces only at the tips of the roughness). or the Cassie state. Herein, we show from large-scale molecular dynamics (MD) simulations that the transition between the Cassie and Wenzel states can be controlled by one-scale trapezoidal nanostructures on a surface.[1] Further, the behavior of droplets on a dual-scale nano/submicro hierarchical structured surface is studied by devising slab model systems with a variety of dual-scale surface structures and with different degrees of intrinsic wettability.[2] Our MD simulations reveal five possible wetting/dewetting states for a water droplet and obtain wetting diagrams. Further, we show MD simulation evidence of a previously unreported wetting behavior, i.e., the rise of multiple Wenzel states on the structured surfaces whose flatsurface counterparts are superhydrophilic (i.e., complete wetting surfaces with the hallmark of zero contact angle for water droplets). [3] Specifically, we show that on the structured surfaces with topology of closed-loop nanowalls/nanochannels, the water droplet can exhibit multiple Wenzel wetting states with the apparent contact angles > 0o , named as "topological wetting states" because their existence can be attributed to the topology of the closed-loop nanowalls/nanochannels. On different shaped closed loops, such topological wetting states can always arise due to the topological invariant. This unusual wetting behavior is contrary to the conventional view, namely, a rough hydrophilic surface should behave stronger hydrophilicity than its flat-surface counterpart.

Keywords: droplet, trapezoidal nanostructures, dual-scale, nano/submicro hierarchical structure

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Keyword: droplet, trapezoidal nanostructures, dual-scale, nano/submicro hierarchical structure

最终交流类型: Oral

Negative or positive? Loading area dependent correlation between friction and normal load in structural superlubricity

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Structural superlubricity (SSL), a state of ultra-low friction between two solid contacts, is a fascinating phenomenon in modern tribology. With extensive molecular dynamics simulations, for systems showing SSL, here we discover two different dependences between friction and normal load by varying the size of the loading area. The essence behind the observations stems from the coupling between the normal load and the edge effect of SSL systems. Our results reveal the importance of loading conditions in the friction of systems showing SSL, and provide an effective way to reduce and control friction.

Recent studies show that the area experiencing prominent normal load only occupies a small part of the entire contact area. Given that AFM is commonly used in SSL experiments, it is of great significance to clarify the effect of loading area on friction.

As shown in Figure 1A,B, we choose a model consisting of five layers of graphene. The lower three layers are considered as the substrate. The upper two layers are hexagonal flakes with the side length of 5 nm. The misfit angle between the flake and the substrate is fixed to be 0 degree. Thus, to achieve a robust superlubric state, 4% in-plane biaxial stretching strains are applied to the substrate. Periodic boundary conditions are applied to the x and y-direction.

Figure 1C, D show the dependence between the friction f and the pressure P for the small and large loading area respectively. It is worth pointing out that for small loading area cases, friction shows a non-monotonic variation with the normal load, while a linear dependence is observed for large loading area cases.

Fig. 1 Simulation model and main results. (A) Schematic sketch of the simulation model. A hexagonal graphene flake (purple) on the strained graphene substrate (red). The area enclosed by the dashed hexagon is the loading area. L is the side length of the loading area of the hexagon. (B) Side view of the simulation model. (C-D) Dependence between the friction force f and the loading pressure P for (C) the small loading area and (D) the large loading area.

Keyword: graphene, normal load, superlubricity, friction, simulation

最终交流类型: Invited

Theoretical Design of Functional Nanomaterials Featured with Inverse Sandwich Structures

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Cluster assembly is very powerful and promising in designing nanomaterials with specific behavior, due to the multi-dimensions in regulating the characteristics and functions of the assembled materials. Using the stable clusters as assembling units is of significance for constructing new nanomaterials. Inspired by the observation of inverse sandwich structures of $[La(\eta^{x}\text{-}B_{x})La]^{-}$ (x = 7–9) clusters in experiments [*Proc. Natl. Acad. Sci. USA* 2018, 115(30), E6972-E6977; *Chem. Sci.* 2019, 10(8), 2534-17713.], we first confirmed the high stability of two non-lanthanide boron clusters, Ti_2B_8 ($D_{8}h$) and $K_2B_9^{-}$ ($D_{9}h$) of inverse sandwich structures, and then designed two-dimensional (2D) TiB_2 ($P2_1/c$) and K_2B_9 (P-62m) monolayers featuring inverse sandwich structures by means of first-principles calculations. Our computations revealed that the 2D TiB_2 sheet possesses very high stability and exhibits both electron and phonon Dirac points at the same k point, which can be assigned to the $C_{2}x$ protection; and that the K_2B_9 monolayer is the global minimum of the same chemical stoichiometry in the 2D space, and is a topological superconductivity with the transition temperature (T_c) of 12.56 Kelvin due to the high electron density near Fermi level caused by the van Hove singularity, and the T_c can be increased by manipulating the ratio of K and B. Furthermore, the inverse sandwich configuration was extended to homonuclear and heteronuclear metal dimers vertically anchored vacant graphene and BN monolayers, with the aid of density functional theory calculations and machine learning approach, the stable structures were found to show very good promise as gas sensors or electrocatalysts for CO_2 reduction reaction or N_2 reduction reaction, prevailing the performance of the systems with single-atom and double-atom parallel to graphene or BN plane. This study provides a novel design strategy of functional nanomaterials for topological semimetals and superconductors, electrocatalysts and beyond. We hope experimental community pay attention to the “unexploited” nanomaterials of inverse sandwich structures for the “unexpected” features.

Keyword: Inverse sandwich structure, cluster assembly, Dirac point, superconductivity, catalytic performance

最终交流类型: Invited

How Bulk Nanobubbles are stable

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How Bulk Nanobubbles are stable

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We will discuss in this talk the stability mechanisms for bulk nanobubbles, primarily focusing on those from our group. First, we demonstrate with thermodynamic analysis that the affinity of negative charges onto the nanobubble interface causes charge enrichment, and the resulting electric field energy gives rise to a local minimum for the free energy cost of bubble formation, leading to thermodynamic metastability of the charged nanobubbles. Secondly, we propose that the adsorbed surfactant-like contaminant molecules, with their amphiphilic character, will affect the dissolution of the existing bulk nanobubbles under low gas supersaturation environments. Our molecular dynamics simulation results show that with gas dissolution, the formed bubble shrinks and the adsorbed insoluble surfactants form a monolayer with an increasing areal density until an extremely low (close to 0) surface tension is reached. Two basic conditions for stable nanobubbles at low gas saturation are identified: vanishing surface tension due to bubble dissolution and positive spontaneous curvature of the surfactant monolayer. Then, we will discuss the similarity of bulk nanobubble stability with that of microemulsions, and proposed that stable bulk nanobubbles can be regarded as gaseous analogues of microemulsions. The similarity also leads us to conclude that for stable nanobubbes, the nanobubble phase and the bubble-containing solution phase coexist with the external gas phase. The three-phase coexistence is validated by molecular dynamics simulations. Finally, we will show how to combine them to interpret stability of bulk nanobubbles.

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Keyword: Bulk nanobubble, Stability, Thermodynamics, Molecular dynamics

最终交流类型: Invited

Tunable exotic states in two-dimensional Kagome materials

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Since the unique atomic arrangement of Kagome lattice usually lead to electronically destructive interference, many exotic physical phenomena have been explored promising for novel states in electronic topology, strong correlation, superconductivity etc. Most of the current research interest focus on the Kagome metals suggesting the desired emergence of Kagome semiconductors. Here we report several kinds of Kagome semiconductors with inorganic or organic frameworks. We predicted that the two-dimensional inorganic system has a rich variety of non-collinear magnetic structures, which determine their topological states of Kagome materials. Intriguingly, large Chern numbers can be obtained in noncollinear and noncoplanar magnetic structures leading to the quantum anomalous Hall effect and the quantum spin Hall effect even if the time-reversal symmetry is broken [1]. We further discovered that achiral conjugated organic molecules can form a chiral Kagome lattice, which is completely derived from the intermolecular electronic state without atomic occupation. These results were confirmed by density functional theory calculations and scanning tunneling microscope experiments. This unusual phenomena can be called electronic chiral Kagome crystals [2]. Lastly the Kagome lattice with strong spin-orbit coupling is selective to the chirality of the light field, and its spin channel and chirality of the light field will be strongly coupled, which can transform the non-local dispersive energy band in real space into highly localized topological flat bands, which are expected to realize high-temperature fractional quantum Hall effect states [3]. The use of periodic light fields to tune the spin topological states of inorganic and organic systems and their strong correlation effects is of great significance for realizing the novel topological states in Kagome materials.

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Keyword: Kagome lattice, topological states, charge density of wave, conjugated organic molecules, spin-orbit coupling, light-matter interaction

最终交流类型: Invited

Rational Design 2D Functional Heterojunctions and Database Construction for Ionic Layered Materials

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Two-dimensional (2D) layered materials offer exciting prospects for designing miniaturized electronic, optoelectronic, and flexible devices at the nanoscale. The sheer openness of 2D magnetic materials makes them possess gate/interface tunability and integrated flexibility. Assembling different 2D layers into heterostructures can lead to enhanced/emergent performance. Thus, discovering such heterostructures with superior performance, and understanding the correlation between structure, composition, and properties are crucial for advancing the design of high-performance devices.

In this presentation, I will present our recent efforts on the relational design of 2D layered heterojunctions and ionic layered materials. Firstly, I will explain the design strategies used to achieve the nonvolatile electrical control of spin polarization of 2D magnets, which is highly desirable for future low-dissipation spintronic nanodevices. We predict that 2D VSeF is an intrinsic bipolar magnetic semiconductor (BMS) featured with opposite spin-polarized valence and conduction band edges. By considering the band alignment, we find that the spin-up/spin-down polarization of VSeF can be controlled by the electric dipole of ferroelectric monolayer and bilayer Al_2Se_3. We have achieved two types of spin field effect transistors, namely multiferroic memory and spin filter, in VSeF/Al_2Se_3 and VSeF/Al_2Se_3/Al_2Se_3 multiferroic heterostructures, respectively.

Next, I will introduce the database construction of ionic layered materials. Unlike van der Waals (vdW) layered structures where the 2D units are charge neutral, ionic layered structures are constructed by charged layers. Stacking different functional vdW units is an effective way to modulate the interplay of charge and spin correlations with enhanced and emergent properties. Using our homemade topological-scaling algorithm, we identify 1028 charged 2D ionic layered units from Materials Project database. We constructed new ionic layered materials by assembling these ionic units while considering valence state and lattice mismatch and predict 353 stable ionic layered materials by high-throughput density functional theory calculations. These materials can inherit their functionalities and show enhanced or emergent properties compared with their parent materials. This database expands the design space of functional materials for fundamental research and potential applications.

Keyword: nonvolatile electric control, spin polarization, ionic layered materials, database, 2D functional materials

最终交流类型: Invited

First principles calculation of nanomaterials using quantum Monte Carlo

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First principles calculation is widely used to understand and design new nanomaterials. However, traditional methods such as the density functional theory have accuracy limitations for complex nanomaterials because of the approximations required for the exchange correlation functional. Electronic structure calculation using quantum Monte Carlo has witnessed an appealing advancement in the last couple of years, which allow for more accurate first principles calculations. I this talk will introduce new developments of state-of-the-art quantum Monte Carlo methods using machine learning techniques such as neural network, including the generalization of the neural network wavefunction based methods to solid systems [1]; the accuracy improvement via diffusion Monte Carlo [2]; implementation of effective core potentials within neural network wavefunction to further reduce the computational cost of realistic chemical systems [3]; extending neural network wavefunction to interatomic force [4] and other quantities. These methodological advances allow us to approach the true ground state of molecules and materials in all dimensions. I will also show applications of accurate first principles calculations to improve our understanding of various nanomaterials, including the structure, phase transition, and dynamics of nano-confined two-dimensional ice [5-7]; molecular adsorption and reaction on nano-materials [8-9]. The studies show that improving the accuracy of first principles calculations are fundamental to understand complex emergent phenomena of nanomaterials.

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Keyword: quantum Monte Carlo; First principles; neural network; nanomaterials

最终交流类型: Oral

Intrinsically scale-free ferroelectricity in two-dimensional M2X2Y6

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Discovery of novel two-dimensional ferroelectric materials and understanding the mechanism are of vital importance for the design of nanoscale ferroelectric devices. In this work, distinct geometric evolution mechanism of newly reported $M_2Ge_2Y_6$ monolayers is explained using $Hf_2Ge_2Y_6$ monolayers as examples, and a large group of two-dimensional ferroelectric candidates are found based on first-principles calculations. The origination of the ferroelectricity of $M_2Ge_2Y_6$ is the vertical displacement of Ge-dimer in the same direction driven by a soft phonon mode of the centrosymmetric configuration. By analyzing the vibrational modes of the flat phonon bands, a centrosymmetric-II phase of $M_2Ge_2Y_6$ monolayers are found. Interestingly, these centrosymmetric configurations are found to be dynamically stable. The metastable centrosymmetric phase of $M_2Ge_2Y_6$ monolayers allows a new two-step ferroelectric switching path and may induce novel domain behaviors. When reversing the polarization of $M_2Ge_2Y_6$ monolayer, both the ferroelectric phase and centrosymmetric-II phase may be obtained. Moreover, the ferroelectric $M_2Ge_2Y_6$ monolayers show intrinsic scale-free ferroelectricity, i.e., the polarizations in adjacent $M_2Ge_2Y_6$ unit cell can be reversed independently. The independently switchable polarization of ferroelectric $M_2Ge_2Y_6$ monolayer showed its potential applications in high-density storage, in which the size of the memory unit, in principle, can decrease to one unit-cell length. The ferroelectric $M_2Ge_2Y_6$ monolayers maintain their ferroelectricity after contacting with graphene electrodes, indicating their high application potentials in high-density storage. Furthermore, 16 ferroelectric $M_2Ge_2Y_6$ and 28 potential ferroelectric $M_2Sn_2Y_6$ monolayers are identified through high-throughput calculations considering 378 possible combinations. The negative ΔH of ferroelectric $M_2Ge_2Y_6$ monolayers, as well as the comparable E_{hull} of ferroelectric $M_2Ge_2Y_6$ monolayers with that of $Cr_2Ge_2Te_6$ monolayer, indicated the high possibility of synthesizing these two-dimensional ferroelectric $M_2X_2Y_6$. The findings provide a new strategy for future discovery of novel two-dimensional ferroelectric materials and also platforms for experimental design of related functional devices based on the understanding of the mechanisms.

Keyword: two-dimensional (2D) materials, mechanism of ferroelectricity, scale-free ferroelectricity

最终交流类型: Invited

Theory of Wetting and Capillarity on the Nanoscale

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Wetting and capillary phenomena on the macroscale are ubiquitous and have been well understood. However, the relevant physics and mechanics on the nano-scale still remain mysterious. In this talk, I would like to discuss the exploration of capillarity from a nanoscopic perspective, including wetting, evaporation and condensation. At the solid/liquid interface, the liquid exhibits a pronounced layered structure that extends over several intermolecular distances from the solid surface. Our recent studies have shown that such molecular detail could provide some new understanding on century-old classical theory in this field, such as Young's equation and Kelvin equation. In specific, we offer a novel approach to describe and quantify the capillary force on the liquid in coexistence with its vapor phase. Our findings not only provide a theoretical insight into capillary forces at the contact line, but also validate Young's equation based on a mechanical interpretation. Microscopic details regarding the mechanism of wetting and capillarity, such as the layering structure of liquid near solid and overlapping of two interfaces, were elucidated. Moreover, we provide a more generalized form of Kelvin equation which can describe the capillary condensation under extreme confinement down to the angstrom-scale. Since the contact angle and the meniscus curvature can not be precisely defined, we introduced the size effect of solid-liquid surface energy. The deviations in the solid–liquid surface energy from its bulk value may be considered as extra work spent to rearrange water molecules into the strongly layered structures. Using the generalized Kelvin equation and the numerically calculated solid–liquid surface energy under extreme confinement, it is straightforward to calculate the relative humidity required for water condensation inside atomic-scale capillaries, which gives good agreement with the experiment. The abnormal structure formed at solid-liquid interface and the molecular interactions are crucial to understand theories of wetting and capillarity on the nanoscale.

Keyword: Wetting, Capillarity, Condensation, Nanoscale, Interfaces

最终交流类型: Oral

Theoretical studies on magnons in two-dimensional magnets

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Two-dimensional (2D) van der Waals magnets possess long-range magnetically ordered ground states. The magnetic excitation (magnon) in 2D materials can be used for next-generation information device. Magnons can interact with other particles, such as photons, electrons and phonons. In this talk, we will present two of our recent works, namely (1) negative thermal expansion due to magnons; and (2) inelastic Raman scattering due to magnons.

(1) Negative thermal expansion. The thermal expansion phenomenon is of both engineering and fundamental interest. The conventional theory of thermal expansion of solids considers the anharmonic phonon effect, but largely neglects other kind of elementary excitations. In general, considering the contribution of phonons alone is sufficient to describe the thermal expansion behavior of materials. A recent experiment reported a negative thermal expansion (NTE) of a two-dimensional magnet CrBr3 at low-temperatures.[1] However, through first-principles calculations, we found that [2] the NTE caused by phonons of CrBr3 at low temperatures is several orders of magnitude lower than the experimental. Considering that CrBr3 is a magnetic semiconductor, we believe that magnon is important to the NTE of CrBr3. Therefore, we have added the contribution of magnons to Helmholtz free energy into the thermal expansion theory, and confirmed the dominate role of magnon in the negative thermal expansion of CrBr3, and predicted the thermal expansion behavior of CrI3 and CrCl3 at low temperature.

(2) Raman scattering due to magnons. Theories of magnon-induced Raman scattering can be dated back to Moriya and Fleury-Loudon etc. Analysis based on crystal structure symmetry predicts the selection rule of Raman scattering. Unsolved problems in magnon Raman effect include the magnon Raman scattering in low-symmetry crystals and the dependence of Raman intensity on photon energy. In this work, we developed a first-principles theory of the Raman scattering due to magnons and applied it for CrI3 monolayer and bilayers. Our first-principles calculations predict selection rules of magnon Raman scattering in CrI3 monolayer and rhombohedral bilayer, which is understood using pseudo-angular moment of magnon. The monoclinic bilayer CrI3 on the other hand is symmetry broken. The calculated Raman intensities in different scattering channels confirm the

violation of selection rule. The calculated Raman intensity reaches maximum when the photon energy coincides with the electronic excitation from I-p orbitals to Cr-d orbitals.

Keyword: magnon, two-dimensional materials

最终交流类型: Invited

Elemental Amorphous Carbon versus Binary Amorphous Boron Nitride Monolayers

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Amorphous materials, unlike their crystalline counterparts, have no long-range order. They have rich applications, e.g., hydrogenated amorphous silicon in photovoltaics and thin-film transistors in liquid-crystal displays; amorphous SiO2 in microelectronics and chromatography; and amorphous metal-oxide semiconductors like indium–gallium-zinc oxide (IGZO) in thin-film transistors in organic light-emitting diodes. Though crystalline materials are accurately characterized by crystallographic techniques, the atomic structure of amorphous materials has been intensely debated. The structure of amorphous materials has been debated since the 1930s as a binary question: Zachariasen continuous random networks (Z-CRNs) vs. Z-CRNs containing crystallites. It was recently demonstrated, however, that amorphous diamond can be synthesized in either form. Here we address the question of the structure of single-atom-thick amorphous monolayers by kinetic Monte Carlo simulations that emulate chemical-vapor deposition (CVD) growth on a substrate. We find that crystallite-containing Z-CRN is by far the energetically preferred structure of elemental monolayer amorphous carbon (MAC), as recently fabricated, whereas the most likely structure of binary monolayer amorphous BN (ma-BN) is altogether different than either of the two long-debated options: it is a compositionally disordered “pseudo-CRN” comprising a mix of B−N and noncanonical B−B and N−N bonds and containing “pseudocrystallites”, namely, honeycomb regions made of noncanonical hexagons [1]. We also find that the thermal conductivities of both monolayer amorphous carbon and monolayer amorphous boron nitride are about two orders of magnitude smaller than their crystalline counterparts. Moreover, the ultralow thermal conductivities are independent of the temperature and strain due to their extremely short heat carrier mean free paths. The relation between the structure disorder and the reduction of the thermal conductivity is analyzed in terms of the vibrational density of states and the participation ratio. The ma-BN shows strong vibrational localization across the frequency range, while the MAC exhibits a unique extended G* diffuson mode due to its sp2 hybridization and the broken E2g symmetry [2].

Keyword: amorphous materials, monolayer materials, kinetic Monto Carlo

最终交流类型: Invited

Computational Study on Filament Growth in Microstructure-Controlled Storage Media of Electrochemical Metallization Memories

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Resistive switching memories exhibit multiple and tunable states depending on their operation history, and they have attracted widespread interest to realize brain-like computing beyond the traditional von Neumann architecture. At present, the conductive-filament-type resistive switching memories (i.e., electrochemical metallization, ECM, memories) occupy the mainstream. Remarkably, the filament growth processes within these memories, crucial to their performance, have been widely investigated to realize the device optimization. With the combination of the kinetic Monte Carlo (KMC) simulations and restrictive percolation model, three different growth modes in ECM cells were dynamically reproduced, and am important factor, the relative nucleation distance, was defined to measure their transition.1 In our KMC simulations, the inhomogeneity of storage medium is realized through introducing evolutionary void versus non-void sites within it to mimic the real nucleation during filament growth. Finally, the renormalization group (RG) method was used in our proposed restrictive percolation model to well illustrate void-concentration-dependent growth mode transition, fitting the KMC results quite well.1 Later, an organic-inorganic hybrid resistive switching memory based on a nanoporous zinc-based hydroquinone (Zn-HQ) thin film has been fabricated with a Pt/Zn-HQ/Ag sandwich structure.2 The porous Zn-HQ functional layer ensures a typical electroforming-free bipolar resistive switching characteristic with the multilevel storage capability, lower operation voltages, higher on/off ratio above 102, and excellent endurance/retention properties for this device.2 Our KMC simulations confirm that the existence of nanopores in the Zn-HQ thin films facilitates the Ag filament formation, contributing to the high performance of this hybrid device.2 Our study spotlights a vital factor, void concentration (relative to defects, grains, or nanopores) of storage media, to significantly affect the growth of conducting filaments in storage media and even induce the growth mode transition. This factor inspires the experimental specialist that an effective strategy, nanostructure processing, can be adopted to realize the device optimization of resistive switching memories. This strategy was also experimentally confirmed.2

Keyword: Keywords: kinetic Monte Carlo (KMC) simulations, percolation theory, resistive switching memories, electrochemical metallization, microstructure manipulation

最终交流类型: Oral

The way to 2D diamond. Recent experimental results and theoretical insights

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With the developments in the field of 2D materials, nowadays of growing interest is synthesis and investigation of 2D diamond or diamane [1], whose potential properties put it in par with the most promising nanostructures such as graphene, h-BN or MoS2. Diamane films inherit from their bulk ancestor a number of remarkable properties that are highly desirable in materials research and applications. These include ultrahard coatings with broad-range optical transparency, the ability to act as a host-material for single-photon emitter defect-centers for quantum computing, superconductivity, biologically active substrates, biosensors, and more. The electronic properties of diamane strongly depend on the type of surface termination and surface orientation, making it a promising platform for nanooptics and nanoelectronics, as well as micro- and nanoelectromechanical systems [2].

The synthesis of diamane is currently a priority goal, but it remains rather challenging. It has been proposed that the thinnest "ultimate diamond slab" can be achieved by purely chemical means, without any pressure, in striking contrast to bulk graphite-diamond transformation.

Here I will show how a few-layer graphene can undergo phase transformation into ultrathin diamond film under reduced or no pressure, if the process is facilitated by hydrogenation or fluorination of the surfaces. Such “chemically induced phase transition” [3] is inherently nanoscale phenomenon, when the surface conditions directly affect thermodynamics, and the transition pressure depends greatly on film thickness. Ab initio computation of Gibbs free energy of the subsequent adsorption of reference atoms allows us to directly observe a nanoscale diamondization process and estimate a nucleation barrier. I show that diamond formation considerably depends on graphene layers number, their

stacking, type and arrangement of adatoms, as well as external parameters, and therefore requires fine tuning in experiments [4]. I will also show that the adsorption of various functional groups can lead to films with different structures (and properties) [5]. Finally, I will discuss recent experimental data in which 2D diamond has been obtained both by chemically induced phase transition and by other approaches.

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Keyword: graphene, 2D diamond, diamane, chemically induced phase transition

最终交流类型: Oral

Rational Design of Heteroanionic Two-Dimensional Materials with Emerging Topological, Magnetic, and Dielectric Properties

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Designing and tuning the physical properties of two-dimensional (2D) materials at the atomic level are crucial to the development of 2D technologies. In transition metal compounds (TMCs), anion engineering is one very effective method, because the anions hybridize with metal cations and greatly influence the band gaps, band dispersions, crystal field splitting, etc. Understanding how the variation of anions affects the electronic structures and physical properties is crucial for guiding the architecture of new functional 2D materials. Besides, the heteroanionic compounds containing multiple anions with different anionic characteristics, such as charge, ionic radii, electronegativity, and polarizability, add new dimensions for controlling and tuning the physical properties of materials.

Here, we introduce heteroanions into metal-centered octahedral structural units of a 2D crystal breaking the O_h symmetry, together with the synergistic effect of anions' electrons and electronegativity, to realize ternary 2D materials with emerging topological, magnetic, and dielectric properties. Using an intrinsic heteroanionic van der Waals layered material, VOCl, as a prototype, 20 2D monolayers VXY (X = B, C, N, O, or F; Y = F, Cl, Br, or I) are obtained and investigated by means of first-principles calculations. The anion engineering in this family significantly reshapes the electronic properties of VOCl, leading to nonmagnetic topological insulators with nontrivial edge states in VCY, ferromagnetic half-semimetals with a nodal ring around the Fermi energy in VNY, and insulators with dielectric constants in VOY higher than that of h-BN.

This work demonstrates the rationality and validity of the design strategy of multiple-anion engineering to achieve superior properties in the 2D monolayers with potential application in electronics and spintronics. Our design strategy can be further applied to those systems, not only to largely enrich the current family of 2D materials but also to explain general trends over broad compositional spaces.

Keyword: Materials design; 2D ternary heteroanionic compounds; Topological insulators; Magnetic nodal-ring semimetals; 2D dielectrics

最终交流类型: Oral

Designing two-dimensional ferroelectric materials from phosphorus-analogue structures

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Two-dimensional (2D) ferroelectric (FE) materials with relatively low switching barrier and large polarization are promising candidates for next-generation miniaturized nonvolatile memory devices. Herein, we screen out 39 new 2D ferroelectric materials, MX (M: Group III-V elements; X: Group V-VII elements), in three phosphorus-analogue phases including black phosphorene-like α-phase, blue phosphorus-like β-phase and GeSe-like γ-phase using high-throughput calculations. Seven materials (α-SbP, γ-AsP, etc.) exhibit FE switching barriers lower than 0.3 eV/f.u., ferroelectric polarization larger than 2×10^{-10} C/m, and high thermodynamic stability with energy above hull smaller than 0.2 eV/atom. We find that the larger the electronegativity difference between M and X, the larger the ferroelectric polarization. Moreover, larger electronegativity differences result in lower in-plane piezoelectric stress tensor (e_{11}) for MX consisting of Group IV and VI elements and larger e_{11} for those consisting of Group V elements. Further calculations predict a giant tunneling electroresistance (TER) in ferroelectric tunnel junction α-Sb(Sn)P/α-SbP/α-Sb(Te)P

(1.26×10^4%) and large piezoelectric strain coefficient (d_{11}) in α-SnTe (396 pm/V), providing great opportunities to the design of non-volatile resistive memories, and high-performance piezoelectric devices.

Keyword: two-dimensional (2D) materials, ferroelectricity, piezoelectricity, ferroelectric tunnel junction

最终交流类型: Oral

Nonvolatile electrical control of spin polarization in the 2D bipolar magnetic semiconductor VSeF

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Two-dimensional (2D) magnetic materials, showing great potential in information storage, transmission and processing by utilizing the spin degree of freedom, have attracted extensive interests since the experimental discovery of atom-thick magnetic materials CrI_3, $Cr_2Ge_2Te_6$, and Fe_3GeTe_2. Meanwhile, the sheer openness of 2D magnetic materials makes them possess gate tunability and integrated flexibility, which is appealing for next-generation nanoscale spintronic devices.

In order to develop high-performance 2D spintronic nanodevices, the flexible manipulation of carriers' spin polarization is highly desirable. As compared with the traditional external magnetic field control of spin orientation in materials, electric field control is an extremely exciting research area, both in fundamental science and technology application. As a result, nonvolatile electrical control of spin polarization in 2D magnetic semiconductors is greatly appealing toward future low-dissipation spintronic nanodevices. Here, we report a 2D material VSeF, which is an intrinsic bipolar magnetic semiconductor (BMS) featured with opposite spin-polarized valence and conduction band edges. BMSs, whose valence band maximum (VBM) and conduction band minimum (CBM) are derived from opposite spin channels, offer an ideal platform to achieve the electrical manipulation of both spin orientation around Fermi energy.

We then propose a general nonvolatile strategy to manipulate both spin-polarized orientations in BMS materials by introducing a ferroelectric gate with proper band alignment. The spin-up/spin-down polarization of VSeF is successfully controlled by the electric dipole of ferroelectric bilayer Al_2Se_3, verifying the feasibility of the design strategy. The interfacial doping effect from ferroelectric gate also plays a role in enhancing the Curie temperature of the VSeF layer. Two types of spin field effect transistors, namely multiferroic memory and spin filter, are further achieved in VSeF/Al_2Se_3 and VSeF/Al_2Se_3/Al_2Se_3 multiferroic heterostructures, respectively. This work will stimulate the application of 2D BMS materials in future spintronic nanodevices.

Keyword: 2D bipolar magnetic semiconductor, multiband Hubbard model, spin-exchange splitting, van der Waals multiferroic heterostructure, spin field effect transistors

最终交流类型: Invited

Tuning the Magnetic and Electronic Properties of Electrenes by Doping and Janus Engineering

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Electrenes, also known as monolayer electrides, possess distinctive characteristics stemming from the presence of anionic electrons. These anionic electrons, owing to their loosely bound and unrestricted nature, exhibit a low work function and an extended distribution, transcending the limitations imposed by atomic orbitals. Besides, electrenes showcase a range of remarkable physical properties, including superconductivity, topological matters, and Dirac plasmons. In our previous research, we introduced a novel magnetic mechanism exclusive to magnetic electrenes, which arises from the dual nature of the anionic electrons—localized and extended. The former engenders the spontaneous formation of local magnetic moments, while the latter gives rise to an extraordinary extended ferromagnetic direct exchange between them. Nonetheless, magnetic electrenes with intrinsic magnetism are scarce. In this presentation, we will elucidate how doping and Janus engineering facilitate the development of magnetic anionic electron states in non-magnetic electrenes.

Our initial proposition involves a stable non-magnetic semiconducting electrene, $ZrCl_2$, which can be effortlessly exfoliated from its experimentally grown layered bulk form. Intriguingly, we unveil a spontaneous spin splitting of the anionic electrons in monolayer $ZrCl_2$, leading to a nonmagnetic-to-magnetic phase transition at a critical doping concentration. By utilizing a low-energy effective model, constrained random phase approximation simulation, and Anderson's theory, we explicate the mechanism behind d magnetism in doped monolayer $ZrCl_2$ and validate the dual localized and extended nature of these magnetic anionic electrons. Our findings establish the potential for electric-field controllable magnetism in electrenes, presenting exciting prospects for novel spintronic applications.

Additionally, we will present a new category of Janus structures called Janus electrenes, which comprise different cation layers. By substituting one of the two zirconium cation layers in Zr_2Cl_2 with elements from groups I to III, we generate nine Janus 2D materials, denoted as $ZrXCl_2$ (where X = Na, K, Rb, Ca, Sr, Ba, Sc, Y, or La). The phonon spectra analysis verifies the dynamical stability of $ZrScCl_2$, $ZrYCl_2$, and $ZrCaCl_2$, affirming the feasibility of forming cationic Janus electrenes. Notably, the introduction of group III elements induces ferromagnetic behavior in the anionic electrons of the $ZrX^{III}Cl_2$ systems, $ZrX^{I}Cl_2$ materials manifest as ferromagnetic half-metals. These results introduce a new dimension of freedom to effectively manipulate the electronic and magnetic properties of electrenes, paving the way for innovative applications.

Overall, our investigations corroborate the dual localized and extended nature of anionic electrons in these extrinsic magnetic electrenes, thereby affirming the widespread presence of the unique magnetic mechanisms observed in magnetic electrenes.

Keyword: DFT, electride, magnetism, 2D materials

最终交流类型：Oral

Theoretical insight of pyrite bimetallic transition metal diselenides for oxygen reduction reaction

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Oxygen reduction reaction (ORR) plays a crucial role in fuel cell and metal–air batteries, making it a topic of great significance in electrochemical energy applications. Recently, transition metal dichalcogenides (TMDs) have emerged as promising materials for ORR due to their active surface or edge sites. However, the over-binding of O^* species significantly limits the intrinsic catalytic performance of TMDs. The single active center in TMDs poses challenges in surpassing the inherent limits of multi-intermediate reactions due to the simple structure and lack of synergistic activity centers. In this work, we provide a strategy to enhance ORR catalytic activity by introducing pyrite bimetallic transition metal diselenides ($ABSe_4$, A = Mn, Fe, Co, Ni, B = Cu, Cd, Sn) as catalysts. By employing first-principle calculations, we confirm the structural stability of all $ABSe_4$ based on the negative formation energies. We further calculate the free energies of the intermediates (O^*, OH^*, and OOH^*) adsorbed on $ABSe_4$, and find that the different elementary steps of ORR indeed occur on distinct metal active sites. Introducing other metal element weakens the adsorption of O^* intermediate on $ABSe_4$, leading to a significant improvement in the ORR catalytic activity.

The scaling relationships between the adsorption energies of three intermediates (ΔG_{*OOH} vs. ΔG_{*OH} and ΔG_{*O} vs. ΔG_{*OH}) in the $ABSe_4$ are well established. Furthermore, we noticed that the remarkable changes in adsorption energies and configurations of three oxygenating species in the bimetallic $ASnSe_4$ upon introducing Sn, compared to monometallic ASe_2 and $SnSe_2$. The partial density of states (PDOS) analysis and Bader charge confirms the altered electronic state of Sn because of the relatively strong interaction between A and Sn elements. In contrast, the relatively weak interaction between A and Cu or Cd elements in the $ACuSe_4$ and $ACdSe_4$ catalysts make it possible for the tandem catalysis of ORR. These findings provide valuable insights for designing optimum ORR catalysts.

Keyword: first-principle calculations, pyrite bimetallic transition metal diselenides, oxygen reduction reaction, electrocatalysis

最终交流类型: Invited

From reaction mechanism to computational screening in nanostructure catalysts

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Nanostructure catalysts have emerged as a highly promising field for achieving efficient and selective catalytic conversion of biomass, CO2, and nitrogen into value-added chemicals and fuels. Among various reactions, electrocatalytic nitrogen reduction and ammonia decomposition have attracted significant attention due to their potential in mitigating the energy and environmental crisis. To design and optimize high-performance nanostructure catalysts, it is necessary to understand the reaction mechanism and develop novel computational screening methods that can predict the catalytic activity and selectivity of various catalysts.

In the first part of this report[1], we discuss the screening of transition metal single-atom catalysts supported by a WS2 monolayer for electrocatalytic nitrogen reduction reaction. The nitrogen reduction reaction (NRR) is a key reaction that enables ammonia synthesis with high energy efficiency, and the use of single-atom catalysts can significantly enhance the selectivity and activity of the reaction. Here we systematically investigate the NRR activity and selectivity of transition metal (TM) single-atom catalyst (SAC) anchored WS2 monolayers (TM@WS2) by means of first-principles calculations and microkinetic modeling. We analyze the activity trend and descriptor and demonstrate how computational screening can provide insights into the reaction mechanism and factors affecting catalytic performance, such as the electronic structure, charge transfer, and coordination environment of the active site.

In the second part of this report[2], we present the computational screening of bimetallic catalysts for ammonia decomposition. By using density functional theory calculations and ab initio molecular dynamics, we can predict the activity and stability of different bimetallic catalysts and elucidate the underlying mechanisms that govern their performance. We also discuss the effect of various factors, such as the composition, morphology, and stability of bimetallic catalysts and provide guidance for experimental synthesis.

In conclusion, this report highlights the importance of combining fundamental studies of reaction mechanism with computational screening methods in the design of efficient and stable nanostructure catalysts. We believe that this work will provide valuable insights for researchers in the field of catalysis and materials science and facilitate the development of sustainable and energy-efficient catalytic processes.

1. Phys. Chem. Chem. Phys., 2022, 24, 13384
2. J. Phys. Chem. C 2022, 126, 192−202

Keyword: computational screening, catalyst, ammonia decomposition, nitrogen reduction reaction

最终交流类型：Invited

Pagoda Instability at the Chemo-Mechanical Coupled Solid-Liquid Interface

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When inserting a cylinder soluble solid into the liquid, we find a new type of interfacial instability, i.e. the periodic instability of solid-liquid interface on the surface of soluble solids. Because the geometry and function of the dissolved solid surface is similar to the Chinese pagoda, we name this new phenomenon to be the Pagoda Instability. We examined different solid-liquid pairs, such as liquid@soluble solid, acid@metal, electrolyte@metal under electric field, all of which would occur similar phenomena. The final morphology of the Pagoda Instability is classified in detail based on a large number of experimental results.

Unlike the formal instability occurred at solid-liquid interface, Pagoda Instability is controlled by both mechanical and chemical fields, therefore the strong interactions between solid and liquid should be considered. Liquid dissolves solid and changes the geometry and properties of solid, while solid dissolves into liquid and changes the properties of the liquid. A cross-scale combined method of experiments, simulations, and theories is developed to reveal the chemo-mechanical coupled mechanism and governing laws of the Pagoda Instability driven by interfacial energy and chemical potential. The influences of the moving boundary condition, the contact angle hysteresis, and the energy dissipation are uncovered. By elucidating the evolution of free energy during the periodic instability of contact lines, we established the criteria for the Pagoda Instability.

Based on the Pagoda Instability, we design and fabricate the Dry-Tip AFM tips, which have the ability to shield capillary forces and pressure perturbations induced by the solid-liquid interfaces. The Dry-Tip AFM can achieve accurate force-displacement curves, morphology and surface properties shielding the effects caused by wet environments or liquid films. It is hoped that our work can enrich the understanding of the chemo-mechanical coupled solid-liquid interfaces, and provide theoretical basis and design guidance for the development of new techniques in the applications such as micro-nano processing, biomedicine, ultra-sensitive sensors and etc.

Keyword: Pagoda Instability, Solid-liquid interface, Chemo-mechanical coupling, AFM

最终交流类型: Invited

Theoretical investigation on the light-activated mechanism of gas sensing with density functional embedding theory

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The traditional literature assumes that the light-activation effect on sensors is due to the excitation of quantum dot sensors, which regulates the sensor's performance through photo-generated charges and holes. Then, the response wavelength of light is determined based on the quantum dot bandgap. However, our work found that visible light significantly improves the NO_2 gas sensor performance with different bandgaps. All the activating effects on the sensors are highest in the violet region, consistent with the NO_2 absorption spectrum. The wavelength is determined by the adsorbed molecule. To unravel this contradiction, we applied the density functional embedding theory (DFET) and the embedded correlated wavefunction method (ECW) to study the excited states of adsorbed molecules and understand the light-activated mechanism of gas sensing. This method combines the periodic

DFT method describing the inert solid environment and the high-level CW method describing the active center involved in the reaction. By comparing the ground state and excited-state properties of NO_2 molecules on three quantum dot gas sensors (PbSe, CdSe, and CdS), It is found that all three systems have strong light adsorption in the violet region. However, the violet adsorptions of CdS and CdSe systems result from the excitation of adsorbate NO_2. On the contrary, the PbSe-NO_2 is due to the excitation of sensor PbSe. We proposed a new light-activated mechanism in collaboration with experimental groups, breaking inherent cognition. For covalent systems, we used the capped-DFET method to theoretically simulate the adsorption and desorption properties of gas molecules on graphene and PdN3 single atoms loaded on graphene, further confirming this light-activated mechanism. We also studied the chemical mechanism of photocatalytic synthesis of singlet oxygen ($^1O_2$) with single-atom catalyst (M-N-C). The emb-CASPT2 method is applied at the active center, which accurately describes the multi-reference characteristics and excited-state properties. Compared with commonly used DFT and CW methods, the DFET method effectively combines high precision and high speed, achieving high-precision theoretical simulation of complex systems.

Keyword: density functional embedding theory, gas sensor, light-activate, single-atom catalyst

最终交流类型: Oral

Selective activation of four quasi-equivalent C–H bonds yields N-doped graphene nanoribbons with partial corannulene motifs

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Carbon-hydrogen (C–H) bond activation in a molecule is an efficient yet challenging route towards synthesis of complex organic compounds due to the existence of multiple reactive sites. By introducing heteroatoms, such as nitrogen and sulfur atoms into the organic skeleton, the ortho C atoms can be more reactive than other C atoms. This strategy, however, lacks selectivity among equivalent/quasi-equivalent ortho C atoms, as previous studies show all the ortho C atoms have almost equal probability to be activated. Therefore, in route towards fine control over C–H selectivity, the selective activation of equivalent/quasi-equivalent ortho C(sp3)-H would be a major achievement in the field.

In recent years, on-surface chemistry has become a quickly developing field and provides an important route for synthesizing complex organic compounds benefiting from extraordinary controllability over the molecular formation process. In addition, surface characterization techniques, such as scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) combined with density functional theory (DFT) calculations, have been demonstrated to be an invaluable strategy to allow unambiguous characterization of the complex chemical structures and further elucidation of their underlying mechanism. The surface could provide the equivalent functional groups with variable activity due to different binding affinity, which has the potential to induce asymmetric active sites in symmetric molecules. By carefully designing the molecular symmetry, geometric size and orientation on a substrate, it is possible to realize selective activation of C–H bond among equivalent/quasi-equivalent sites.

Here, we successfully achieve the selective activation of four quasi-equivalent C–H bonds in a specially designed nitrogen-containing polycyclic hydrocarbon (N-PH). Density functional theory calculations reveal that the adsorption of N-PH on Ag(100) differentiates the activity of the four ortho C(sp3) atoms in the N-heterocycles into two groups, suggesting a selective dehydrogenation, which is demonstrated by sequential-annealing experiments of N-PH/Ag(100). Further annealing leads to the formation of N-doped graphene nanoribbons with partial corannulene motifs, realized by the C–H bond activation process. Our work provides a route of designing precursor molecules with ortho C(sp3) atom in an N-heterocycle to realize surface induced selective dehydrogenation in quasi-equivalent sites.

Keyword: selective C-H activation, polycyclic aromatic azomethine ylide, on-surface synthesis, graphene nanoribbons, density functional theory

最终交流类型：Oral

Electrically tunable optical PUF based on BaTiO3 nanoparticles

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Nowadays, with the expansion of the Internet-of-Things (IoT) ecosystem, it is fundamental to ensure the security of the equipment in the IoT. Moreover, the prevalence of counterfeit products often brings adverse effects to society, such as breaking the intellectual property law to shake the social economy [1], manufacturing counterfeit drugs that endanger human safety [2], hence it is of great significance and urgency to develop robust, unclonable tokens with the features of large-capacity, one-way anti-counterfeiting, reconfigurability for social and economic benefits [3]. Here, a novel electrically tunable optical physically unclonable function (O-PUF) is proposed, which has excellent potential applications in anti-counterfeiting, security authentication, data encryption, etc.

As a security identifier for hardware [4], PUFs have unique and unclonable physical characteristics due to the inherent randomness during manufacturing. Among various types of proposed physically unclonable functions (PUFs), Pappu R et al. introduced the definition of physical one-way function (POF) and designed the first form of O-PUFs [5]. Their O-PUF based on optical scattering has a high angle and wavelength dependence on scattering. Therefore, it is effective to extract physical features from the laser speckle images, and a slight change of the excitation light could bring a large change of the laser speckle. O-PUFs are also proved to be more resistant to machine learning attacks than electronic PUFs [6]. Further, integrated O-PUF was proposed by Rührmair U et al. [7] by constructing a tunable coherent light source array instead of modulating a single light source. No matter what type of O-PUF is, most of its scattering structures are linear, that is the refractive index of the medium does not change significantly with low light intensity. In this regard, the linear scattering of the excitation light array makes the extracted physical properties of O-PUF vulnerable, and there are still risks under machine learning attacks. In our proposed electrically tunable O-PUF, $BaTiO_3$ nanoparticles are used as the scattering medium. The characteristic of a larger refractive index of $BaTiO_3$ (2.4) makes the scattering very strong, which is a desired feature of O-PUFs. Besides, $BaTiO_3$ has the ferroelectric phase at room temperature as well as significant electro-optic effects [8,9], so changing the voltage will significantly change the refractive index. Essentially, Maxwell's equations of particle scattering are nonlinearly superimposed by changing the medium parameters through the electric field. Therefore, the introduced tunable electric field in combination with the modulation of optical excitation makes our O-PUF have both the advantages of resistance of machine learning attacks and integration capabilities.

We used COMSOL to simulate the scattering field of the two-dimensional random structure based on $BaTiO_3$ nanoparticles. TE wave (λ=632 nm) incidents perpendicularly on the O-PUF with a particle diameter of 200 nm, and the porosity factor of 0.7. Fig. 1 shows its schematic diagram and the output electric field distribution. The speckle pattern-response distribution is collected and extracted as a binary key by Gabor filtering [10]. Adjusting the voltage changes the output speckle, and thus changes the extracted binary key. A new independent code is generated if the normalized Hamming distance between two binary keys is equal to 0.5. We focus on the dependence of the independent coding times on the voltage range as well as the thicknesses of O-PUFs. Fig. 2(a) depicts the relationship between Hamming distance and voltage of ten different pieces of O-PUFs with a thickness of 5 μm. Due to the relationship between Hamming distance and voltage is approximately linear near the null voltage, the voltage change required to generate a new independent code can also be determined by the full width at half maximum (FWHM) of the curve. Therefore, the independent coding times within a given voltage range can be measured by $\delta V/FWHM+1$, where is the tuning voltage range, and it can be used to estimate the variation of entropy induced by the changing voltage. Fig. 2(b) shows the independent coding times of O-PUFs with a thickness varying from 1 μm to 10 μm (δV=100 V). It can be seen from that there is a linear proportional relationship between the thickness of O-PUFs and the independent coding times, and the entropy also goes up by increasing the O-PUF thickness. For example, the entropy of the O-PUF with a thickness of 5 μm and the δV of 100 V enhances by four times over that of the case without voltage.

In conclusion, our proposed electrically tunable optical PUF based on $BaTiO_3$ nanoparticles effectively enhances the entropy and generates more binary keys by changing the voltage and O-PUF thickness. It is well expected that this O-PUF has more excellent security in the integration field.

Keyword: Physically unclonable function, electrically tunable, BaTiO3 nanoparticles, independent coding times

最终交流类型: Oral

A stable rhombohedral phase in ferroelectric Hf(Zr)1+xO2

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Hafnium oxide-based ferroelectric materials are promising candidates for next-generation nanoscale devices because of their ability to perfectly integrate into silicon electronics. However, the intrinsic high coercive field of the fluorite-structure oxide ferroelectric devices leads to the incompatible operating voltage with advanced technology node and the limited endurance performance. By employing density functional theory (DFT) calculations, we discover a rhombohedral ferroelectric Hf(Zr)1+xO2 material rich in Hf(Zr). The formation energy of the r-phase is lower than those of the o-phase and monoclinic phase (m-phase) in Hf(Zr)-rich Hf(Zr)1+xO2 films when increasing the ratio of Hf(Zr) to O, which is more conducive to the formation of the r-phase. The ferroelectric polarization in r-phase HfO2 is believed to be induced by the lattice expansion in the [111] direction. Similarly, the polarization of Hf(Zr)1+xO2, like that of stoichiometric r-phase HfO2, depends on the d111 value. Comparing with the well-known Hf(Zr)O2-x with oxygen vacancies, Hf(Zr)-rich Hf(Zr)1+xO2 exhibits distinct characteristics. We have further investigated the ferroelectric properties of the Hf(Zr)-rich Hf(Zr)1+xO2, including the phase transition mechanism, ferroelectric switching pathway, and the origin of its ferroelectricity. Different from the ferroelectric HfO2 in o-phase with localized dipoles or the r-phase Hf(Zr)O2-x involving oxygen migration during switching process, the ferroelectric Hf1+xO2 with spread dipoles has quite broad domain walls which contribute to a low switching barrier, and a relatively small Ec. X-ray diffraction (XRD) and scanning transmission electron microscopy (STEM) experiments confirm the existence of the r-phase Hf(Zr)1+xO2. High angle annular dark field (HAADF) image of the Hf(Zr)1+xO2 film clearly shows the intercalation of excess Hf/Zr atoms, confirming the Hf/Zr-excess structure. Further device experiments reveal a high remnant polarization, a small saturation polarization field, an ultra-low coercive field, and a large breakdown electric field. Most importantly, a long device lifetime of more than 1012-cycles has been achieved at saturation polarization. This discovery may help to realize low-cost and long-life memory chips.

Keyword: first-principle calculations, ferroelectricity, hafnium oxide-based material, phase transition, ferroelectric switching

最终交流类型: Invited

Quantum Phase Engineering of Two-Dimensional Post-Transition Metals by Substrates

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Quantum anomalous Hall insulators (QAHIs) are a highly promising class of quantum materials for spintronic and quantum computational devices owing to their incredibly precise quantization and robustness against defects along spin-polarized edge electron channels. Realization of the high-temperature QAH effect has been hindered by the difficulty of simultaneously controlling both magnetization and spin-orbit coupling (SOC), and the critical temperatures for the QAH effect are fundamentally limited by the SOC gap and the ferromagnetic (FM) Curie temperature (Tc). Thus, it is of great significance to discover new QAHIs with both larger SOC gaps and higher Tc. Here, we propose a new realistic strategy to engineer topological and magnetic properties of two-dimensional (2D) hexagonal lattices consisting of post-transition metals such as Ge, Sn, and Pb, as examples, and to achieve room-temperature QAHI. Our first-principles calculations demonstrate that substrates serve as templates to form 2D lattices of a wide range of lattice constants with high thermodynamic stability, where their topological properties as well as magnetic properties sensitively change as a function of lattice constants: the system undergoes a first-order phase transition from nonmagnetic to ferromagnetic state above a critical lattice constant. Consequently, substrates can be used to explore versatile magnetic, electronic, and quantum topological properties. We establish phase diagrams of versatile quantum phases, including quantum spin Hall insulators (2D topological insulators), magnetic Weyl semimetals, QAHIs, and ferromagnetic semiconductors, in terms of key governing parameters (exchange coupling and SOC) effectively tuned by the lattice constants. We reveal the room-temperature QAH effect: Sn on 2√3×2√3 graphane is a QAHI with a large spin-orbit coupling gap of ~0.2 eV and a Tc of ~380 K by using the 2D anisotropic Heisenberg model. Using a four-band tight-binding Hamiltonian based on first-principles calculations we reproduce these four phases and further establish their phase diagrams in terms of exchange coupling and SOC. Our results should be instrumental in finding new 2D high-temperature QAHIs.

Keyword: quantum anomalous Hall insulators, ferromagnetic semiconductors, graphane, post-transition metals, first-principles calculations

最终交流类型: Invited

Active Nanoparticles Strengthened and Toughened Gel of Noncovalently-Bonded Supramolecular Chains

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Supramolecular materials are ubiquitous and increasingly employed in many modern industries from solid-state-batteries, drug delivery to rubber tyres. Targeted biomedical and industrial applications of synthetic supramolecular materials require a pre-definition of both their mechanical strength and toughness, which however, are hard to balance. In particular, materials made of supramolecular gels that have a crosslinked and/or entangled structure usually exhibit a high mechanical strength but also a limited toughness. To operate within specification even under extreme conditions such as high pressures and rapid forced-deformations, these supramolecular materials have to be sufficiently strong and tough to resist and dissipate the damaging effect of external impacts. Achieving strong mechanical strength combined with large toughness is one of the most challenging tasks for designing some function-specified supramolecular materials that can stay undestroyed when being forced to deform strongly and quickly. Through scrutinizing statistically the static and dynamical behaviors of nanoparticles (NPs) and noncovalently-bonded supramolecular chains (NBSCs), together with performing Rouse mode analysis to quantify the relaxation spectra of NBSCs, we show and demonstrate using numerical simulations that active NPs immersed in an entangled and crosslinked network of NBSCs induce delayed segmental relaxation and strand-crossing of NBSCs, which thereby contributes to enlarging mechanical strength as well as toughness of the studied supramolecular gel. The dynamic mechanical improvements introduced by active NPs will have broad interests for expanding further the practical applications of gels of NBSCs in emerging areas ranging from aerospace and automobile industries to wearable electronics and displays, among many others.

Keyword: Active Nanoparticles; Supramolecular Chains; Crosslinked Network; Viscoelasticity; Mechanical Strength

最终交流类型: Oral

Effect of surface modification on interfacial properties of fiber reinforced polymer

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Glass fiber-reinforced (GFR) epoxy resin is widely utilized in various applications such as insulating materials, adhesives, electronic packaging materials, and matrices for functional composites. This is due to its thermal stability, lightweight nature, superior mechanical properties, excellent corrosion resistance, and outstanding electrical insulation. The adhesion between the fiber and matrix plays a crucial role in determining the performance of the composite, as it ensures the transfer of stress from the weaker matrix to the stronger fiber. However, achieving efficient stress transfer from the matrix to the glass fiber (GF) remains a challenge, hindering the complete utilization of the reinforcing capabilities of the fibers. To address this, extensive research has been dedicated to the surface modification of glass fiber, including methods such as plasma treatment, chemical treatment, and electrochemical

oxidation and polymerization, aimed at improving the interfacial properties of composites. In recent years, carbon nanomaterials, such as graphene and carbon nanotubes (CNTs), have garnered significant attention due to their exceptional properties. They have been widely applied as nanoscale reinforcements in composites to enhance their properties. Coating glass fiber with CNTs or graphene, for example, can create mechanical interlocking between the fiber and the matrix. Studies have shown that incorporating CNT-coated glass fiber can lead to over 30% improvement in the Young's modulus of GFR epoxy, while graphene-coated GF can increase fracture strength by approximately 30%. Despite numerous experimental investigations into the effect of carbon nanomaterial coatings on the mechanical properties of GFR epoxy, the underlying mechanisms governing the improvements and failures of such nanocomposites at the atomistic scale remain unidentified due to limitations in experimental approaches. Molecular dynamics (MD) simulations have been widely employed to explore the physical behaviors of materials at the atomistic scale, offering an in-depth understanding of molecular interactions while controlling experimental variables. MD simulations enable the depiction of surface modifications' impact on the structural evolution of the interface during deformation and help identify the reasons behind variations in interfacial properties.

In this study, we investigate the influence of graphene and single-walled carbon nanotubes (SWCNTs) on the interfacial properties of glass fiber-reinforced epoxy at the atomistic scale. Specifically, we sandwich graphene and SWCNTs between epoxy and silica to examine the debonding behavior of the sandwiched structures. Our findings reveal a significant improvement in interfacial energy with the incorporation of graphene and SWCNTs between epoxy and silica, resulting in enhanced adhesion stress for graphene coating and increased debonding displacement for SWCNT coating. Unlike the epoxy/silica without coatings, where the silica and epoxy detach from the contact surface, the sandwiched structures exhibit different failure modes. The sandwiched structure with graphene coating fails at the epoxy matrix close to the interface, displaying a cohesive failure mode attributed to relatively stronger interfacial interactions. On the other hand, the structures with SWCNTs fail at the interface between silica and SWCNTs, representing an adhesive failure mode due to the interlocking between SWCNTs and polymer chains. This work offers theoretical insights into optimizing the interface adhesion of coated glass fiber-reinforced epoxy through structure design and surface modification of coating materials.

Keyword: Interfacial failure; Carbon nanotube, Graphene; Glass fiber-reinforced epoxy composite, Molecular dynamics simulations

最终交流类型: Invited

Computational Design of Nano-materials for Hydrogen Energy Application

张亮
清华大学

Recently, hydrogen has been widely studied as an energy carrier that can simultaneously meet the requirements of clean and low-carbon emissions, as well as flexible and efficient energy use under the "30-60" goal. Using renewable energy to produce and utilize hydrogen through electrocatalysis is a key pathway for efficient and safe utilization of hydrogen energy and achieving sustainable development. However, the catalysts currently used for electrocatalytic water splitting and hydrogen fuel cells heavily rely on precious metal catalysts (such as Pt, Ir, Ru, etc.). Therefore, it is particularly necessary and urgent to develop high-performance and low-cost electrocatalysts for hydrogen conversion. Alloy catalysts can effectively reduce the loading of precious metals and even further improve catalyst performance. The degree of order in which different atomic elements occupy lattice sites is a key characteristic of the atomic arrangement of alloy catalysts, which has an important influence on the activity and stability of the catalyst. This work will introduce our recent theoretical work on accelerating alloy catalysts based on active learning. By combining density functional theory methods with Bayesian optimization, we can quickly and efficiently search for and optimize the composition and structure of new alloy catalysts. Using this model, we have optimized the key reaction oxygen reduction catalysts, hydrogen oxidation catalysts, and oxygen evolution catalysts in electrolytic hydrogen production and fuel cells. The optimized alloy catalysts exhibit excellent activity and stability, and have lower costs and better sustainability compared to traditional precious metal catalysts. This work has developed an efficient and accurate prediction model for the stability and activity of alloy catalysts, providing new ideas and methods for the development of high-performance and low-cost electrocatalysts for hydrogen conversion.

Keyword: Hydrogen and Fuel Cell，Machine learning, Alloy, Gas Sensing

最终交流类型: Oral

Theoretical and experimental study on temperature field distribution of superlarge vacuum furnace

肖振华
东北大学

Superlarge vacuum furnace is widely used for large structural parts under heat treatment due to the advantage of large effective heating area and high production efficiency and has become established as one of the most critical parts in the ceramic, steel and metallurgy industrial areas. However, the effect of structural parameters on temperature uniformity of superlarge vacuum furnace still is unclear. Hence, we proposes a method for the design optimization of superlarge vacuum furnace by computational fluid dynamics. The temperature distribution in furnace was calculated under different boundary conditions and structural sizes to optimize the structure and temperature field of the furnace. This work focuses on temperature change of the heating area, focusing on a superlarge vacuum sintering furnace used in a factory, establishes a three-dimensional CFD numerical simulation model of the energy-mass transfer in this region. The key thermodynamic parameters used in the simulation calculation are further optimized through monitoring data and experimental results. Then, a parametric study is conducted to investigate the effects of furnace geometrical characteristics on temperature distribution inside the furnace. These factors including a variety of different parts such as the structure, quantity and layout of the heating elements, thickness of insulation layer, vent location etc. Besides, the relevant database of the internal temperature and quality of the workpiece is established by the visualization of the internal temperature of the workpiece. It is helpful for process parameter optimal design. Through the transient nonlinear thermal analysis of the superlarge vacuum furnace, the real-time visualization of the temperature field in the furnace under vacuum environment is realized. Combined with the experimental measurement data of the vacuum furnace under the optimized design scheme, the feasibility of the optimization scheme can be verified, which can provide a theoretical reference for the design of the superlarge vacuum heat treatment equipment.

Keyword: Vacuum furnace，Numerical simulation，Temperature distribution theory，Optimal design

最终交流类型：Invited

Materials Informatics: AI in Materials Science

LEI SHEN
Department of Mechanical Engineering, National Univeristy of Singapore

There is no doubt that technology will be the key driver of future world economy. New technologies may also bring solutions to many of the world challenges we are facing currently, such as energy crisis. Developing most new technologies are on the basis of new materials. For example, Si-based electronics and Li-based batteries. Unfortunately, it takes typically 15-20 years to move a newly discovered advanced material from the laboratory to the commercial market place in the traditional approach. The high-throughput calculation is an essential idea to shorten this materials development continuum and reduce its cost.

Our ability to generate and collect vast volumes of materials data has significantly outstripped our capacity to analyse it, leading to the emergence of a new paradigm in materials science and engineering - data-driven materials innovation utilising machine learning (ML). 'Big data' is driving significant changes across all scientific and engineering fields and is beginning to revolutionise the way materials researchers operate and interact. For instance, scientists can discover and design new materials using failed experiments with the assistance of ML techniques.

In this talk, I will review the state-of-the-art developments in high-throughput calculations and machine learning within the field of materials science. This will include a special focus on the discovery of new materials existing as two-dimensional (2D) crystals with tunable electronic properties, i.e., development of 2DMatPedia database and the development of explainable ML models for discovering materials.

Keyword: Machine learning, 2D materials database, high-throughput calculations, materials informatics, explainable deep learning, electrode materials

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最终交流类型：Invited

Molecular dynamics simulation of molecular design and property prediction of novel elastomer

刘军
Beijing University of Chemical Technology, China

Polymer nanocomposites (PNCs) are widely used in automobile tire manufacturing industry. Concerning the long-standing energy crisis, designing and fabricating PNCs with both high strength and low energy consumption has gained numerous scientific interests.

Inspired by nanoparticle-based supramolecular materials, the processed nanoparticles (NPs), as one of the synthetic monomers to build polymer chains, can essentially enhance the strength and stability of the filler network, thus achieving high strength and low energy consumption in the novel PNCs. We constructed the novel nanopolymer composites by embedding nanoparticles into polymer chains through coarse-grained molecular dynamics simulations. The structural, dynamic, mechanical and viscoelastic properties influenced by the content and size of the NPs are systematically explored. Compared to traditional PNCs, this novel PNCs exhibits a relatively higher glass transition temperature at the same content of NPs. Moreover, by analyzing the microstructure evolution during deformation, it was found that the formation of a zigzag-interlock structure with an intermediate strength, namely between the physical and chemical interaction, allows for a more prominent mechanical reinforcing efficiency than traditional PNCs. Besides, the NP size and the crosslink density play an important role in tailoring the mechanical properties. Finally, the dynamic mechanical properties of this novel PNCs, such as the loss factor and hysteresis loss, exhibit a much smaller energy dissipation than those of traditional PNCs, which is attributed to much lower friction between NPs-polymer brought by the more stable filler network. The slip rate between NPs-polymer can be reduced by 30%~60% in the nanopolymer system compared to the traditional PNCs. In general, our work confirms that this novel PNCs is an excellent candidate to exceed the traditional PNC by possessing a more significant nano-reinforcing effect and a much less dynamic hysteresis, opening a good avenue for the design and fabrication of next-generation elastomer nanocomposites tailored for green automobile tires.

Keyword: elastomer, simulation, structure-property relation

最终交流类型: Invited

Wetting with Thin, Deformable Boundaries: From Graphene to Lubricated Surfaces

戴兆贺
北京大学

In various biological and micro/nanomechanical systems, droplets are frequently constrained between or adhered to thin fluid or solid films, giving rise to a novel category of wetting problems characterized by two key factors: 1) small scales and 2) large slenderness. The crucial characteristic of small scales is the impact of intermolecular forces, which can even dominate over elastic forces in solid films or capillary forces in liquid films. The large

slenderness enables the simplification of three-dimensional theories in fluid and solid mechanics along the thickness direction. However, it also calls for a reevaluation of the fundamental principles of classical wetting problems. In the case of solid films, the large slenderness entails nonlinear elastic deformation, fundamentally modifying the equilibrium conditions at the liquid-solid contact line. For fluid films, the deformation of liquid-liquid interfaces experiences geometric constraints.

This presentation aims to demonstrate the establishment of theoretical models that simultaneously account for small-scale forces and thin, deformable boundaries. Two examples will be introduced: 1) the statics of liquid cells formed by droplets confined at bilayer graphene interfaces, and 2) the dynamics of droplets on ultrathin liquid lubricated surfaces. The discussion will encompass several geometric and physical parameters (groups) that govern these static/dynamic systems. Through a combination of theory and experiment, the presentation will elucidate how the deformation of slender boundaries leads to "long-range" interactions between droplets or the self-merging of droplets.

Keyword: Wetting, Elastocapillarity, Lubricated surfaces, Graphene

最终交流类型: Invited

Magnetic and Topological Excitonic Insulators from First-principles

李元昌
北京理工大学

Magnetic/Topological excitonic insulators combine magnetism/nontrivial-topology and spontaneous exciton condensation, with dual functionality of magnetic/topological insulators and excitonic insulators. Yet, they are very rare and little is known about their formation. In this presentation I will describe our recent progress in finding and designing two-dimensional magnetic excitonic insulators and topological excitonic insulators using first-principles GW-BSE calculations in accordance with the selection rule. We reveal an unusual electronic state (dubbed as half excitonic insulator) in monolayer $1T\text{-}MX_2$ (M = Co, Ni and X = Cl, Br). Its one spin channel has a many-body ground state due to excitonic instability, while the other is characterized by a conventional band insulator gap. We predict the semi-hydrogenated graphene (known as graphone) as a spin-triplet excitonic insulator with a critical temperature of 11.5 K. We find that a mechanism dubbed as parity frustration prevents excitonic instability in usual topological insulators, and those whose band inversion is independent of spin-orbit coupling are possible candidates. We verify this on four monolayer double-transition-metal carbides (MXenes), which show a robust thermal-equilibrium exciton condensation, being sufficient for topological applications at room temperature.

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Keyword: Excitonic insulator; Bose condensation; First-principles calculations; Two-dimensional semiconductors

最终交流类型：Invited

Rational Design of Electrocatalysts for Oxygen Evolution Reaction

王璐
Soochow University, China

The oxygen evolution reaction (OER) is the key process that severely limited the overall efficiency of electrochemical water splitting, so exploring the highly efficient electrocatalysts for OER is an urgent issue. Two strategies are suggested to develop more active catalysts to promote OER reaction. (1) we propose a strategy to regulate the magnetic behavior of Fe atoms in hematene by introducing structural defects to enhance its OER activity. The most stable DVFe1−O defect in hematene exhibits superior OER activity, which originates from the unique spin state of the active Fe atom. A novel descriptor of the magnetic moment difference on active Fe is proposed to efficiently evaluate the OER activity; (2) we develop a strategy by combination of high-throughput density functional theory (DFT) and machine learning (ML) techniques for material discovery on IrO2-based electrocatalysts with enhanced OER activity. Utilizing the neural network language model (NNLM), we associate the atomic environment with the formation energies of crystals and free energies of OER intermediates, and finally a series of potential candidates have been screened as the superior

OER catalysts. This strategy could efficiently explore promising electrocatalysts, especially for evaluating complex multi-metallic compounds.

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Keyword: oxygen evolution reaction, metal oxides, spin-modulated, high-throughput calculations, machine-learning

最终交流类型: Invited

Material Simulations in 2D Limit for Non-volatile Data Memory

李贤斌

吉林大学

With the rapid development of the data-intensive industry, such as machine learning, Internet of Things, and piloted driving in recent years, high-performance computing and memory hardware are therefore required [1]. For implementation of these technology, various kinds of nonvolatile data memory such as phase-change memory, ferroelectric memory, resistive memory with excellent performances are being developed. One advantage for them is able to miniatured ultra-scaling of corresponding semiconductor materials to achieve high-density integration for the big-data requirements. In this talk, I will introduce a series of DFT simulation studies recently in the 2D material limit for phase-change memory [2,3], ferroelectric memory [4], resistive memory [5].

Keywords: phase-change memory, ferroelectric memory, resistive memory, 2D limit, ultra-scaling

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最终交流类型：Invited

Solvent evaporation driven interface segregation of single-chain nanoparticles in all-polymer nanocomposite films: its formation mechanism and application

钱虎军
吉林大学

In athermal all-polymer nanocomposites (all-PNC), single-chain nanoparticles (SCNPs) are often considered to be well miscible with polymer matrix due to their similarity in chemical composition. However, internal cross-linking units of SCNPs must have different chemistry from the backbone monomers or matrix. Therefore, a hypothetically uniform dispersion of SCNPs in the polymer matrix have to be reconsidered, especially under the action of solvent. Here, we use large-scale molecular dynamics simulations to study the influence of the solvent selectivity on dispersion state of SCNPs in all-PNC film upon solvent evaporation. Surprisingly, we find distinct dispersion states of SCNPs in drying films with different solvent selectivity. When the solvent is both good for cross-linkers and backbone/matrix monomers, SCNPs can be uniformly dispersed. However, when the backbone/matrix monomers have a better solvophilicity than the cross-linker and the solvophilicity of the latter is weak enough, we find segregation of SCNPs in surface regions. A mean-field theory calculation demonstrates that the increase of the chemical potential of SCNPs in the bulk region drives its interface segregation along with the solvent evaporation. Detailed analysis of chain conformations shows that after the surface accumulation of SCNPs, the conformation of matrix chains will be largely influenced. In particular, when SCNPs are accumulated at the interface, chain end of free matrix chains can penetrate into inter-particle spaces between neighboring SCNPs, therefore aligning free matrix chains vertically to the surface. In addition, in a blend system of SCNP and block copolymers (BCP), we found that the interface segregation of SCNPs can be well utilized to control the perpendicularly orientation of the self-assembled BCP domains. The interface segregation of SCNPs is found to neutralize the interface selectivity for the distinct blocks in BCP. We believe that such a strategy can be useful in regulating the orientation of BCP films in practical applications.

Keyword: all-polymer nanocomposites, single-chain nanoparticles, interface segregation, solvent evaporation, self-assembly orientation of block-copolymers.

最终交流类型:

Molecular mechanisms of efficient organic photovoltaics

易院平

中国科学院化学研究所

For organic solar cells, the photoelectric conversion needs a series of electronic processes, including light absorption, exciton diffusion, exciton dissociation, charge migration, and charge collection. At the same time, there also exist competitive energy loss processes including exciton decay and charge recombination. Here, we will focus on the charge generation, charge migration, and charge recombination processes in the efficient organic solar cells based on the A-D-A type acceptors, discuss the effect of electronic polarization, super-exchange transport, and triplet channel recombination, and then propose a new mechanism of free charge generation and effective strategies for promoting charge transport and reducing charge recombination.

Keyword: photoelectric conversion, charge transfer, exciton dissociation, excited state, organic semiconductors

最终交流类型: Invited

Friction and Wear Beyond Hertzian Contact

刘小明

Chinese Academy of Sciences

The Hertzian contact model has been a nonlinear interfacial law used for over a century. However, there are situations where the Hertzian assumption fails to adequately capture the contact behavior for advanced interfaces. In this talk, we delve into the scenarios where the multiscale nature of solid surfaces comes into play. These surfaces, widely employed in various applications, may be coated with films, exhibit roughness consisting of numerous small contact spots, or possess thin thicknesses with strain gradient and dynamic wave effects. The focus of this presentation is our recent work on the effects of these microstructural characteristics on friction and wear at interfaces. Our findings demonstrate that the size effect stemming from strain gradients can significantly influence the contact stiffness and hardness. Additionally, the dynamic effects associated with decreasing solid thickness can induce

abnormal contact behavior. Moreover, at small scales, novel behaviors may arise, leading to the breakdown of the Archard wear law.

Keyword: Dynamic impact, stress wave, friction and wear, thin film

最终交流类型：Keynote

When Metal-Support Interaction is Strong?

李微雪
University of Science and Technology of China, China

The activity, selectivity, and stability of supported nanocatalysts is crucial to meeting environmental and energy challenges and necessitates fundamental theory to relieve trial-and-error experimentation and accelerate lab-to-fab translation. Among others, metal-support interaction is thought as one of the fundamental concepts and vital to the overall performance of supported nanocatalysts. In particularly, strong metal-support interaction received long standing attention since it was proposed in 1969, though the description was phenomenal and qualitative. Here we report a Sabatier principle of metal-support interaction (MSI) for stabilizing metal nanocatalysts against sintering based on the kinetic simulations of 323 metal-support pairs based on MSI scaling relations extracted from 1252 energetics data (Science 374 (2021) 1360-1365). For the first time, MSI and criterion for strong MSI are quantified and established, respectively. Too strong of an interaction is shown to trigger Ostwald ripening whereas too weak of an interaction stimulates particle migration and coalescence. The identified optimum MSI enables high-throughput screening of supports to stabilize the nanocatalysts (~3nm) to reach the Tammann temperature on single functional supports. For high temperature reactions, cluster catalysts and those with poor chemical stabilities, bifunctional supports is proposed to break the scaling relationships. This theory is substantiated by first-principles neural network molecular dynamics simulations and available experiments.

Keyword: Metal-support interaction; stability; scaling relationship; Tammann Temperature; Bifunctional Support

最终交流类型：Keynote

Getting Published in Nature Computational Science

Jie Pan
Nature Computational Science

This talk will give an overview of Nature Portfolio journals and the editorial process involved in publishing. The discussions will especially cover the aims and scope of Nature Computational Science, the editorial process, and our vision for this journal in the growing field of computational science. We will also discuss what editors do, what they look for, and how they make decisions, together with some practical tips for writing and submitting a paper to a Nature Portfolio journal.

Topics covered:

- Overview of Nature Portfolio journals
- Editorial Process at Nature Computational Science
- Preparing your manuscript for submission
- Handling editor and reviewers' comments and rejection
- Publishing Interdisciplinary Research in Nature Computational Science

Keyword: Computational Science, Publishing, Nature Portfolio

最终交流类型: Invited

Moiré Engineering of Correlated Topological Systems

冼乐德

松山湖材料实验室

Twisted two-dimensional materials are one of the popular research topics in the field of 2D materials and condensed matter physics. Twisted stacking allows one to turn 2D materials into strongly correlated systems, providing unpretending opportunity to investigate strongly correlated physics in a relatively simple but highly tunable setup. While early research started from twisted graphene systems, using large-scale Density Functional Theory calculations, we extend the study to various other 2D materials, such as twisted BN， MoS_2, GeSe, etc [1-3]. Basing on the electronic structures and atomic symmetry of 2D materials, we can not only design twisted moiré systems to realize various strongly correlated lattice models, but also be able to engineer correlated systems with non-trivial topology [4-5]. We believe these highly tunable 2D moiré systems will provide novel platforms for the simulation of correlated quantum state of matters [6].

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Keyword: moiré materials, 2D materials, Density Functional Theory calculations, correlated states, topological states

最终交流类型: Invited

Tension-compression asymmetry of the stress-strain behavior of the stacked graphene assembly

Haimin Yao

The Hong Kong Polytechnic University

Two-dimensional (2D) materials as exemplified by graphene have received a bunch of attention for their outstanding properties and enormous application potential. Recently, a macroscopic graphene-based material was fabricated simply by stacking the few-layer graphene flakes. The resulting film, called SGA, exhibits unusual mechanical behavior, which implies the existence of tension-compression asymmetry in its mechanical property. However, direct experimental verification of such unique mechanical property of the SGA remains deficient because of the difficulty in fixturing and applying load on the samples. In this work, we tackle these problems by transferring the SGA film onto a polyethylene (PE) substrate which can elongate and contract in response to the variation of the ambient temperature. Tensile and compressive loads thus can be controllably applied to the SGA samples through the SGA/PE interface by tuning the temperature variation. The stress-strain curves of the SGA, including tensile and compressive, are deduced based on the Stoney equation for thin film-substrate systems, showing the tension-compression asymmetry as expected. Theoretical modeling is carried out and reveals the structural basis of such unique mechanical behavior. This work not only provides a facile yet effective approach to measuring the stress-strain behavior of less-cohesive materials like SGA but also is of great value to the design and applications of SGA and other stacked assemblies of 2D materials in flexible sensors and actuators.

Keyword: Two-dimensional materials, Thin film, Stoney equation, Stacked assembly, Less-cohesive materials

最终交流类型: Invited

Theoretical simulations of CeO2 surface structures and catalytic activities

龚学庆
上海交通大学

Rare earth metal oxides, such as cerium dioxide (CeO_2) have found applications in wide range of areas. However, the detailed understanding of the origins of their unique catalytic performance is still limited. In particular, it is still unclear how the characteristic highly localized 4f orbitals/electrons can affect the catalytic activities. In a series of recent work, by performing density functional theory calculations corrected for on-site Coulomb interactions (DFT+U), we have studied the structures and corresponding physico-chemical properties of CeO_2 surfaces. The processes of O vacancy formation and interactions with other metal oxides such as supported VO_x and WO_x were systematically investigated. In addition, the chemical processes such as CO oxidation, NO reduction, H activation, oxidative dehydrogenation (ODH) and CO_2 hydrogenation were also calculated. The results of these studies helped reveal the "electron reservoir" and "oxygen reservoir" effects of ceria-based nanomaterials in catalysis, which heavily rely on the electronic properties of the Ce species.

Keyword: CeO2, DFT+U, Catalytic oxidation, Catalytic hydrogenation, Selective catalytic reduction

最终交流类型: Invited

A Finite Deformation Continuum Model for Strain-Driven Phase Transition of Transition Metal Dichalcogenide Monolayers

韦小丁
北京大学

Phase transition, 2D materials, Finite deformation, Mechanical instability.

Tuning the electronic properties of transition metal dichalcogenides (TMDCs) through phase engineering is promising for their applications in electronic devices, energy conversion, etc. Here, we present a phase-field continuum mechanics model that accounts for the finite deformation and mechanically induced phase transition of monolayer molybdenum disulfide (MoS2) and molybdenum ditelluride (MoTe2). With key parameters calibrated by first-principles calculations, our model can accurately prescribe not only the nonlinear mechanical behavior but also the strain-induced phase transition process. When applied to the nanoindentation experiments on MoS2 drum specimens, the model can precisely reproduce the force vs. depth curves and provides a wealth of information regarding how the phase change originates and evolves around the contact region. Moreover, based on the analysis of mechanical instability, our study suggests that MoS2 monolayers will fail prematurely during indentation tests due to mechanical instability in shear mode before the phase transition is complete. MoTe2, on the other hand, can complete the phase transition without risking mechanical instability, as has been demonstrated in previous experimental studies. The model and methods presented in this paper would serve as a powerful guide for the phase engineering of two-dimensional TMDCs.

Keyword: Transition Metal Dichalcogenide Monolayers, Phase transition, Mechanical Stability, Strain Engineering

最终交流类型: Invited

Chiral optical/electrical properties in hybrid nanostructures: strong coupling and collective effects

张伟
Institute of Applied Physics and Computational Mathematics, China

Chirality plays important roles in many fields and has various applications. Hybrid nanostructures made of metallic nanoparticles and (chiral) molecules provide more opportunities for exploring the mechanism of chirality and realizing multi-functionalities. I present our recent studies on the optical/electric properties of hybrid nanostructures, focusing on the strong coupling and collective effects. We develop a plexcitonic Born−Kuhn model to explore the strong coupling dynamics of the chiral hybrid nanostructures made of corner stacked nanorod dimers and molecules from the chiroptical perspective. As a consequence of strong interaction between plasmons and excitons, double normal mode splittings/Rabi splittings and an anti-crossing phenomenon appear in circular dichroism (CD) spectroscopy. The character of dual plexciton (symmetric and anti-symmetric plexciton) and associated chiroptical properties have been demonstrated. The interplay between mirror symmetry breaking and plasmon−plasmon/plasmon−exciton interaction leads to an optimal configuration with the maximal chiroptical response. Moreover, chirality (of incident light) selective excitation of plexcitonic modes has been achieved by structural design. The theory agrees with the experiment based on the synthesized chiral plasmonic nanodimers coated

with Jaggregate dye molecules. We study the optoelectronic effects of thin films made of gold nanoparticles and chiral molecules. Based on analytical model and finite-difference time-domain (FDTD) simulation, we reveal the chiroptical characters due to the combination effects of local field enhancement, collective effect and the backaction of chiral molecules (on the nanoparticles). With the help of Poisson–Nernst–Planck equation, the chirality transfer from optical response to electronic response (chiral photocurrent) can be found by using the calculated absorption coefficient.

Keyword: Chirality, plasmon, plexciton, strong coupling effect, collective effect

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最终交流类型: Invited

Theoretical Study on Controllable Synthesis and Property Modulation of Two-dimensional Materials

董际臣
中国科学院化学研究所

The unique structure dimensionality and physical properties of two-dimensional (2D) materials make them hold great potentials in the fields of informatics and energetics. Controllable synthesis of high-quality 2D materials and modulating their properties are of critical importance and the prerequisites for their applications. Currently, chemical vapor deposition (CVD) is one of the most promising methods for massive production of 2D materials. This method involves the synergistic interplay of multi-elements under both thermodynamic and kinetic conditions at multi-scales. An in-depth understanding on the mechanisms of CVD synthesis and property modulation of 2D materials can provide theoretical guidance for their controllable production and application.

Here, I will present recent advances on multiscale simulations of CVD synthesis of 2D materials and their property modulations, including (i) development of multiscale simulation methods and mechanisms of growth kinetics of 2D atomic crystals; (ii) mechanisms of synthesizing wafer-scale single crystalline 2D materials; and (iii) mechanisms on modulating structures and electro-catalytic properties of 2D materials for CO2 reduction and hydrogen evolution reaction.

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Keyword: Two-dimensional materials, Crystal growth, Multi-scale simulation, Property modulation

最终交流类型: Invited

Chemical Doping of Organic Semiconductors: From Thermoelectric Conversion to Spintronic Applications

王冬

Tsinghua University, China

Controllable doping of organic semiconductors (OSCs) not only has improved the performance of organic field-effect transistors and solar cells, but also will enable thermoelectric conversion and spintronic applications. However, the knowledge of chemical doping in realizing desired functionalities remains limited. Herein, I will highlight some recent advances in our theoretical understanding toward the dopant-host interplay in organic and coordination polymers and frameworks, with a focus on thermoelectric and spintronic applications.[1]

First, I will show doping-induced modification to the electronic band of host in an n-type thermoelectric material, potassium-doped coordination polymer.[2] The charge localization due to Coulomb interaction with the ionized dopant led to the formation of an electronic polaron band, which was responsible for the non-monotonic temperature dependence of conductivity and Seebeck coefficient observed in experiment. Next, I will demonstrate that ionized dopants can act as scattering centers of charge carriers via screened Coulomb interaction.[3] After incorporating the ionized dopant scattering mechanism in a p-type thermoelectric polymer, PEDOT:Tos, we were able to reproduce the experimentally measured Seebeck coefficient-electrical conductivity relationship spanning over a wide range of doping levels. In the above two cases, an integral charge transfer between dopant and host has taken place via redox reactions. In the third example, I will present a novel type of OSCs, conjugated covalent organic frameworks (COFs) that can be spin polarized when doped with iodine.[4] The fractional charge transfer between dopant and host and orbital hybridization introduced stable spin centers to non-magnetic COFs. The anisotropic interactions between spins led to the long-range magnetic order as observed in experiment. We conclude that dopant and host should be viewed as an integrated system and the type of charge transfer interaction between them is the key for spin polarization of OSCs with closed-shell electronic structures.

Keyword: doping, polymers, COFs, thermoelectric, spintronic

最终交流类型：

Designing Topological and Correlated 2D Magnetic States via Superatomic Lattice Constructions of Zirconium Dichloride

宋洋
国家纳米科学中心

Designing magnetic materials with novel properties is of broad interest to the communities of nano science and materials science. The combination of magnetism and topology is known as magnetic topological state, and the magnetism offers more freedoms to manipulate topological states. Specifically, the magnetic materials coexisting band topology and electronic correlation have broad prospects in quantum information, spintronics and valleytronics. On one hand, topological magnetic materials have various applications, such as information storage and dissipationless spin and charge transport. On the other hand, correlated magnetic materials, such as AFM Dirac Mott insulator, can be used in valleytronic and optoelectronic nanodevices, based on the properties, such as valley effect and AFM induced metal-to-insulator transition. To our knowledge, 2D Dirac Mott insulator have rarely been reported. It is desired to realize these intriguing magnetic states in new material platforms.

Here, we propose the approach of designing novel 2D magnetic states by using d-orbital-based superatomic lattices. We choose triangular zirconium dichloride disks as superatoms to design the honeycomb superatomic lattices. Using first-principles calculations, we construct a series of 2D magnetic states by tuning the size of superatoms. The non-uniform stoichiometries and geometric effect of superatomic lattice give rise to spin-polarized charges arranging in different magnetic configurations, containing FM coloring triangle, AFM honeycomb and FM kagome lattices. These magnetic states are endowed with nontrivial band topology or strong correlation, and form ideal Chern insulator or AFM Dirac Mott insulator. This work not only reveals the potential of d-orbital-based superatoms for generating unusual magnetic configurations, but also supplies a new avenue for material engineering at the nanoscale.

Keyword: topological state, Chern insulator, Dirac Mott insulator, zirconium dichloride, superatomic lattice

最终交流类型：Invited

Long-lived weak ion pairs in ionic liquids: An insight from all-atom molecular dynamics simulations

江剑
Institute of Chemistry, Chinese Academy of Sciences

The microstructure and local dynamics of ions in room-temperature ionic liquids (RTILs) have drawn a lot of attention due to their extensive potential applications in numerous fields. It is well-known that the widely-used definitions of ion pairs (IPs) cannot reflect the full picture of RTILs. In this study, we find a universal residence time, which is regardless of the number of counterions in the first solvation shell in RTILs. Inspired by this, we propose a weak IP (WIP) model from a spatio-temporal perspective and demonstrate that the WIPs are long-lived and their lifetimes obey a lognormal distribution, which is different from the literature. In addition, the electrostatic interactions are the main factors in the formation of WIPs and the reorientations of ions are vital to the ruptures of WIPs. This research provides a new perspective for understanding the microstructural and dynamical properties of RTILs.

Keyword: Ionic liquids; molecular dynamics simulations; ion pairs

最终交流类型：Invited

Water and electrolytes under nanoconfinement: structure, dynamics and transport properties

仇虎
南京航空航天大学

The behaviors of water and electrolytes confined in nanoscale spaces impact a broad range of biological processes and industrial applications. As an example, ion diffusion across cell membranes through nanoscale tunnels of protein channels has been intensively investigated for several decades due to its essential role in electrical signaling in neurons. Alternatively, advances in nanotechnologies have allowed nanoconfined systems to be routinely examined and manipulated in functional mimics of biological protein channels, namely, nanoscale channels (or nanochannels) created with artificial structures. These systems can have outstanding ion selectivity and permeability, with promising applications in desalination, biosensing and energy conversion. Computation has proved itself a useful tool in predicting structures of nanoconfined systems on the atomic level, understanding molecular-scale interactions, as well as guiding relevant experimental researches. In recent years, our group has used prevailing computational approaches include quantum mechanics (QM) calculations and molecular dynamics (MD) simulations to understand the structure, dynamics and transport properties of these nanoconfined systems. In this talk, I will discuss the progress related to the development of a deep learning potential function for nanoconfined water, as well as a series of confinement-induced new phenomena and mechanisms, such as the relationship between phase and friction of nanoconfined water and a new electroosmotic effect for nanoconfined electrolytes.

Keyword: Nanoconfinement, water, transport, molecular dynamics, nanochannels

最终交流类型: Invited

Organic Solar Cell research from a point view of Literature big data analysing

张兴华
Beijing Jiaotong University, China

The focus of solar cell research lies in the discovery of new photovoltaic mechanisms and the improvement of power conversion efficiency which is a complex system engineering. At the molecular level, this involves the design of new molecules and the screening based on parameters such as band gap, mobility, and processability among a vast number of candidate materials. At the device level, it involves the optimization of device structure and fabrication processes, etc. As a hot research field, solar cells have accumulated a massive amount of literature and considerable work. From the parameter space perspective, the studies are predominantly localized in smaller parameter windows. Due to the overwhelming number of publications, it is no longer feasible for human capacity to comprehensively grasp. The systematic analysis of the correlation between data and ideas in a massive amount of literature can reveal the formation of ideas, bottlenecks in research, and even indicate overlooked areas in this field. This paper builds a complete solar cell knowledge base with the help of natural language processing technology for more than 160,000 literature data of solar cells in Web of Science. Hierarchical Latent Dirichlet Allocation (LDA) is utilized for

topic identification. By projecting the number of papers for each topic along the timeline, the generation, evolution, and interaction of new ideas in the history are revealed. Through correlation analysis of core performance parameters of solar cells such as Voc, Jsc, FF, and PCE, the research bottlenecks and challenges in the field are identified. By utilizing literature data on 163 donor materials and 243 acceptor materials and using the correlation between PCE and donor/acceptor materials as the objective function, a correlation map between donor-acceptor material combinations and PCE is obtained. This research highlights 20 core combinations of donor materials and acceptor materials in organic solar cell research.

Keyword: Organic Solar Cell，big data, Literature

最终交流类型：Invited

Exotic electronic states in low-dimensional super-atomic crystals

季威
中国人民大学

In this talk, I will show exotic electronic states hosted in two super-atomic crystals, one exists in nature and the other is purely artificial, as observed in scanning tunneling microscopic images/spectra and verified/predicted by density functional theory calculations. One example lies in a layered super-atomic crystal of $Au_6Te_{12}Se_8$ (ATS) cubic clusters stacked through noncovalent inter-cube quasi-bonds. We found a sequential-emerged anisotropic triple-cube charge density wave (TCCDW) and polarized metallic states below 120 K. The polarized states are locked in an antiparallel configuration, which is required for maintaining the inversion symmetry of the center cube in the TCCDW. The antipolar metallic states are thus interweaved by the CDW and the polarized metallic states, and primarily ascribed to electronic effects via theoretical calculations. Another example was illustrated using post-annealed $MoTe_2$ monolayers. A coloring-triangle (CT) latticed $MoTe_2$ monolayer (see below), termed CT-$MoTe_2$, was constructed by controllably introducing uniform and ordered mirror-twin-boundaries into a pristine monolayer. This CT-$MoTe_2$ monolayer has an electronic Janus lattice, i.e., an energy-dependent atomic-lattice and a pseudo-Te sublattice, and shares the identical geometry with the Mo_5Te_8 layer. Dirac-like and flat electronic bands inherently existing in the CT lattice are identified by two broad and two prominent peaks in STS spectra, respectively, and verified with DFT calculations.

Keyword: kagome bands; superatomic crystal; layered materials; MoTe2; Au6Te12Se8

最终交流类型：Invited

Artificial Intelligence Design of Advanced Electrolyte for Lithium batteries

陈翔
清华大学

Lithium metal batteries are considered as promising next-generation energy storage devices due to their ultrahigh energy densities. However, the high reactivity of lithium metal toward organic solvents and salts renders inevitable side reactions, which further leads to undesirable electrolyte depletion, cell failure, and the evolution of flammable gas. Tremendous efforts from experiments have been devoted to the exploration of advanced electrolytes mainly through trial-and-error approaches, which are both time-consuming and cost-expensive.

Herein, the ion–solvent chemistry was developed to prove the intrinsic instability of normal organic electrolytes towards lithium metal anodes through multiscale calculations and in situ microscopic observations. The formation of cation−solvent complexes decreases the reductive stability but increases the oxidative stability of solvent molecules according to frontier molecular orbital theory, whereas the introduction of anions into the Li+ solvation shell has the opposite function in regulating solvent stability compared with cations. The competitive coordination of anions and solvent molecules with cations directly determines the salt solubility in electrolytes and the formation of ion pairs and aggregates, which widely exist in high-concentration electrolytes and stabilize Li metal anodes. Although anions are hardly solvated in routine solvents, solvents with a high acceptor number or an exposed positive charge site are highly expected to enhance the anion−solvent interaction. The solvation of anions will have a strong influence on electrolytes, including regulating the electrolyte solvation structure and stability, increasing the cation transference number, and promoting salt dissociation.

Based on the ion–solvent model, several strategies were further proposed to build stable electrolytes for alkali metal anodes, including additive design and regulating anions in electrolyte solvation shells. Furthermore, a high-throughput computation platform has been established and an electrolyte database including more than 200 thousand electrolyte molecules has been established. Finally, emerging electrolytes are designed through the electrolyte database and artificial intelligence approaches.

Keyword: Lithium metal batteries, advanced electrolytes, multi-scale simulations, artificial intelligence

最终交流类型: Invited

The multi-phase coacervation of polyelectrolytes

杨爽
Peking University

The liquid-liquid phase separation (LLPS) is a general phenomenon existing in cells, which is closely related to the partitioning inside a cell, various biochemical reaction related microenvironments and the formation of membrane-less organelle. The complexation of oppositely charged polyelectrolytes (also refer to coacervation) in solutions is an important representation of LLPS. The electrostatic interaction plays a key role in determining the phase separation. At present, more attention has been paid to the two-component polyelectrolyte system containing simple polyanion/polycation. In real cellular environments, there are numerous components and the resulting phases includes a dilute phase coexisting with multiple condensed phases, such as nucleoli. However, there is a lack of theoretical exploration on the physical mechanism about the multiphase separation. Here, for multi-component polyelectrolyte mixtures, we investigated the multiphase separation process. Our calculations indicate that the multiphase coacervation can be induced by the asymmetry of linear charge density or the asymmetry of charge sequence, which results from the different electrostatic correlations. The theoretical results may help to understand the mechanism of polyelectrolyte complexation, and can provide insights towards the designing of polyelectrolyte molecules in their application.

Keyword: phase separation, polyelectrolyte complexation, coacervation, electrostatic correlation, random phase approximation

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最终交流类型: Invited

Theoretical Study on the Electrocatalytic Mechanism and Enhanced Performance of Two-Dimensional PI-Conjugated Materials

朱嘉
国家纳米科学中心

Obtaining sustainable energy and important chemicals through electrochemical reactions is an important solution to the energy crisis. The development of 2D materials as highly active electrocatalysts have attracted wide attention, among which the determination of the atomic structure of the active center, the catalytic mechanism, and the activity descriptor are critical for understanding the activity origin and further improving their electrocatalytic performance. The first-principles calculation was adopted to systematically study the electrocatalytic active sites, activity descriptors, and "structural-property" relationships of two representatives π conjugated materials, i.e., doped graphdiyne and 2D conducting metal-organic framework (Metal-BHT), in the electrocatalytic processes of hydrogen evolution reaction, oxygen reduction reaction, carbon dioxide reduction reaction. The modulation of intramolecular and intermolecular charge transfer properties was verified to be effective in activating the electrocatalytic active sites of 2D conjugated materials. The results of theoretical calculation provide theoretical insights into the origin of activity, facilitating the rational design and experimental explorations of high-performance electrocatalysts.

Keyword: 2D materials, doped graphdiyne, metal-organic framework, electrocatalyst, first principles calculations

最终交流类型: Keynote

"Construct exchange-correlation functional via machine learning and delta-learning method“

Guanhua Chen
The University of Hong Kong

Density-functional theory has been widely used in quantum mechanical simulations. Despite of its success, the universal exchange-correlation (xc) functional has been elusive. About twenty years ago, neural networks has been introduced to construct the xc functional or potential. Due to the emergence of deep learning, this effort has gained the renewed momentum in recent years. In this perspective, I review the early efforts to approximate the xc functional or potential with neural networks. A key challenge was the transferability from the knowledge learnt from small molecules to larger systems. The transferability problem was recently resolved by adopting quasi-local density-based descriptors, which is rooted rigorously in the holographic electron density theorem. I discuss then the recent developments to employ the deep-learning techniques to learn the exact xc functional. It is important that the high-level ab initio molecular energy and as well as the corresponding electron density are targeted for the training. All these efforts can be encompassed under a general framework. In addition, the delta-learning method will be discussed.

Keyword: AI; Quantum Chemistry; DFT; Exchange-correlation functional

最终交流类型:

Design of Novel Two-Dimensional Carbon Materials Based on Chemical Rules

刘伟
浙江农林大学

Structure design based on chemical rules is an important method in designing novel materials, which has achieved great success in predicting structures of bulk materials. Here, I will show several examples of two-dimensional (2D) carbon allotropes, which are designed by structural and topological analysis based on chemical knowledge and intuition. In the first example, we propose a strategy to arrange defect structures in the graphene lattice based on a careful analysis of the topological distribution of minima, maxima, and saddle points.[1] Using this method, egg-tray graphenes (Fig. 1a) are constructed by arranging non-hexagon defects (pentagons and heptagons) in the graphene lattice. By anchoring Pd single atom on the N-doped egg tray graphene, we designed a series of Pd@ETG-Nx (x = 0–3) catalysts for formic acid dehydrogenation reaction. In the second example, we introduce innovative 2D carbon materials that combine the unique characteristics of zero-dimensional (0D) fullerenes and one-dimensional (1D) carbon nanotubes (CNTs). We achieve this by incorporating fullerene-like hollow structures, referred to as "bubbles", into the graphene lattice, resulting in a collection of bubble-wrap carbons[2] (see Fig. 1b). Additionally, we create an ensemble of highly anisotropic 2D carbon-based Dirac materials called "nano-makisu" by interlacing an array of CNTs through direct C-C bonds or by employing graphene ribbons[3] (as depicted in Fig. 1c). In the third example, based on the successfully synthesized polyazulene carbon fragment, we have theoretically designed a novel 2D carbon allotrope composed of pentagonal, hexagonal, and heptagonal carbon rings, denoted as anti-polyazulene graphene (APA-graphene, shown in Fig. 1d). These low-dimensional carbon allotropes designed using chemical rules exhibit remarkable properties that even outperform graphene, such as superior mechanical strength, negative Poisson’s ratios, high anisotropy, and potential superconductivity. Our examples show that chemical knowledge and rules can be very important in 2D carbon materials discovery.

Keyword: First-principles calculations, graphene, two-dimensional carbon materials, defects, negative Poisson’s ratios

最终交流类型：

Electrocatalytic properties on axial coordinated spin-regulated structures

明 邱

Central China Normal University

"Transition metal-nitrogen-carbon" materials are a very promising catalyst for carbon dioxide reduction. In order to improve the activity and stability of "transition metal-nitrogen-carbon" catalyst material in the electrocatalysis process, we adopted the way of regulating the active site through axial coordination to improve the catalytic performance of carbon dioxide reduction. Environmental regulation in the active region can not only optimize the catalytic activity in the active region, but also enhance the conductivity of the adsorption/desorption response system of the reaction intermediates, thus improving its catalytic performance.

Keyword: carbon dioxide reduction reaction，CoPc，delocalization，catalystic activity

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最终交流类型：

One-Dimensional van der Waals Polymers with Nonlinear Optical Performance Approaching Theoretical Upper Limit

杨靖宇

中国科学院物理研究所

Nonlinear optical materials (NLO) attract great attention because of their applications in generating coherent laser sources, etc. Many efforts have been devoted to looking for crystals with large nonlinearities to meet the demand for high-power coherent laser sources. However, crystals with NLO susceptibilities close to the theoretical upper limit are rare.

In recent years, attention has been moved to van der Waals materials, where crystals consisting of low-dimensional building blocks could be a possible solution to realize large NLO susceptibility and high birefringence.[1] And numerous two-dimensional crystals were predicted to own giant optical nonlinearities near the theoretical upper limit. [2] Inspired by a recent report of one-dimensional (1D) material PNF2[1a] with excellent NLO performance, we extend this region to crystals made up of 1D building blocks, where the dipoles along the chain result in strong second harmonic oscillations.

Recently, a novel protocol based on graph theory and density functional theory (DFT) calculations is conducted in the structural classification for atom-scale one-dimensional materials,[3] allowing us to look for 1D polymer patterns with NLO properties. In this work, by high throughput calculations, we searched new NLO crystals from 244 materials constructed by vdW stacking of one-dimensional (1D) polymers. Besides, the weak vdW interaction of these 1D building blocks allows them to be easily exfoliated from bulk to two-dimensional flakes and 1D chains. We found 14 experimentally synthesized bulk vdW materials, 11 2D and 11 1D forms as NLO candidates. Nearly half of their NLO susceptibilities approach the theoretical upper limit, and their working frequencies cover ultraviolet, visible, and infrared regions. Moreover, we found that their NLO susceptibilities are positively related to the charge difference of atoms on the chains. Finally, we proposed a design strategy that superior NLO polymers can be obtained with proper bandgap and large charge difference on the chain.

Keyword: nonlinear optical crystals, 1D motifs, first-principles calculations, second harmonic generation, materials design

最终交流类型：Keynote

Clusters as building blocks towards assemblies with precise band engineering

赵纪军
大连理工大学

Clusters, having a definite number of atoms as well as precise and controllable geometric and electronic structures, represent a new hierarchy between microscopic atoms, molecules and macroscopic condensed matter. Due to rich tunability of elements, structures, and electronic properties, clusters are expected to provide infinite possibilities for material assembly and device design at atomic level. In recent years, our group have also studied a series of cluster assembled systems, and realized the material design and band engineering using clusters as building blocks, A number of interesting electronic properties have been observed, such as strongly correlated electronic states [1], coexistence of Dirac states and flat bands [2], bipolar Magnetic semiconductor [3], one-dimensional multiferroic [4], and giant exciton energy [5, 6].

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Keyword: cluster, band engineering, assembly, Dirac state, strong correlation

最终交流类型: Invited

Nanoconfined Water and Carbon from First Principles

Ding Pan
Hong Kong University of Science and Technology

This talk presents a study on the impact of nanoconfinement on the physical and chemical properties of aqueous solutions, with a particular focus on the reactions of CO2 in water under extreme pressure-temperature conditions. Carbon storage and transport below Earth's surface have significant implications for the carbon budget in the atmosphere, and underground aqueous solutions are often confined to the nanoscale. However, the molecular-scale chemical speciation and reaction mechanisms of these systems are not yet fully understood.

To address this issue, extensive ab initio molecular dynamics simulations were performed to investigate aqueous carbon solutions confined by graphene and stishovite (SiO2) at 10 GPa and 1000 ~ 1400 K. The results show that CO2(aq) reacts more in nanoconfinement than in bulk, and the stishovite-water interface increases the acidity of the solutions, shifting the chemical equilibria and significantly affecting the reaction mechanisms. These findings suggest that CO2(aq) in deep Earth is more active than previously thought, and confining CO2 and water in nanopores may enhance the efficiency of mineral carbonation.

Furthermore, first principles methods were employed to compute the Raman and infrared spectra of water confined by graphene in a broad pressure-temperature range. By comparing these spectra with those of bulk water, the effects of spatial confinement on hydrogen bonds and proton transfer were studied. The results provide a novel understanding of the molecular structure of nanoconfined aqueous solutions and offer valuable insights for interpreting related experimental data.

Keyword: water, CO2, nanoconfinement, Raman, IR

最终交流类型:

Identification of S-Au bonds in Thiolate-protected Gold Nanoclusters with a Deep-Learning Models

李永徽
天津大学

The concept of chemical bonds has been taught generation by generation for centuries but the connection between such human-intelligence-based idea and quantum mechanical world. If one wants to interpret a molecule or a bulk system via the traditional “ball-stick” model, the sticks (bonds) should be multiple feature sticks instead of simple ones with several quantities such as bond-length bond type and etc. Though earlier works rationalized bond types to electron wave functions and derivatives, chemical bond has not fully been captured by features. In this work, the ELFnet, a novel convolutional neural network (CNN) model is trained and tested to bring chemical bond feature extracting to the next level. Based on this model, each chemical bond can be mapped to a feature vector with 256 features with superior properties such as high-resolution, better comprehensiveness, and great discontinuity. From the perspective of feature identification and utilization, the machine-learning-level feature extractor surpasses human-level chemical bond identification dramatically. Such idea is testified based on sulfur-gold bonds in “Thiolate-protected gold nanoclusters” while human-level bond recognition fails in the identifications of those sulfur-gold bonds.

Keyword: Machine Learning, electron structures, nanoclusters, feature extraction, bond characteristics,

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最终交流类型: Invited

Understanding Assembly of Nanoparticles from Computations

刘亚伟
中国科学院过程工程研究所

Nanoparticle assembly is an important approach for constructing advanced materials with specific microstructures. With the proliferation of nanoparticles of different shapes, compositions, patterns, and functionalities, interpreting the corresponding experimental data becomes more difficult, and significant limitations appear with regard to size, shape, concentration, time scale, and polydispersity. Computer simulations, due to their precise control of particle attributes and direct information about particle motion, have played a key

role in interpreting experimental results and in validating theories. In this talk, we will present two recent studies on our recent computational and experimental work on nanoparticle assembly: i) computational simulations and in situ experimental characterization of controllable self-assembled structures of gold nanoparticles on SiN solid substrates [Figure 1(a)]; ii) computational simulations and experimental work on the electric field-driven assembly of large-scale vertical arrays of gold nanorods [Figure 1(b)]. From computations, we revealed the significant influence and control mechanisms of nanoparticle assembly by the solid-liquid interface structure, including nanoparticle crystal facets, surface ligand distribution, and interface ion clouds.

Keyword: nanoparticle assembly; superlattices; colloids; electrophoretic deposition; computer simulation;

最终交流类型: Invited

Two-Dimensional Conjugated Organic Framework for Overall Water Splitting under Visible Light

武晓君
University of Science and Technology of China, China

Using solar energy to dplit water to prepare hydrogen and oxygen is an important way to obtain clean hydrogen energy and solve energy and environmental problems. Among them, direct catalytic decomposition of water using semiconductor photocatalytic materials absorbing solar energy is a promising way, but it is necessary to find photocatalysts that are low-cost, highly stable, and effectively absorb visible or near-infrared light. To address this challenge, it is required to design photocatalysts with appropriate bandgap, band-edge positions, and surface reactivity. We developed a material design strategy based on topological assembly of molecules and first-principles calcualtion. Starting from functional molecules, we used molecular units and toplogical structure to modulate the energy band structure of the materials, designed a series of 2D covalent organic framework photocatalysts that can fully decompose water using visible light, revealed the reaction mechanism in the process of photodegradation of water, and further modified the photocatalytic performance of the materials through chemical modification. The photocatalytic performance of the materials was further modulated by chemical modification. Several 2D covalent organic frameworks that can fully decompose water under visible light irradiation were reported.

Keyword: first-principles calculation, overall water splitting, photocatalysts, covalent organic framework, visible light

最终交流类型：Keynote

Combining Coarse-grained Molecular Dynamics with Monte Carlo Method to Describe Reaction at Larger Spatial/Temporal Scales in Simulations: Applications in Constructing Nanostructures

吕中元
Jilin University, China

Microscopic ordered structures of nanomaterials can be regulated via controlling thermodynamic factors or by coupling multiple kinetic influences. To appropriately describe the coupling among various kinetic influences in a coarse-grained simulation, it is essential to suitably represent chemical reactions, mass transportation, and other kinetic factors at the same time. We will show the stochastic reaction model for use in coarse-grained simulations via combining molecular dynamics and Monte Carlo to especially study the influences of chemical reactions on the construction of ordered nanostructures. The hybrid simulation model together with technical details will be presented and illustrated by several representative applications.

Keyword: coarse-grained molecular dynamics; reaction model; nanostructures

最终交流类型：Invited

Prediction Theory for Medical Functions of Nanomaterials

高兴发
National Center for Nanoscience and Technology, China

The activities of inorganic nanomaterials (NMs) in catalytically tuning reactive oxygen species (ROS) underlie many medical functions of the materials, which are therefore of great importance in both basic chemistry and therapeutic applications of the materials. However, although many NMs have been experimentally demonstrated to catalyze the chemical conversion of ROS such as H_2O_2, O_2, and $O_2^{\bullet-}$, the principles governing the activities remain elusive, hindering the in-depth understanding of the biological effects of the NMs and the rational design of the NMs for medical applications. The complexity of these catalytic systems has added to the difficulties in developing the principles. In the past several years,

we have studied the mechanisms for inorganic NMs to catalyze the dismutation of H_2O_2 and $O_2^{\bullet-}$ and the oxidation of organic molecules by H_2O_2 and O_2. On the basis of the microscopic thermodynamics and kinetics of these catalytic processes, we have developed the prediction models for the activity of NMs in catalyzing the reactions between H_2O_2 and organic molecules. We have recently developed two principles, namely, an energy level principle and an adsorption energy principle, for the activity of nanomaterials catalytically decomposing $O_2^{\bullet-}$. The first principle quantitatively describes the role of the intermediate frontier molecular orbital in transferring electrons for catalysis. The second one quantitatively describes the competition between the desired catalytic reaction and undesired side reactions. Both principles can thus be easily implemented in computer programs to computationally screen NMs with the intrinsic catalytic activity to predict their medical functions. In this presentation, these progresses will be reviewed. The power of computation in exploring the mechanisms and predicting medical functions for NMs will also be prospected.

Keyword: medical function, reactive oxygen species, computational chemistry, virtual screening, prediction theory

最终交流类型: Invited

Toughening and crack healing mechanisms in nanotwinned diamond composites

李晓雁
清华大学

Recently synthesized nanotwinned diamond composites with various polytypes embedded in nanoscale twins exhibit unprecedented fracture toughness without sacrificing hardness, overcoming the hardness versus toughness trade-off of diamond. But the toughening and crack healing mechanisms at the atomic scale remain mysterious. Here, we present large-scale atomistic simulations of crack propagation in nanotwinned diamond composites. Our simulation results show that nanotwinned diamond composites have a higher fracture energy, compared with the single-crystalline and nanotwinned diamonds. Such enhanced fracture energy is attributed to multiple toughening mechanisms, including twin boundary and phase boundary impeding crack propagation, crack deflection and zigzag paths in nanotwins and sinuous paths in polytypes, and the formation of disordered atom clusters. Our simulations further reveal that crack healing occurs due to the rebonding of atoms on fracture surfaces during unloading. Our current study provides a fundamental understanding of toughening and crack healing mechanisms in nanotwinned diamond composites.

Keyword: nanotwinned diamond, toughening, crack healing, atomistic simulations, twin boundary

最终交流类型：Invited

Multiscale Mechanical Behaviours of van der Waals Layered Materials

Yilun Liu
State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace Engineering, Xi’an Jiaotong University

Van der Waals layered materials are usually assembled by 2D materials in layer-by-layer manner, demonstrating complex hierarchical structures and multiscale mechanical degrading. The featured mechanical properties of van der Waals materials are extreme anisotropy due to strong in-plane and weak interlayer interactions, which bring anomalous mechanical behaviors. We have comprehensively studied this type of materials in the viewpoint of multiscale mechanical analysis from monolayer 2D materials, multilayer 2D materials and assemblies of 2D materials. First, the measure of the failure of atom bond of graphene and hBN is proposed. Then, a universal strength criterion is developed which can accurately describe the failure surface of graphene and hBN with vast types of defects under complex stress states. For the multilayer 2D materials, the continuum mechanical model by considering the extreme anisotropy and surface elasticity of 2D materials is developed. Based on which, a series of mechanical behaviors for the laminate-like and nacre-like multilayer 2D materials are studied. At the assembly scale, a multiscale mechanical model is proposed to describe the mechanical degrading of graphene assemblies. Then, the optimization strategies, like defect regulation, interlayer crosslinking and microstructure regulation, are proposed to get the graphene membrane with gigapascal strength.

Keyword: Layered materials; Strength criterion; Continuum theory; Strengthening and tough-ening mechanism

最终交流类型：Invited

Peculiar Structures and Properties of Confined Water

张助华
南京航空航天大学

This report will systematically introduce some of our research progress on confined water. First, a new highly stable two-dimensional ice structure is discovered based on a self-developed structure search program combined with first principles calculations. The six water molecules in the model building block are arranged in a helical pattern along the normal direction, which is called a helical monolayer ice. This program also enables us to locate two-dimensional folded ice with folded structure motif. Further, our physical and mechanical analysis shows that water confined in one-dimensional nanochannels with localized perturbation exhibits pronounced density oscillations. The oscillations occur vividly like the Friedel oscillations in electron density resulting from defects in metals. This oscillation behavior was shown to control ion transport remotely. Then, by exploiting the order-disorder structural transition of confined water, we report giant mechanocaloric effect in water confined within slit nanopores, featured by an unprecedentedly high isothermal entropy change of ~1298 J/(kg·K) and an ensuing adiabatic change of temperature up to 50 K near room temperature. Finally, we report our latest advancement in exploiting polar confined water for modulating the bandgap of BN nanoribbons.

Keyword: Confined water, model analysis, molecular dynamics, monolayer ice, mechanocaloric effect

Topical Sessions =》 11.Biological and Bioinspired Nanomaterials

最终交流类型: Oral

Bioinspired Synthesis of Selenomelanin Nanomaterials and its Ionizing Radiation Protecting Properties

曹玮

北京师范大学

Melanin is a ubiquitous nanoscale biomacromolecule in nature. Found across different kingdoms of life, melanins have a myriad of important functions, including thermal regulation, radical scavenging, photoprotection, and radioprotection. Eumelanin and pheomelanin are the most common subtype of melanin in human body. Natural pheomelanin is likely synthesized from L-dihydroxyphenylalanine and cysteine, and has benzothiazine as the main building block. Compared to the extensive research on eumelanin and polydopamine, pheomelanin has been far less studied. We investigate synthetic routes to a close mimic of natural pheomelanin. Each giving rise to structurally dissimilar materials. Only the route employing 5-cysteinyl-dihydroxyphenylalanine (5-CD) as a monomer was verified as a close analogue of extracted pheomelanin from humans and birds. The resulting biomimetic and natural pheomelanins were compared via various techniques, including solid-state Nuclear Magnetic Resonance (ssNMR) and Electron Paramagnetic Resonance (EPR). Previous studies suggest that sulfur-containing pheomelanin absorbs X-rays more efficiently compared to eumelanin. While selenium is a heavier chalcogen than sulfur, we reasoned that if a selenium enriched melanin existed, it would be a better X-ray protector than the sulfur-containing pheomelanin because the X-ray absorption coefficient is proportional to the fourth power of the atomic number (Z). Indeed, selenium is an essential micronutrient, and the amino acid selenocysteine is genetically encoded in 25 natural human proteins. Compared with sulfur, selenium has lower electronegativity, higher nucleophilicity, and selenium compounds have lower bond dissociation energy and unique bioactivities. We introduce this novel selenium analogue of pheomelanin through chemical and biosynthetic routes using selenocystine as a feedstock. The resulting selenomelanin nanoparticle is a structural mimic of pheomelanin as confirmed by ssNMR. We found selenomelanin effectively prevented neonatal human epidermal keratinocytes from G2/M phase arrest under high-dose X ray irradiation. This line of research pushes forward our fundamental understanding of melanin nanomaterials, and showcases that bridging selenium chemistry with polymer synthesis can create new biomaterials for the urgent need of radiation protection.

Keywords:Melanin; Radiation protection; selenium; biomaterials

最终交流类型: Invited

Rational design of ICD-inducing nanoparticles for cancer immunotherapy

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Cancer immunotherapy has changed the paradigm of cancer treatment by mobilizing the host immune system to recognize and destroy cancer cells. Recently, nanoparticles have been increasingly used in cancer immunotherapy due to their abilities to optimize biodistribution, improve circulation stability and reduce the side effects of therapeutic agents. To date, most current research on nano-immunotherapies uses nanoparticles as delivery vehicles. The design of nanoparticles usually focuses on prolonging circulation time and improving delivery efficiency but ignores the potential of nanoparticles to directly regulate the immune system. Although some serendipitous discoveries suggest that certain nanoparticles may have immunoregulatory effects, there is a lack of rationally designed nanoparticles with immunomodulatory capacity. Nanoparticles are a special class of materials with unique particle sizes and highly engineerable surfaces. These properties allow tailor-made nanoparticles to target specific tissues, cells, and even organelles. Moreover, the binding affinity between the nanoparticle and its target can be finely controlled by tuning nano-multivalent interactions, thus offering nanoparticles great potential to modulate immune systems. Inspired by the endogenous endoplasmic reticulum (ER) stress caused by unfolded/misfolded proteins, we present here a rationally designed immunogenic cell death (ICD) inducer named NanoICD, which is a nanoparticle engineered for ER targeting and retention. By carefully controlling the surface composition and properties, we have successfully obtained NanoICD that can overcome the retrotranlocation process and accumulate in the ER, resulting in the effective induction of ER stress and the activation of

ICD-associated immune responses. Our results demonstrated that NanoICD effectively induced bona fide ICD and generated strong anti-tumor responses in vivo. 50% of the mice receiving NanoICD treatment did not show any tumor recurrence or metastasis even after being challenged with tumor cell re-injection. This result demonstrates the potential of NanoICD to effectively induce strong anti-tumor immune responses, and its efficiency is much higher than that of conventional ICD inducers. In addition, the synthesis method of NanoICD is generally applicable to various proteins and enzymes to further enhance the immunomodulatory capacity. This work demonstrates the potential of engineered nanostructures with a tailored surface to autonomously regulate biological processes particularly in the context of cancer immunotherapy, and provides new insights into the development of advanced nanomedicines for cancer treatment.

Keywords:nanoparticle, immunotherapy, surface interaction, immunogenic cell death, biomaterial

最终交流类型: Invited

Bio-inspired mechano-functional gels through multi-phase order-structure engineering

刘明杰

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Adaptive gel materials can greatly change shape and volume in response to diverse stimuli, and thus have attracted considerable attention due to their promising applications in soft robots, flexible electronics and sensors. In biological soft tissues, the dynamic coexistence of opposing components (for example, hydrophilic and oleophilic molecules, organic and inorganic species) is crucial to provide biological materials with complementary functionalities (for example, elasticity, freezing tolerance and adaptivity). Taking inspiration from nature, we developed a series of high mechanical performance soft active materials, so-called organohydrogels, based on multiphase synergistic strategy. Traditional techniques such as post-polymerization modification, interpenetrating network and controlled micro-phase separation are combined with binary complementary concept to design and fabricate new organohydrogels with diverse topology of heteronetworks. Meanwhile, the synergistic effect of heteronetworks provided the organohydrogels with unprecedented mechanical functions such as freeze-tolerance, programmed high-strain shape memory and shaking insulation. Their applications in anti-biofouling, thin-film fabrication, flexible electronics and actuators are also explored.

Keywords:Bio-inspired, mechano-functional gels, multi-phase order-structure

最终交流类型: Invited

Biomacromolecular nanomaterials with unnatural functions

吴钰周

Huazhong University of Science and Technology

Biomacromolecules such as proteins and nucleic acids, as ideal natural sources of biomaterials, have broad application prospects in the field of biomedicine. Traditional biomacromolecule materials are usually extracted from natural source, utilizing their natural functions and undergoing simple modifications. With the development of synthetic biology technology, biomacromolecules can have more and more designed unnatural properties and functions, which greatly expands people's ability to modify and manipulate biomacromolecules rationally and provides new opportunities for the design of biomacromolecule materials. Using the new technology of synthetic biology to develop a new generation of biomacromolecule nanomaterials that can be rationally designed in structure and function is of great significance for the development of biomedical technology. Based on ligand directed chemical modification, genetic codon expansion and in situ polymerization, we have developed a variety of new methods for rational design and modification of biomacromolecules, and achieve precise hybridization and functional cooperation between unnatural entities and natural biomacromolecule scaffold. With these methods, we have constructed nanomaterials with new biological activity, unique physical and chemical properties and fine microstructure. For instance, new methods for the rational construction of protein unnatural activity was established, which realized the efficient cooperation between unnatural active centers and protein backbone and created enantioselective "triplet photoenzyme"; New strategies such as "in situ synthesis of nucleic acid encoding polymers" and "particle adhesion for nucleic acid mineralization" were established to realize the precise combination of biomacromolecules and synthetic materials; New strategies for drug delivery based on unnatural biomacromolecules were developed, such as in situ synthesis, intracellular and extracellular collaborative delivery, and fine

surface structure regulation, and how nanoscale fine surface structure affects biological effects was explored. By regulating the interaction between biomacromolecule materials and the microenvironment of life, smart biomaterials are constructed and their applications in nano medicine, biocatalysis, gene therapy and other fields are explored.

Keywords:biomacromolecule, protein, DNA, artificial enzyme

最终交流类型: Keynote

Bioresponsive Drug Delivery

顾臻

浙江大学

Spurred by recent advances in materials chemistry, molecular pharmaceutics, and nanobiotechnology, stimuli-responsive "smart" systems offer opportunities for precisely delivering drugs in dose-, spatial- and temporal-controlled manners. In this talk, I will discuss our ongoing efforts in developing physiological signal-triggered bioinspired drug delivery systems. I will first present the glucose-responsive synthetic systems for biomimetic delivery of insulin for diabetes treatment. The development of smart insulin patches will be emphasized. I will further discuss the local and targeted delivery of immunomodulatory therapeutics for enhanced cancer therapy. Our latest studies utilizing platelets, cell conjugates, and sprayed gels for the delivery of immune checkpoint inhibitors will be specifically introduced.

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Keywords: Protein delivery, Bioresponsive materials, Immunotherapy, Cell engineering

最终交流类型: Keynote

Conjugated Polymer-Based Assembly Materials for Biomedical Applications

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Water-soluble conjugated polymers (CPs) provide a unique platform for chemical and biological sensors in view of their optical signal amplification effect. Our recent studies showed that CPs/DNA complexes combing with fluorescence resonance energy transfer (FRET) processes could be used for detecting disease-related gene modifications, such as single nucleotide polymorphisms (SNPs), mutations and DNA methylation. In recent years, conjugated polymers (CPs) integrating recognition, imaging and therapeutic functions have attracted more and more attention. A novel photodynamic therapy (PDT) system was developed in which the photosensitizer is activated by chemical molecules instead of outer light source. In this system, luminal, hydrogen peroxide and horseradish peroxidase (HRP) were used as bioluminescent molecules and a cationic oligo (p-phenylene vinylene) (OPV) was used as the photosensitizer. The excited OPV by BRET from luminol sensitizes oxygen molecule in the surrounding to produce ROS that kill the adjacent cancer cells and pathogenic microbes. The BRET system can work in vivo even in the deeper tissue, which comes over the drawback of the deep tissue penetration for PDT with light irradiation. We designed an oligo(p-phenylenevinylene) unit with thiol groups and a paclitaxelunit (OPV-S-PTX). The OPV-S-PTX is capable of diffusing into cells, where π-π interactions lead to aggregation. Crosslinking of the aggregates via oxidation of thiol groups preferentially occurs inside tumor cells because of their higher internal reactive oxygen species (ROS) concentration. Crosslinked aggregates effectively “chemically lock” the multichromophore particle inside the cells and this process decreases the diffusion of the molecules out of the cell. The formation of the chemically locked particles enhances drug efficacy and helps in reducing resistance. Recently, we have also described a supramolecular antibiotic switch to reversibly “turn-on” and “turn-off” its antibacterial activity, which provides a proof-of-concept to regulate antibacterial activity and avoid accumulation of active antibiotics in the environment. This supramolecular antibiotic switch could be a potential strategy to fight bacterial infections and drug-resistance.

Keywords:conjugated polymers, sensors, nanomedicine, self-assembly, antibacterial activity

最终交流类型: Keynote

Fluoropolymer-MOF Hybrids with Switchable Hydrophilicity for 19F MRI-Monitored Cancer Therapy

Andrew Whittaker

The University of Queensland

Fluoropolymer-MOF Hybrids with Switchable Hydrophilicity for 19F MRI-Monitored Cancer Therapy

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ABSTRACT

The principal challenges in delivery of therapeutics in nanoparticle vehicles are selective and efficient delivery to the desired target tissue, and confirmation of delivery. These challenges have driven the field of nanomedicine to extraordinary lengths, with many delivery vehicles being developed and demonstrated in pre-clinical small animal models. Despite these efforts, these key challenges persist, and new approaches to ensuring efficient and effective delivery of therapeutic agents are required. In this study we introduce theranostic nanoparticles with unique design features aimed are enhancing delivery and retention in diseased tissue (Figure 1). A pH-responsive metal organic framework material, zeolitic imidazolate framework-8 (ZIF-8), was decorated with a low fouling fluoropolymer

which enables extended blood serum lifetimes and hence maximizes the probability of the nanoparticles reaching the target tissue. The fluoropolymer, poly(N-(2-((2,2,2-trifluoroethyl)sulfinyl) ethyl)acrylamide) (PFSAM), gives an intense 19F MRI signal, enabling in vivo tracking of injected nanoparticles. The ZIF-8 core degrades in the acid tumour microenvironment, releasing zinc ions, which associate with the sulfinyl group of the PFSAM chain thereby reducing their hydrophilicity and promoting retention within the tumour tissue. Finally the large pore volume of the ZIF-8 can be loaded with a chemotherapeutic drug, doxorubicin, also released within the tumour volume. Effective treatment of a murine xenograph model of breast cancer was demonstrated [1].

Figure 1. (a) Synthetic route of ZIF-8-PFSAM-DOX. (b) Schematic illustration of magnetic resonance imaging-guided chemotherapy of cancer.

Keywords:MOF, ZIF-8, polymer conjugate, breast cancer, 19F MRI

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最终交流类型: Oral

透气电子皮肤及人体健康监测应用

Permeable electronic skins for health monitoring

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One limitation of commercialized wearables, such as smartwatches and bands, is that they cannot form conformable contact with human skin due to their rigid form factor, thereby limiting their monitoring capabilities. Soft bioelectronics, on the other hand, is touted as an ideal platform for personalized health care owing to unique characteristics, such as thinness, lightweight, good biocompatibility, excellent mechanical robustness, and great skin conformability. Permeable skin-mountable electronics that are capable of long-term applications have emerged as promising tools for early disease prevention, screening, diagnosis, and treatment. Dr

商业化的可穿戴设备，如智能手表和手环的一个局限性在于其坚硬厚重的外形，导致不能与人体皮肤形成共型贴合，从而限制了其人体健康监测能力。然而，电子皮肤器件由于诸多优势，如薄、轻、良好的生物相容性、机械柔韧性和皮肤适应性，被认为是未来个性化医疗保健的理想平台。可长期使用的透气电子皮肤器件已经在早期疾病预防、筛查、诊断和治疗等应用方面展现了重要潜力。王燕博士的研究兴趣主要是开发应用于人体健康监测的超薄/透气柔性材料和柔性可穿戴电子。在今天的演讲中，王燕博士将介绍基于超软纳米网格的高性能皮肤生物电子，该电子可以在不干扰自然皮肤运动和感觉的情况下实现对人体微弱变化的精确测量以及人体健康的长期监测。

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Keywords:电子皮肤 electronic skins；纳米网格 nanomesh；健康监测 health monitoring；透气电子 permeable electronics

最终交流类型: Oral

Programmable DNA nanocomposites

胡勇

同济大学

Biomedical applications require substrata that allow for the grafting, colonization and control of eukaryotic cells. Currently available materials are often limited by insufficient possibilities for the integration of biological functions and means for tuning the mechanical properties. We report on tailorable nanocomposite materials in which silica nanoparticles are interwoven with carbon nanotubes by DNA polymerization. The modular, well controllable and scalable synthesis yields materials whose composition can be gradually adjusted to produce synergistic, non-linear mechanical stiffness and viscosity properties. The materials were exploited as substrata that outperform conventional culture surfaces in the ability to control cellular adhesion, proliferation and transmigration through the hydrogel matrix. The composite materials also enable the construction of layered cell architectures, the expansion of embryonic stem cells by simplified cultivation methods and the on-demand release of uniformly sized stem cell spheroids.

Then, using the example of the functionalization of silica nanoparticle-modified DNA polymer materials with agonists or antagonists of the epidermal growth factor receptor EGFR cell membrane receptor, we demonstrate that hierarchically structured interfaces to living cells can be established. Owing to the modular design principle, even complex DNA nanostructures can be integrated into the materials, thereby enabling the high-precision arrangement of ligands on the lower nanometer length scale. We believe that such complex biohybrid material systems can be used for new applications in biotechnology.

Eventually, we report on novel hierarchically structured composite materials from silica nanoparticles and DNA polymers that can be obtained by self-assembly through the clamped hybridization chain reaction. The nanocomposite materials can be assembled into thin layers within microfluidically generated water-in-oil droplets to produce mechanically stabilized hollow spheres with uniform size distributions at high throughput rates. The fact that cells can be encapsulated in these microcontainers suggests that our concept not only contributes to the further development of supramolecular bottom-up manufacturing, but can also be exploited for applications in the life sciences.

Keywords:Nanomaterials, DNA assembly, cell-material interaction, stem cells

最终交流类型: Keynote

School of Materials Science and Engineering

Xiaodong Chen

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Biological senses are indispensable for the survival and thriving of living organisms. They represent an intricate network of mechanisms that enable organisms to perceive and interact with their surroundings. Over the years, a considerable amount of scientific effort has been dedicated to unravelling the complex physiological processes that underpin these senses. However, despite the significant progress made, there remains a chasm between biological senses and the existing conventional sensing techniques. In response to this, we have conceptualized a new paradigm of artificial sense technology. This approach seeks to mirror the abilities of biological senses, but it differentiates itself in terms of its capacity for objective sensing and the provision of intelligent feedback. Harnessing the power of nanotechnologies, artificial sense technology can augment the abilities of biological senses and, in certain aspects, even surpass their capabilities. We envisage this technology becoming a potent perceptual interface that will be instrumental in a range of fields. These include sensation substitution, digital healthcare, animal interactions, plant electronics, intelligent robotics, and other areas that aim to deepen the interconnections between the physical and virtual worlds. This concept has given rise to the emerging interdisciplinary field of conformal sense digitalization. This field aims to revolutionize the way we sense and interact with our surroundings by synergistically blending digital technology with physical objects, environments, and human experiences. In this talk, I will delve deeper into the fundamental principles of conformal sense digitalization, exploring its potential applications as well as the formidable challenges it must overcome to realize its full potential. Among the topics I will discuss are recent advancements in materials science and soft electronics. These advancements have set the stage for the development of conformal sensors and interfaces - devices capable of adapting to complex geometries, surfaces, and biological systems. By effectively bridging the gap between the digital and physical realms, conformal sense digitalization has the potential to redefine the way we interact with our environment. It could unlock a new epoch characterized by seamless, intuitive human-machine interactions, enriching our lives in myriad ways that we are just beginning to envisage.

Keywords:soft electronics; conformal sensors; biological systems

最终交流类型: Invited

Construction of ice-binding materials for cryopreservation of cells and tissues

王健君

中国科学院理化技术研究所

Cryopreservation is currently the only effective method to realize long-term storage of biological samples, e.g., cells, tissues and organs, and it plays a crucial role in areas of biomedicine such as cell therapy, regenerative medicine and organ transplantation. As the water content of cells and tissues can be as high as 70% ~ 90%, ice formation inevitably occurs both intracellularly and extracellularly, which can be lethal because of the mechanical damage, the osmotic shock and excessive solute accumulations. Therefore, the scientific challenge of cryopreservation is to inhibit or control ice formation. Traditional cryopreservation strategies use large amounts of small organic molecules, such as dimethyl sulfoxide (DMSO), as cryoprotectants (CPA) to completely inhibit the ice formation, which to some extent is successful in the cryopreservation of cells. However, although cryopreservation of biological samples, especially tissues and organs, has long been intensively pursued, limited progress has been achieved due to the cytotoxicity and tissue destructive effect as well as the low efficiency in controlling ice formation of the conventional cryoprotective agents (CPAs) used for the cryopreservation of cells. Many living organisms in nature can express ice-binding proteins (IBPs) to regulate the site and temperature of the occurrence of ice nucleation and the afterwards ice growth, so as to protect the living organisms from ice-related damages. We have revealed the ice-controlling mechanisms of the IBPs, which guides to construct a series of ice controlling materials (ICMs); the constructed ICMs in-turn consolidate our understanding of the mechanism of living organisms in protecting themselves from freezing damage. Unlike the conventional CPAs which vitrify the water in biological samples, the ICMs allow the formation of ice crystals in cryopreservation but control the location and temperature of ice nucleation and the shape and size of the formed ice crystals, thus alleviating the ice-related damages. By using the ICMs, efficient and safe cryopreservation of cell suspensions as well as cell monolayers have been achieved.

Keywords:Ice nucleation, ice-binding proteins, cryopreservation, ice-controlling materials, frozen tolerance

最终交流类型: Oral

Bioinspired small interfering RNA nanocarriers for synergistic treatment of neurodegenerative diseases

李燕

北京科技大学

Gene therapy has shown great potential for neurodegenerative diseases with complex pathology. However, its therapeutic effect is limited due to the delivery barriers and its own single function.[1] Herein, bioinspired small interfering RNA (siRNA) nanocarriers were developed to promote the delivery and treatment process of siRNA for synergistic treatment of neurodegenerative diseases. Firstly, to enhance the target cellular uptake of siRNA, as shown in Figure 1, neurophilic virus-inspired siRNA nanocarriers S/Ce-PABMS were developed.[2] On the one hand, the rough surface of the S/Ce-PABMS mediated by ceria (CeO_2) nanozymes could catalyze the cellular uptake in the delivery process, so that S/Ce-PABMS with acetylcholine analogs penetrated the blood-brain barrier (BBB) and entered the neurons more effectively. On the other hand, the CeO_2 nanozymes could catalyze the treatment process by scavenging excess reactive oxygen species (ROS), and cooperated with siRNA-targeting SNCA to decrease the α-synuclein (α-syn) aggregation and alleviate the Parkinsonian pathology. Moreover, the S/Ce-PABMS treatment reduced the number of activated microglia and regulated the release of inflammatory cytokine, thereby relieving neuroinflammation. After treatment with S/Ce-PABMS, dyskinesia in Parkinson’s disease (PD) model mice was significantly alleviated. Secondly, to overcome the endosome trapping, synaptic vesicle-inspired nanocarriers RT-PPB with spatiotemporally controlled release ability were developed.[3] After efficiently crossing the BBB and targeting/docking to the neurons, the lipid shell of the RT-PPB fused with the cell membrane and directly released the drug core into the cytoplasm, which avoided endosome trapping and exocytosis. More importantly, the drug core with dual ROS-responsive ability could achieve controlled release of rapamycin and siRNA for reducing the intracellular α-syn aggregate level and neuron-to-neuron transmission of α-syn aggregates *via* the aggregates themselves and exosomes.

Therefore, the RT-PPB played the role of a guard to clear the toxic α-syn aggregates in diseases neurons and prevent the culprits from escaping to affect other normal cells. The RT-PPB could significantly rescue the dopaminergic neurons and recover the motor behavior of PD model mice. These finding showed that the bioinspired siRNA nanocarriers had the great potential in the treatment of PD, as well as other neurodegenerative diseases.

Keywords:gene therapy, delivery barriers, bioinspired nanocarriers, synergistic treatment, neurodegenerative diseases

最终交流类型: Keynote

Organ-on-a-Chip for the Substitution of Animal Tests

顾忠泽

Southeast University, China

Organs-on-a-chip (OOC) system, or microphysiological system (MPS), is a new type of biomedical research method that aims to recapitulate organ-level tissue structures and functions for drug evaluation and disease modeling. The MPS can be used to simulate the microstructure, microenvironment, and functional features of human organs, and applied in drug screening and clinical diagnosis and treatment. In previous studies, we have developed multiple organ-on-a-chip systems including biomimetic blood vessels, kidney, liver, heart, etc. Our previous work demonstrated that the miniature organs made with advanced microfabrication, 3D printing, microfluidics and tissue engineering techniques could form tissue-specific structures and could maintain some desirable organ functions for drug screening and disease modeling purposes.

In this presentation, we report the development of a two-photon/multi-photon based 3D printing systems for the OOC fabrication and microenvironment formation, and the fabrication of multiple microphysiological systems for disease modeling, and the development of an automated high-content organs-on-a-chip imaging system for automated drug screening together with deep-learning based AI-algorisms for data analysis. Regarding the challenges of cross-scale high-precision manufacturing and fluid control in organ-on-a-chip, research has been conducted on controlled microstructure fabrication and the interaction between microstructures and liquids. The concept of focal editing using two-photon polymerization combined with a lattice has been proposed, enabling efficient processing at a

centimeter scale with sub-micrometer precision, making it possible to achieve additive manufacturing at low fill ratios across multiple scales. To achieve automatic organ-on-a-chip evaluation, six tumor organ-on-a-chip image evaluation indices were proposed, and micro-organ intelligent classification algorithms and devices were created. The systems that we reported here have been widely applied in drug discovery and toxicity evaluation in collaboration with top-tier pharmaceutical companies in China, and have been used for precision medicine in collaboration with top-tier hospitals. We also report the design and development of a functional Lung-on-a-Chip system for lung bacterial/viral infection, inflammation studies. Lastly, our system and platform have been successfully applied in Covid-19 and other virus infectiousness evaluation, testing of efficacy for drug, neutralizing antibodies (including vaccines from Pfizer, BioNTech, etc.), and other protective measures. In summary, our work demonstrated the usefulness and progressive applications of OOC in multidisciplinary fields in China.

Keywords:Organs-on-a-chip; Tissue engineering; 3D printing; Artificial Intelligence

最终交流类型: Keynote

SONOPHARMACOLOGY AND SONOGENETICS: ACTIVATING DRUGS, PROTEINS AND GENES BY ULTRASOUND MEDIATED BY NUCLEID ACID NANOSTRUCTURES

Andreas Herrmann

DWI Leibniz Institute e.V.

Remote controlling biological systems is an exciting endeavour because it is the offspring for new therapies and allows answering fundamental biological questions. In this context, the field of optogenetics has enabled the understanding of neural circuits and disorders.[1,2] However, current optogenetic techniques are hampered by the low penetration of light in tissue and hence often require invasive surgical procedures to deliver light to target cells. Therefore, ultrasound (US) was used as alternative trigger since US can deeply penetrate tissue with high spatiotemporal control.[3] Our group develops general molecular technologies based polynucleic acid aptamers and mechanochemistry to control protein activity by US.[4] High molar mass polynucleic acids fabricated by enzymatic reactions

undergo covalent and non-covalent bond cleavage induced by shear forces originating from US-induced cavitation bubbles. These nucleic acid carriers allow the activation of small bioactive molecules and drugs that can initiate gene expression, kill pathogens or cure diseases.[5,6,7] A particular emphasis is paid to reducing US energies to make these sonogenetic and sonopharmacological systems compatible with living matter.

Keywords:nucleic acids, nanotechnology, ultrasound

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最终交流类型: Keynote

Protein Assembly: A Platform to Develop Biomimetic Enzymes

Junqiu Liu

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Sophisticated protein self-assemblies have attracted great scientific interests in recent few decades due to their various potential applications. The design and control of proteins into hierarchical nanostructures via self-assembly strategies offers unique advantages in understanding the mechanism of naturally occurring protein assemblies and in creating various functional biomaterials with advanced properties. Protein self-assembly into exquisite, complicated yet high-ordered architectures represents the supreme wisdom of nature. However, precisely manipulating protein self-assembling behaviors in vitro is a great challenge. By taking advantage of supramolecular strategies such as the metal ion chelating interactions, host-guest interaction and non-specific protein-protein interactions, accuracy control of the orientation of protein self-assembly has been achieved. The designed nanostructures have been used as biomimetic scaffolds for developing biomimetic enzymes. We first developed a series of methods for the preparation of antioxidative selenoenzyme. Based on the protein assembly strategy, we constructed multi-enzyme and multi-enzyme integration, as well as a multi-enzyme cascade protein assemblies [1-6].

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Keywords:Protein Assembly；Biomimetic Enzymes

最终交流类型: Oral

Intelligent Delivery System of Living Microorganism Carrier

吴锦慧

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The process of drugs from entering the body to playing a role faces many obstacles. The traditional delivery system mainly relies on simple packaging of drug molecules to reduce their loss in circulation. With the development of targeted drug delivery, nano-delivery systems have shown significant advantages in improving the accuracy of drug delivery. For example, liposomes have been one of the most successful examples for improving drug delivery. In addition, exosomes as novel drug delivery carriers have also attracted extensive attention. However, existing delivery systems are unable to meet the demand for precise delivery of the novel therapeutic entities and therapeutic strategies that have emerged in recent years. In the future, the ideal delivery carrier should be able to achieve more accurate in vivo delivery. Bio-intelligent living carriers is one of the important strategies to achieve this goal. The use of bacteria as vehicles for drug delivery in oncology therapy has attracted widespread interest. In recent years, with the rapid development of synthetic biology, some properties of bacteria, such as gene operability, excellent tumor colonization ability, and host-independent structure, make them ideal intelligent drug carriers and have attracted extensive attention. Compared with traditional drug delivery, the usage of bacteria for drug loading has better targeting ability and controllability, and can cope with the complex delivery environment of the body to achieve the intelligent delivery of drugs. Our concept is to design microbial living vectors that can sense the microenvironment in vivo and make responsive release. For example, hypoxia-directed drug delivery can be achieved by designing hypoxic chemotaxis biological living carriers that sense hypoxia in vivo. Secondly, directed gas delivery can be achieved by designing light-sensing photosynthetic bacterial live carriers. In addition, we use chemical biology, synthetic biology and other methods to further optimize the microbial live vectors, and focus on the in situ antigen delivery in vivo, in order to improve the immune activation effect of in situ vaccine, and provide a new solution for anti-tumor immunotherapy based on in situ vaccine.

Keywords:Microorganism; carrier; vaccine

最终交流类型: Keynote

Solvo-Driven DNA-Directed Nanoassembly with Strong Coupling

邓兆祥

中国科学技术大学

Strong nearfield coupling between plasmonic nanounits is the basis of a versatility of functioning optical devices fabricated by bottom-up processes. Despite various wet chemistry methods reported in literature to make nanoparticle assemblies, DNA-directed supramolecular self-assembly offers an ideal way to build structurally programmable nanoassemblies toward desired functions. The accurate and predictable pairing between complementary nucleobases of DNA represents an inherent advantage of the DNA-based nanofabrication techniques, making them outperform many existing strategies. We have previously relied on DNA-based structural programming and colloidal chemistry to achieve strongly coupled plasmonic metastructures with highly promising functions. In particular, a technique termed Ag ion soldering is able to make sub-nm-coupled plasmonic “nanomolecules” as well as various derived structures, with or without the help of DNA molecules. This method, while highly promising, has not been adopted to make structures with increased complexities. This talk introduces a different process to build strongly coupled nanostructures under the direction of DNA “bonds”. The rationale of this strategy is that DNA offers an unrivaled ability to make programmable nanostructures which fail to deliver functions different from what possessed by their non-interacting nanounits. Contrary to the commonly adopted aqueous chemistry, this new method gets into a largely unexplored aspect of DNA-directed nanoassembly in non-aqueous media with an intention to address the coupling dilemma of DNA-assembled nanostructures and the complexity issue encountered by previously methods including Ag ion soldering. The key achievement is that the coupling of nanoparticles selectively and immediately happens between DNA-linked nanoparticles due to enhanced double layer neutralization and suppressed hydration, which is unachievable in an aqueous solution. Following this success, we are now being able to work on more complicated nanostructures toward prescribed plasmonic coupling in one-, two-, and three-dimensional spaces. This progress opens up immense opportunities to pursue novel DNA-guided nanomaterials, and to explore their structure-activity relationship toward real-world applications.

Keywords:DNA, nanoparticle, self-assembly, plasmon coupling, non-aqueous solvent

最终交流类型: Oral

Rational design of nano-based hydrogel composite scaffolds for bone and cartilage repair

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上海大学

With the accelerated aging process, the incidence of bone-related diseases such as osteoporosis, osteoarthritis and bone defects is increasing, which intensifies the requirement for novel biomaterials of bone and cartilage repair. In recent years, nano-based hydrogel composite scaffolds guided by stem cell therapy and tissue engineering strategies, have been widely applied for tissue regeneration. Hence, novel neutrophil-erythrocyte hybrid membrane-modified hollow CuS nanoparticles, in-situ nanocomposite hydrogel loaded with ROS-controlled drug release and multifunctional hydrogel composites scaffolds were rational designed for bone and cartilage repair. Firstly, we extracted erythrocyte and neutrophil membranes using membrane protein lysis and gradient centrifugation techniques. And then, biocomposite membrane-modified hollow CuS nanoparticles were obtained for photothermal/anti-inflammatory therapy of osteoarthritis. Furthermore, in the advanced stages of osteoarthritis, there are often concomitant damages to the articular cartilage and subchondral bone. To address that, a novel in-situ nanocomposite hydrogel were prepared through ultrasound disruption of ROS-responsive nanoliposomes. In which, controlled release of KGN and generation of augmented ROS were achieved for cartilage repair. In addition, based on a soft-hard concept, multifunctional CuS nanoparticle-PEG composite soft hydrogel-coated 3D hard PCL scaffolds were prepared using 3D printing and infiltration coating to achieve efficient bone regeneration. In conclusion, this study could provide new materials and strategies for clinical treatment of bone-related diseases.

Keywords:Bio-membranes modification, in-situ gelation, 3D printed scaffold, bone and cartilage repair.

最终交流类型: Invited

Supramolecular Cell Engineering

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Cells are a basic unit of living organisms and using them as drug carriers or therapeutics has unique advantages. For instance, it can significantly improve the targeting efficiency due to the homing effects (e.g. immune cells and stem cells) or improve the systemic circulation (e.g. red blood cells). There are currently several strategies to engineer cells to afford therapeutic capability. The most common one is genetic engineering, which however involves tedious and complicated process, leading to expensive cell-based therapeutics. Non-genetic cell engineering may rely on either endocytosis of medicines intracellularly, or covalent conjugation of medicines onto the surface of cells. Additionally, biological ligand-receptor interactions can be leveraged to conjugate nanomedicine to the surface of live cells. Nevertheless, the cells that phagocytize medicines may degrade the drug before reaching the target. Covalent binding involves a complex synthetic process on the cell surface, which may impair the physiological function of the carrier cells. The ligand-receptor interaction is often limited to specific cells, and competitive ligand displacement occurs in vivo as well.

During the past several years, we have developed unique supramolecular cell engineering approaches via synthetic host-guest interactions that are mostly bioorthogonal, to tackle these above-mentioned issues and to enable targeted delivery of various nanomedicines to specific tissues, driven by the inflammatory tropism of immune cells or wound-targeting properties of platelets.1 When required, other cells such as red blood cells may also be engineered and employed to deliver nanomedicine for extended circulation and targeted accumulation in tissues with specific microenvironment.2 Two general, supramolecular cell engineering strategies were designed and development to achieve the above-discussed purpose: 1) extracellular supramolecular engineering;3 and 2) intracellular supramolecular engineering.4 We show that these unique systems, when designed for individual purposes, may effectively treat several key diseases including acute pneumonia,5 atherosclerosis,6 solid tumors,7 and ischemic stroke,8 respectively.

Keywords:cell engineering, nanomedicine, supramolecular chemistry, targeted delivery, therapeutics

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最终交流类型: Oral

Self-pumping wound dressing

时连鑫

中国科学院理化技术研究所

Capillary adhesion and anti-adhesion problems caused by the interfacial fluid layer are hot issues in the area of interfacial research. In recent years, we have developed a series of self-pumping textiles/dressings and wet adhesive fibers focusing on the problems of impeded healing caused by excessive exudate wetting and dis-attachment caused by the interfacial liquid layer. 1) We propose a biofluid "self-pumping" model and develop a self-pumping dressing with unidirectional transportation of wound exudates to promote overhydrated wound healing (Adv. Mater. 2019, 31 (5), 1804187); 2) We construct a bio-inspired "self-pumping" textiles with asymmetry wettability and structure, which effectively removes sweat from the skin surface and solves the problem of wet stickiness and coldness by the wetted conventional cotton textile (Adv. Mater. 2019, 31 (41), 1904113); 3) A series of self-pumping dressings based on aligned channels and fractal channels are developed to achieve rapid and continuous unidirectional transportation of wound exudates, promoting the healing wound, such as diabetic wounds and burns (Macromol. Rapid Commun. 2022, e2200814, Front. Bioeng. Biotechnol. 2023,11, 10.3389/fbioe.2023.1188782).4) Inspired by the wet adhesion and low-temperature toughness of spider silks, a series of core-sheath/side-by-side hydrophilic fibers are fabricated to achieve omni-wet adhesion on oil/water wetted surfaces and ultra-low temperatures tolerance (-196°C) for the storage of wet-adhesive materials at extremely low temperatures (Adv. Mater. 2021, 33 (14), e2007301, Nano Today 2023, 48, 101748).

Keywords: Self-pumping, Unidirectional Draining, Janus Materials, Wet Adhesion, Super-cold Tolerance

最终交流类型: Oral

Gene therapy based on chemical modification and controlled self-assembly of nucleic acid

刘建兵

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Life system follows the rule of central dogma. DNA is transcribed into mRNA, and then mRNA is translated into target protein to perform specific biological functions. In the treatment of various diseases, most therapeutic targets of small molecule and antibody drugs are the downstream proteins. With the continuous development of nucleic acid manipulation technology and nucleic acid chemical biology, we can directly achieve effective intervention and precise treatment of diseases at the DNA or RNA levels, the upstream of proteins.

As a novel type of treatment, gene therapy, developed from these nucleic acid manipulation technologies, possesses a wide range of application values. However, how to efficiently build a precise gene therapy system to achieve in vivo therapy is a key scientific problem in the field of gene therapy at this stage. Due to the addressability, site-specific modifiability, and biocompatibility, nucleic acid nanostructure can be designed as an ideal drug carrier. Meanwhile, nucleic acid drugs can also be co-assembled through complementary base pairing, which makes the construction of gene therapy system based on nucleic acid chemical modification and controllable self-assembly possible.

We focused on the construction of gene therapy system based on chemical modification and controlled self-assembly of nucleic acid. We have achieved a series of distinctive scientific results from three aspects: (1) establishing new methods for precise assembly of chemically modified nucleic acid nanostructures;[1] (2) developing new technologies for controllable loading of gene therapy drugs;[2] (3) building new systems for precise gene therapy in vivo.[3-5] This biocompatible nucleic acid nanoplatform presents a new promising strategy for the development of gene therapy.

Keywords:Gene therapy, nucleic acid chemical modification, nucleic acid self-assembly, nucleic acid drug, drug delivery

最终交流类型: Invited

Rationally Designed Synthetic Protein Hydrogels with Predictable and Controllable Mechanical Properties

曹毅

Nanjing University

Our bodies are composed of soft tissues made of various proteins. In contrast, most hydrogels designed for biological applications are made of synthetic polymers. Recently, it is increasingly recognized that genetically synthesized proteins can be tailored as building blocks of hydrogels with biological, chemical, and mechanical properties similar to native soft tissues. In this talk, we summarize recent progress in synthetic protein hydrogels. We compare the structural and mechanical properties of different protein building blocks. We discuss various biocompatible cross-linking strategies based on covalent chemical reactions and non-covalent physical interactions. We introduce how stimulus-responsive conformational changes or intermolecular interactions at the molecular level can be used to engineer responsive hydrogels. We highlight that hydrogel network structures are as important as the protein sequences for the properties and functions of protein hydrogels and should be carefully designed. Despite great progress and potentials of synthetic protein hydrogels, there are still quite a few unsettled challenges and unexploited opportunities, providing abundant room for future investigation and development, particularly as this field is quickly expanding beyond its initial stage. We will discuss our recent efforts in designing synthetic hydrogels with predictable and controllable mechanical properties. Specifically, we use single-molecule force spectroscopy, protein engineering and theoretical modeling to prove that the mechanical properties of protein hydrogels are directly linked to the mechanical hierarchy of the crosslinkers and the load-bearing modules at the molecular level and the network structures.

Keywords:Hydrogel, protein, mechanical properties, single molecule force spectroscopy

最终交流类型: Invited

Fabrication of Physical Unclonable Function Using DNA

Dong Ki Yoon

KAIST

Controversy over the artwork's authenticity is ongoing despite numerous technologies for copyright protection. Artists should build their own ways to protect the authority, but piracy is still open. Here, we propose a platform for developing anticounterfeiting labels based on physical unclonable function (PUF), in an artist-friendly manner, brushstrokes. Deoxyribonucleic acid (DNA), which is nature-born, biocompatible, and eco-friendly, can be applied as a paint that shows the entropy-driven buckling instability of the liquid crystal (LC) phase. Brushed and wholly dried DNA exhibits line-shaped zig-zag textures with inherent randomness as a source of PUF, and its primary performance and reliability are systematically examined. This breakthrough enables the utilization of these drawings in broader applications.

Keywords DNA, Physical Unclonable Function, Meniscus-induced Self-Assembly, Shearing, Brushing, Liquid Crystal

最终交流类型: Keynote

Self-Assembly on the Nano-Bio Interface

Qiangbin Wang

Suzhou Institute of Nano-Tech and Nano-Bionics, CAS, China

In this talk, I will introduce our recent efforts to precisely fabricate inorganic nanostructures by templating the inorganic nanoparticles on the rationally designed DNA origamis and protein nanostructures.

Keywords:self-assembly, DNA nanotechnology, protein, inorganic nanostructures

最终交流类型: Oral

Intracellularly gelated macrophages for targeted therapy of inflammatory diseases

高成

澳门大学

Membrane protein disintegration and spatial disorder on membrane camouflaged nanomedicine, caused by separation and reassembly of membrane fragments during the coating process, often affect their cytokines neutralization and targeting efficiency. Herein we show that intracellularly gelated macrophages (GMs) preserve cell membrane structures, including protein content, integration and fluidity, as well as the membrane lipid order. Consequently, GMs can act as cellular sponges to efficiently neutralize various inflammatory cytokines via receptor-ligand interactions, and serve as immune cell-like carriers to selectively bind inflammatory cells in culture medium, even under a flow condition. In a rat model of collagen-induced arthritis, GMs alleviate the joint injury, and suppress the overall arthritis severity. Upon i.v. injection, GMs efficiently accumulated in the inflammatory lungs of acute pneumonia mice for precise anti-inflammatory therapy. Conveniently, GMs are amenable to lyophilization and can be stored at ambient temperatures for at least 1 month without loss of integrity and bio-activity.

Keywords:Cytokine neutralization, membrane protein, hydrogel, antiinflammation, cell-based carrier

最终交流类型: Oral

The Precise Construction and Functionalization of Self-assembled DNA Nanostructures

李娜

国家纳米科学中心

Chemical self-assembly is an important method to create new substances with new functions. The trend of chemical self-assembly is from the early simple-assembled system to the controllable precise construction of multi-functional system. How to accurately construct functional self-assembled system to realize the customized applications has become a key challenge in the field of chemical self-assembly. Controllable self-assembly is an effective way to accurately construct nanosystems. Biological molecules, especially DNA molecule, which has precise recognition sites, simple self-assembly conditions, and controllable sizes and structures, can be used to achieve the precise construction of multi-functional self-assembly systems. Aiming at the major challenge of chemical self-assembly, we first

developed a novel method to accurate construction of multi-component system using DNA molecules, especially the controllable assembly of heterogeneous-shaped nanoparticles. Meanwhile, we also realized the site-specific controllable growth of a variety of nanomaterials, and our method can facilitate the customized pattern growth of nanomaterials. Subsequently, we also constructed many multi-component systems with unique physical and chemical properties, and elucidated the structure-property relationship. Finally, we further promoted the application of novel functionalized nanosystems assembled by DNA molecules for the regulation of bio-functions. We designed a novel self-assembly system to realize molecular recognition and signal amplification of specific ligand on the surface of tumor cells, and provided a new strategy for disease diagnosis and treatment. Our work extends the scope of controllable self-assembly systems, and promotes the application of DNA self-assembly systems in biological detection and sensing. Moreover, our work provides a new idea for the construction of functional self-assembly systems with potential application value.

Keywords:Chemical self-assembly; DNA; multifunction; Structure-function relationship; biological detection and sensing

最终交流类型: Oral

Glyco-engineered Biomimetic Nanosponge to Promote Broad-spectrum SARS-CoV-2 Inhibition

艾相昭

上海交通大学

The COVID-19 pandemic caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) poses a significant challenge to global health. Although the vaccines have been widely administered, their protection rate may decrease with the emergence of SARS-CoV-2 variants. Moreover, most of the drugs approved in clinics are potentially confronted with a decline in therapeutic efficacy against various variants. Therefore, innovative therapeutic approaches are highly demanded to inhibit the SARS-CoV-2 viral infection. Recently, the biomimetic nanosponge camouflaged with cell membrane acts as a broad-spectrum countermeasure based on its promising capability to neutralize the spike (S) protein of SARS-CoV-2 by multiple membrane receptors. In addition, the complex glycocalyx covering the surface of the cell membrane acts as an important co-receptor for viral infection

of host cells, which enhances binding to angiotensin-converting enzyme 2 (ACE2) by altering the open conformation of receptor binding domain (RBD) in the S1 subunit. Herein, we demonstrated that increasing the density of surface glycans (e.g., heparin) on the cellular nanosponges can greatly promote their inhibition against SARS-CoV-2 (**Figure 1**). This glycol-engineering approach of host-mimicking cellular nanosponges is a facile method to enhance SARS-CoV-2 inhibition. It can be readily generalized to promote the broad-spectrum treatment of mutations in coronaviruses and other glycan-dependent viruses in the future.

Keywords:biomimetic, nanosponge, coronavirus, glycan, broad-spectrum

最终交流类型: Invited

The Raising of Bioinspired Asymmetric Micro-nanochannel Membrane

闻利平

中国科学院理化技术研究所

Learning from nature has inspired the creation of intelligent devices to meet the increasing needs of the advanced community and to better understand how to imitate biology.[1-2] As one of biomimetic nanodevices, nanochannels or nanopores aroused particular interest because of their potential applications in nanofluidic devices, biosensing, filtration, and energy conversions. Here, inspiration from biological ion channels in nature, we developed some biomimetic smart nanochannels and then applied those smart nanochannels in practical applications such as energy conversion, [3,4] ion separation. [5,6] Such applications with biomimetic nanochannels can not only help people to know and understand the living processes in nature, but also inspire scientists to study and develop novel nanodevices with better performance for the mankind.

Keywords:Bioinspired nanomaterials; Nanochannel; Micro-nanopore membrane; energy conversion; ion separation.

最终交流类型: Invited

Synthetic α-L-Threose Nucleic Acids as Biocompatible Materials for Diagnosis and Therapy

Pik Kwan Peggy Lo

City University of Hong Kong

α-L-Threose nucleic acids (TNAs) is composed of a backbone repeating of four-carbon threose sugar group with phosphodiester linkages taking place at the 2’- and 3’- vicinal positions of the sugar ring. We and other groups have reported a cost-efficient strategy to synthesize TNA phosphoramidite and used them for solid phase synthesis of sequence-designed TNAs in high synthetic yield. Compared to natural DNAs, synthetic TNAs exhibited high stability in pH extremes, human blood serum, fetal bovine serum and even under storage in various buffer solutions at room temperature for half a year. In the first part, we will report TNA being as a promising alternative to traditional antisense oligonucleotides for suppressing target gene suppression and inhibiting tumor growth in vitro and in vivo with no harmful effects due to its higher specificity and stronger binding affinity towards its complementary RNAs over DNAs. In the second part, we will present stable and reliable detection and imaging of target nucleic acids in vivo using biosensors composed of chemically modified TNA capture probes. Compared to natural DNA probes used in conventional techniques, this TNA-based biosensor not only enables simple and rapid detection, identification and quantification of target nucleic acids, but also allows to monitor the dynamic change of the expression of target nucleic acids in living cells at different status. Importantly, this TNA-based biosensor can specifically discriminate single nucleobases mismatch, resulting in high specificity and selectivity.

Keywords:TNA, capture probe, miRNA biosensor, antisense drugs, cancer therapy

最终交流类型: Oral

Platelet-inspired Nanomedicine

张银龙

University of Chinese Academy of Sciences

Apart from playing important roles in thrombosis and hemostasis, platelets also play significant roles in tumor progression and metastasis. They secrete various cytokines that promote tumor proliferation and angiogenesis. By secreting TGF-ß, platelets induce tumor

cells to acquire invasive properties. In the bloodstream, platelets bind to circulating tumor cells, providing protection against immune system attacks and high-speed blood flow during their journey to distant sites. Platelets also secrete chemotactic factors that assist metastatic cells in establishing themselves at these distant sites. Moreover, platelets help to maintain the integrity of tumor blood vessels through the secretion of inflammatory protective factors or physical adsorption. Understanding these diverse roles of platelets holds promise for developing effective treatment strategies. Combined with the special pharmacokinetic properties of nano-carriers, a variety of nanomedicines targeting platelets for disease treatments have been developed. Here, we presented intelligent nanomedicines for local platelets regulation to navigate cancer-related diseases, e.g. tumor embolization therapy, tumor metastasis prevention and tumor targeted drug delivery. Besides, we have developed nanomedicines for reversing the effects of antiplatelet drugs, particularly in cases where urgent surgery is required to avoid life-threatening bleeding. These explorations offer novel options for disease treatment that demonstrate advantages over traditional strategies.

Keywords:Platelet regulation, Nanomedicine, Antiplatelet drug reversal

最终交流类型: Invited

Multi-Dimensional Manipulation of Solid/Liquid Interaction

邓旭

电子科技大学

olid/Liquid interaction play important role in many research and application fields. In this presentation, we will introduce a radically new strategy that resolves the bottleneck through the creation of an unexplored gradient in surface charge density (SCD) [1]. By leveraging on a facile droplet printing on superamphiphobic surfaces as well as the fundamental understanding of the mechanisms underpinning the creation of the preferential SCD, We envision that our work enriches and extends our capability in the manipulation of droplet transport and would find numerous potential applications otherwise impossible. We will also show that robust superhydrophobicity can be realized by structuring surfaces at two different length scales, with a nanostructure design to provide water repellency and a microstructure design to provide durability[2]. We apply this strategy to various substrates—

including silicon, ceramic, metal and transparent glass—and show that the water repellency of the resulting superhydrophobic surfaces is preserved even after abrasion by sandpaper and by a sharp steel blade. This design strategy could also guide the development of other materials that need to retain effective self-cleaning, anti-fouling or heat-transfer abilities in harsh operating environments.

Keywords: Solid/Liquid Interaction,Surface charge density

最终交流类型: Oral

Peptidyl Virus-Like Nanovesicles as Reconfigurable "Trojan Horse" for Targeted siRNA Delivery and Synergistic Inhibition of Cancer Cells

王跃飞

天津大学

Gene-based therapeutics have wide-reaching clinical potential, such as in the prevention and treatment of COVID-19. However, genetic drugs need efficient carriers to deliver them into cells. Peptides and peptide derivatives provide an attractive platform for gene drug delivery due to their flexibility, versatility, and facile synthesis. Recently, we developed a series of peptide carriers for the delivery of gene drug based on the rational design and self-assembly of peptides. For example, we report the self-assembly of peptidyl virus-like nanovesicles (pVLNs) composed of highly ordered peptide bilayer membranes that encapsulate the siRNA. The targeting and enzyme-responsive sequences on the bilayer' s surface allow the pVLNs to enter cancer cells with high efficiency and control the release of genetic drugs in response to the subcellular environment. By transforming its structure in response to the highly expressed enzyme MMP-7 in cancer cells, it helps the siRNA escape from the lysosomes, resulting in a final silencing efficiency of 92%. Moreover, the pVLNs can serve as reconfigurable "Trojan horse" by transforming into membranes triggered by the MMP-7 and disrupt the cytoplasmic structure, thereby achieving synergistic anticancer effects and 96% cancer cell mortality with little damage to normal cells. The pVLNs benefit from their biocompatibility, targeting, and enzyme responsiveness, making them a promising platform for gene therapy and anticancer therapy.

Keywords:anticancer, enzyme response, gene delivery, peptidyl virus-like nanovesicle

最终交流类型: Oral

Virus-like iron oxide minerals inspired by magnetotactic bacteria: the fabrication and application

丁春梅

四川大学

Magnetic iron oxides, as the typical photothermal material, possess the advantages of low cost, easily prepared and biocompatible, that are given great expectations in broad application prospects. However, the limited photothermal efficiency of iron oxides restrict their further use. To address this problem, inspired by magnetotactic bacteria, we develop a liquid film-confined strategy assisted by magnetic field for mineralization and assembly of iron oxides on surface at room temperature. Virus-like hierarchically micro/nanostructured iron oxides can be obtained on universal substrates which exhibit excellent photothermal performance, highest among all iron oxides coatings and even comparable with carbon-based material. Theoretical simulation demonstrates the promotion of light capture by this particular structures. Taking advantage of this strategy, iron oxides can be integrated with other minerals (e.g. bismuth sulfide) with the maintaining of hierarchical structures.

By virtue of the outstanding photothermal properties and micro/nano-structures, the surface is endowed with superhydrophobicity by simple modification to construct photothermal superhydrophobic platform. This application of composite materials is verified in three challenging scenarios: (1) high-efficient antibacterial activity, (2) defrosting/deicing ability controlled remotely and (3) floating water cleaning robots with the synergy of light and magnetism.

No need for harsh experimental conditions and templates, the strategy reported here is mild, environmental-friendly and adopts trace amount of liquid (55 μL per cm2), which can provide reference for the fabrication and application of other photothermal materials.

Keywords:Bioinspired mineralization, Liquid film-confined, Virus-like iron oxide minerals, Photothermal, Superhydrophobic

最终交流类型: Invited

Analysis and Detection Based on Solid Nanopore/Channel

夏帆

中国地质大学（武汉）

Various types of transmembrane pores and ion channels in the range of 1-100 nm are found in each biological cell, playing crucial roles in varieties of significant physiological activities such as maintaining cell osmotic balance and stabilizing cell volume. Inspired by this natural phenomenon, different biomimetic nanodevices (nanopore/channel) with different characteristics have emerged as an attractive and powerful platform and have been used for a wide range of applications. Generally, the principle of analysis applications based on solid nanopore/channel can be described as follows: molecules access or attach on the inner surface of a nanopore/channel, change the effective diameter of the nanopore/channel, or affect the charge transfer as well as the wettability of the inner surface of the nanopore/channel, leading to ionic current changes that can be detected.

Keywords:nanopore/channel, biomimetic, analysis, molecular recognition

最终交流类型: Invited

Mechanism and Function of Interfacial Dynamic Superspreading

田野

中国科学院理化技术研究所

Interface dynamic superspreading has a wide range of applications in many fields [1]. The study found that the surface of the animal cornea has a very significant ultrafast spreading property (the super spreading time is 830 ms), this special property is endowed by the unique microchannel surrounding the nanowire array structure on the corneal surface [2], the spreading behavior is induced by the three-dimensional nanocapillary forces between the nanowire arrays, while the dynamic velocity of super-spreading is dominated by the microchannels. In addition to life systems, there is also a very classic superspreading phenomenon in the field of artificial materials. For example, Chinese Xuan paper prepared by our ancestors can preferentially achieve superspreading on the two-dimensional plane and not penetrate in the longitudinal direction [3].

At the molecular scale, the superspreading behavior of water at the interface is mainly affected by the intermolecular forces between the liquid and the substrate, such as hydrogen bonds, electrostatic forces, van der Waals forces, and so on. Studies have found that the spreading behavior of liquid depends on the arrangement of the first layer of water at the interface, that is, the hydrogen bond network structure of water molecules at the interface [4]. By simultaneously controlling the intermolecular interaction and the size of the interfacial space, the superspreading process can be realized on the interface of different dimensions, and then the application in the field of molecular ion transport can be realized [5].

Keywords:interface; dynamic; superspreading; intermolecular force

最终交流类型: Invited

Virus inspired mimetic DNA origami frameworks

杨洋

Shanghai Jiao Tong University

Through hundreds of millions of years, viruses have evolved precise and efficient host cell infection capabilities, which are closely related to their nanoscale dimensions, densely genetic material packaging, and specific surface protein exhibition. Mimicking viruses to build nanodevices is expected to provide new toolbox for biomedical research and applications. We have designed and assembled a few DNA origami frameworks with regular icosahedral symmetry. By modifying the receptor-binding domain of the virus S protein outside the framework, the thermodynamic and kinetic behavior of the interaction between the imitation virus particle and the cell was studied, and the efficient activation of immune cells was induced. Through the internal modification of the frame, the high-density genome packaging behavior of the virus is simulated, and the infection of the pseudophage is realized. Through modification at both inside and outside of a frame, a safe and efficient siRNA delivery vector was constructed. Relevant studies have proved the advantage that the virus-like DNA origami framework can be precisely modified, suggesting its great potential in the fields of cell engineering and new vaccines.

Keywords:DNA origami, virus mimetic device, genome packaging, surface modification, gene delivery

最终交流类型: Keynote

Super-wettability and Beyond——Quantum-confined Superfluid: Biological Energy Conversion, Chemical Reaction and Information Transfer

江雷

中国科学院理化技术研究所

Life system presents an ultralow energy consumption in high-efficiency energy conversion, information transmission and bio-synthesis. The total energy intake of human body is about 2000 kcal/day to maintain all our activities, which is comparable to a power of ~ 100 W. The energy required for brain to work is equivalent to ~ 20 W, while the rest energy (~ 80 W) is used for other activities. All in vivo bio-syntheses take place only at body temperature, which is much lower than that of in vitro reactions. To achieve these ultralow energy-consumption processes, there should be a kind of ultralow-resistivity matter transport in nanochannels (e.g., ionic, molecular channels), in which the directional collective motion of ions or molecules is a necessary condition, rather than the traditional Newton diffusion. Directional collective motion of ions and molecules are considered as ionic/molecular superfluid. The research of ionic/molecular superfluid will promote the development of neuroscience and brain science, develop quantum ionic technology, construct future chemical reactors with high flux, high selectivity and low energy consumption, and produce a series of disruptive technologies.

Keywords:Super-wettability, Quantum-confined Superfluid, Energy Conversion, Chemical Reaction, Information Transfer

最终交流类型: Invited

Oral Delivery of Bioactive Glass-Loaded Core–Shell Hydrogel Microspheres for Effective Treatment of Inflammatory Bowel Disease

Hon Fai Chan

Chinese University of Hong Kong

Resolving inflammation and promoting intestinal tissue regeneration are critical for inflammatory bowel disease (IBD) treatment. Bioactive glass (BG) is a clinically approved bone graft material and has been shown to modulate inflammatory response, but it is unknown whether BG can be applied to treat IBD. Here, it is reported that BG attenuates pro-inflammatory response of lipopolysaccharide (LPS)-stimulated macrophages and hence reduces inflammatory damage to intestinal organoids in vitro. In addition, zein/sodium alginate-based core–shell microspheres (Zein/SA/BG) are developed for oral delivery of BG, which helps prevent premature dissolution of BG in the stomach. The results show that Zein/SA/BG protects BG from a gastric-simulated environment while dissolved in an intestinal-simulated environment. When administered to acute and chronic colitis mice model, Zein/SA/BG significantly reduces intestinal inflammation, promotes epithelial tissue regeneration, and partially restores microbiota homeostasis. These findings are the first to reveal the therapeutic efficacy of BG against IBD, which may provide a new therapeutic approach at low cost for effective IBD treatment.

Keywords bioactive glass, microsphere, oral delivery, macrophage, inflammatory bowel disease

最终交流类型: Invited

Synergistic Interactions of Semi-Stable Domains in Biosystem

杨雨荷

National Center of Nanoscience and Technology

Multivalent interactions are crucial in biological recognition and signaling processes, such as immune recognition, cell adhesion, virus-host interactions, and protein-protein interactions. This study focuses on the synergistic enhancement effect and mechanism of weak interactions in two scenarios: folding and assembly of nucleic acid molecules and antigen-antibody interactions. DNA and RNA assembly structures contain many unstable and complementary building blocks. Studies have shown that these unstable building blocks tend to form a single closed loop dimer due to the synergistic enhancement effect between two complementary building blocks in a dimer. In antigen-antibody interactions, the synergistic effect of multivalent interactions also depends on the optimal spatial matching between multiple ligands and receptors. The structure of antigen-antibody complexes was analyzed using cryo-electron microscopy, which showed that bivalent binding of IgG to three RBDs on the Spike protein promotes enhanced binding affinity and specificity, resulting in the formation of higher-order multivalent complexes. Multivalent interactions are especially critical in whole virus systems. These research results reveal the synergistic enhancement effect and mechanism of multivalent interactions of unstable building blocks in the biological system, which has important implications for understanding the nature of life systems.

Keywords:nanotechnology， immunology， vaccine， virology

最终交流类型: Invited

Lipid-modified DNA platform for biological drug delivery: Self-assembly and dynamics

Minseok Kwak

Pukyong National University

This presentation will focus on lipid-DNAs with synthetic hydrophobic segments covalently connected to oligonucleotides. The self-assembled lipid-DNA micelle is a versatile delivery platform where biomolecules such as DNA, RNA, and peptide are co-loaded within the carrier for anti-cancer therapeutics or elsewhere. These materials exhibit both the complementary nucleobase recognition of DNA and the aggregation behavior of amphiphilic macromolecules. Here, successful in vivo utilization of the materials in immunology and gene silencing will be demonstrated. Lastly, we performed molecular dynamics simulations to understand the underlying mechanism for phenomena at cell membranes.

Keywords: micelle, cell membrane, immunotherapy, RNAi, biophysics

最终交流类型: Keynote

Bioinspired Chaperone to Control Protein Folding

史林启

Nankai University

Folding and unfolding are essential ways for a protein to regulate its biological activity. The misfolding of proteins usually reduce or completely compromise their biological

functions, which eventually causes a wide range of diseases including neurodegeneration diseases, type II diabetes, and cancers. Therefore, materials that can regulate protein folding and maintain proteostasis are of significant biological and medical importance. In living organisms, molecular chaperone is a family of proteins that maintain proteostasis by interacting with, stabilizing, and repairing various proteins. Herein we report an efficient nano molecular chaperone based on polymeric micelles which bioinspired the intriguing structure and functionalities of the chaperones. The nano chaperone can effectively promote the correct folding of proteins, be used for the renaturation of Inclusion bodies proteins, and significantly improve the efficiency of correct protein folding; It can also protect proteins and improve their stability; Mediate protein transport and improve delivery efficiency; Promote the immune process and improve the therapeutic effect of immunotherapy.

Imbalance of protein homeostasis is the main cause of degenerative neurological diseases. These nano molecular chaperones can effectively promote the correct folding of related proteins, exert normal functions, inhibit their misfolding, reduce aggregation, and reduce neuronal toxicity; Simultaneously mediate the degradation of related protein aggregates and restore the homeostasis of proteins in the body. Animal experiments have shown that nano molecular chaperones can effectively alleviate the symptoms of degenerative neurological diseases such as Alzheimer's and Parkinson's, restore behavioral abilities, and control the development of related conditions.

Keywords: Molecular chaperone; Protein folding; Misfolding, Protein homeostasis

最终交流类型: Invited

Physical Therapy Strategies Based on Assembled Interfaces

罗聃

北京纳米能源与系统研究所

Self-assembly refers to the process in which basic building blocks spontaneously form structurally regular, thermodynamically stable, and functionally specific aggregates through weak forces. A large number of exquisitely designed assembled interfaces in nature, but it is often difficult to simulate these complex and ordered superstructures artificially, and there are challenges such as unclear assembly mechanism, organic-inorganic phase mismatch, and uncontrollable nanoscale morphology. In addition, the mechanisms of how ordered assembly interfaces regulate the behavior of organisms through their unique physical properties need to be further explored. We have constructed inorganic/organic multivariate controllable assembled interfaces through thermodynamic optimization, kinetic modulation, and template confinement regulation strategies, and carried out systematic research and exploration on their potential biological regulation functions. In vitro reconstruction of cross-scale complex biological interfaces, such as bone, tendon, and periodontal tissue have been realized from multiple dimensions such as chemical composition, micro-nano topology, and local microenvironment. More importantly, by exploring the signaling mechanism of the assembly interface, we have revealedthe optimization rules of the "collective properties" of the assembled interfaces and their force regulation mechanism on cell activity and fate. We have also exploited triboelectric and electrostatic induction effects at the assembly interfaces to develop high-performance electrical stimulation medical devices for applications in areas such as drug delivery, tissue engineering, and haptic biomimicry. The above research work revolves around the controlled assembly of functional interfaces and their bioregulatory mechanisms, which are expected to lead to novel tissue engineering materials and high_x0002_performance medical devices with clinical translation potential.

Keywords:assembled interfaces; biomimetic nanomaterials; electronic medical devices; tissue engineering

最终交流类型: Invited

Molecular engineering for structural proteins and material applications

刘凯

清华大学

Protein-based structural biomaterials are of great interest for various applications because the sequence flexibility within the proteins may result in their improved mechanical and structural integrity and tunability. As the two representative examples, protein-based adhesives and fibers have attracted tremendous attention. The typical protein adhesives, which are secreted by mussels, sandcastle worms, barnacles, and caddisfly larvae, exhibit robust underwater adhesion performance. In order to mimic the adhesion performance of these marine organisms, two main biological adhesives are presented here, including genetically engineered protein-based adhesives and biomimetic chemically synthetized adhesives. Moreover, various protein-based fibers inspired by spider and silkworm proteins, collagen, elastin, and resilin, have been studied extensively. The achievements in synthesis and fiber fabrication by microbial biosynthetic technology and chemical regeneration certainly will accelerate the explorations and applications of protein-based materials in wound healing, tissue regeneration, drug delivery, biosensors, and other high-tech applications. Perspectives regarding the study of the interplay of the protein structure, cohesion and adhesion effects, fiber processing, and mechanical performance will be discussed.

Keywords: Artificial proteins, molecular engineering, biosynthesis, nanoassembly, structural protein

最终交流类型: Keynote

Soft Monitoring of Cells, Tissues and Organoids

Wenlong Cheng

Monash University

In the context of telehealth and internet of things (IOT), there are unprecedented needs for developing remote diagnostic tools that can monitor chemical and biological markers remotely anytime anywhere, such as via a smart phone. Such sensing devices are ideally soft and thin so that they can “bio-friendly” interface with soft biological systems. However, traditional biosensing devices are typically constructed by bulk electrodes which are rigid and planar limited electroactive surface areas.

Here, I will present our skin-like sensing devices that can establish intimate “soft contact” with cells, tissues and organoids so that their health can be diagnosed in real-time and in-situ, even remotely via a smartphone.

Keywords: Soft Bioelectronics, Wearable Biosensor, Gold Nanowire, Cardiac Organoid

最终交流类型: Keynote

Anti-tumor vaccine and immunotherapy

胥传来

Jiangnan University

Cancer immunotherapy, which combats tumor cells by activating the immune system, has become a promising strategy for the treatment of tumors; however, this strategy requires a powerful immune system to be effective. Compared with traditional cancer therapy, such as chemotherapy, radiotherapy, and surgical therapy, immunotherapy is efficient and sustainable against cancer with relatively lower toxicity and side effects. The chirality of nanoparticles can influence their interaction with cells and biological systems. How the chirality can exert impact on the immune response are far from to have extensive research attention. We use irradiation with circularly polarized light (CPL) to synthesize nanoparticles with controllable nanometre-scale chirality and optical anisotropy factors (g-factors) of up to 0.4. We find that chiral NPs are shown to enhance both innate and acquired immunity against tumor growth. The therapeutic and preventative effects of chiral NPs against tumors in tumor model are investigated. It is found that L-type NPs have a significant greater ability to induce apoptosis in tumor cells and prolong the survival time of model mice than D-type NPs. Mechanistic studies reveal that the binding of nanoparticles to two proteins from the family of adhesion G-protein-coupled receptors (AGPCRs)—namely CD97 and EMR1—results in the opening of mechanosensitive potassium-efflux channels, the production of immune signalling complexes known as inflammasomes, and the maturation of mouse bone-marrow-derived dendritic cells. Both in vivo and in vitro immune responses depend monotonically on the g-factors of the nanoparticles, indicating that nanoscale chirality can be used to regulate the maturation of immune cells.

Keywords:chiral; nanoparticle; tumor; vaccine; immunotherapy

最终交流类型: Oral

Optically Functional Organic Crystal in Biomineralization

张甘

兰州大学

Living organisms regulate organic molecules in their body to produce highly refractive crystals through strategies similar to biomineralization. The crystallizations are exerted by the biological control over the crystal structures, morphology and the assembly of the ultrastructural organization, generating different optical phenomena with various functions in nature, such as animal visions and structural colors. These optically functional biogenic crystals exhibit significant optical property, bio-compatibility and eco-compatibility, and provide new insights to biomineralization and bioinspired crystallization. Despite the huge potential to inspire artificial optical materials, little is known about these materials. Here we present biological models constructed by three different types of optically functional biogenic crystals: guanine, isoxanthopterin, and 7,8-dihydroxanthopterin. The lizard generates matte blue structure color arising from a disordered photonic structure constructed by guanine nanocrystals in the pigment cell. This conspicuous angle-independent color in tail can deflect the predator attacks away from vital organs, thus increasing the survival probability. The reflector in the crustacean's eye is constructed from a photonic glass of crystalline isoxanthopterin nanospheres. The nanospheres' size and ordering are modulated to tune the reflectance from deep blue to yellow, enabling concealment in different habitats. Meanwhile, the photonic glass also functions to enhance the acuity and sensitivity of the vision by acting as an optical screen photoreceptor. The tapetum layer in fish eye is composed of randomly packed 7,8-dihydroxanthopterin nanocrystals. These crystals surround the photoreceptors from retina, and back reflect the incoming light to the retina to provide a second chance of photon capture, thus enhancing the vision sensitivity. By discovering the new bio-optical materials and elucidating their functional mechanisms of the biological models, we learned how nature achieve optical functionalities from nanoparticles beyond what is possible with perfectly ordered or ideal system alone, which inspire the fabrication of artificial optically functional materials with significant bio-compatibility and eco-compatibility.

Keywords:Biomineralization, Organic Crystal, Optical Function

最终交流类型: Keynote

Publishing in Nature Materials

李昕

Springer Nature

This talk will give an overview of the editorial process involved in publishing in Nature Materials. The discussions will especially include what editors do, what we look for in a Nature Materials paper, and how we make decisions, together with some practical tips for the submission and the peer-review process.

Keywords:scientific publishing

最终交流类型: Invited

Nanopore based nucleic acid and peptide sequencing

白净卫

Tsinghua University

Recently, with the improvement in performance, high-throughput DNA sequencing technology has become an essential tool for basic life science research and numerous clinical applications. Nanopore sequencing as the latest generation of sequencing technology, has proven to be beneficial due to its long read length, fast speed, and portability. Furthermore, research is being conducted in order to develop detection and sequencing technologies for other macromolecules, such as proteins, based on the basic principles of nanopore stranded sequencing. We will outlines the progress in nanopore DNA sequencing research, clinical applications and industrialization, and the recent development of nanopore based peptide sequencing techniques.

Keywords:nanopore, sequencing, protein, nucleic acid, application

最终交流类型: Invited

Supramolecular Interactions Induced Chiral Assembly of Plasmonic Nanoparticles

刘堃

Jilin University

Chiral assemblies of plasmonic nanoparticles are known for strong circular dichroism but not for high optical asymmetry (g-factor), which is limited by the unfavorable combination of electrical and magnetic field components compounded by strong scattering. In the present talk, we will demonstrate a series of biomolecules induced chiral assembly of gold nanorods by using supramolecular interactions [1-6]. These studies show the long-range orderedness of chiral assembly is critical for achieving high optical asymmetry. The supramolecular interactions of gold nanorods with human islet amyloid peptides catalyze their assembly into metallic superstructures with unusually high cholesteric order. Contrary to current theories, the transition from individual NRs to long straight helices leads to increase

of g-factor (up to 0.12) by 4600 times. These works established the link between the liquid crystals and chiral inorganic nanostructures; provides unifying design principles for organic and inorganic optically active media and opens new modalities for drug discovery of amyloid diseases.

Keywords:Chiral nanostructures；g-factor；Supramolecular；Surface plasmon resonance；Amyloid fibrils

最终交流类型: Invited

Cell-mimetic nanomaterials through dynamic assembly in aqueous phase separating systems

Anderson Shum

The University of Hong Kong

Biological cells are intriguing basic units of life with sophisticated cellular and sub-cellular structures. Besides membrane-bound organelles, such as nuclei and mitochondria, membraneless organelles are discovered to play very important role in many important cellular processes. Membraneless organelles are essentially aqueous droplets with critical constituents within an aqueous environment. In addition, the environment also consists of viscoelastic networks, such as the cytoskeleton, as a dynamic structure. In this talk, I will discuss some approaches to formulate aqueous droplets that mimic these liquid organelles. I will also illustrate how the resultant liquid-liquid interfaces can be used to assemble macromolecules and nanoparticles into functional structures. Furthermore, I will introduce a way to formulate a viscoelastic network within these synthetic cell-mimetic microenvironment. These cell-mimetic solution phases and interfaces will not only provide representative models of cellular and sub-cellular structures, but also introduce ways to generate new functional nanomaterials.

Key Words Cell-mimetic nanomaterials

最终交流类型: Invited

Design and fabrication of bioinspired macroporous materials

柏浩

浙江大学

Biological porous materials, such as wood, bone and polar bear hair, have obtained outstanding mechanical and thermal properties by building hierarchical architectures. Specifically, wood exhibit excellent mechanical strength, highly efficient water and nutrient transport capability, and low density due to their hierarchically aligned porous architecture; polar bears can retain thermal homeostasis in the extremely cold Arctic due to outstanding thermal insulation property of their porous hairs; bone has developed highly mineralized porous architecture to realize both high strength and efficient vascularization channels. Learning from these design motifs is believed to provide an effective way to design novel materials with unprecedented properties to meet the ever-growing demands of a sustainable society.

In this talk, I will present our recent progresses in developing cuttlebone-inspired cellular materials to resist large hydrostatic pressure in the deep-sea environment, thermally stealthy textile inspired by polar bear hair, intrinsically self-healable nacre-mimetic composites, and so on. I will also demonstrate the potential applications of these bioinspired porous materials in areas like lightweight vehicles and equipment, thermally efficient textiles and buildings, mechanically functional materials and so on, to support the development of sustainable society. At the end of my talk, challenges and prospects of bioinspired porous materials will be discussed.

Keywords:macroporous materials, composite, polar bear hair, ice-templating, hierarchical structure

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最终交流类型: Keynote

Bioinspired Sustainable Structural Materials

俞书宏

University of Science and Technology of China, China

Biominerals are well-known composites of inorganic and organic materials in the form of fascinating shapes and high ordered structures, which exist in Nature, for example, pearl, oyster shells, corals, ivory, sea urchin spines, magnetic crystals in bacteria, and human bones, created by living organisms. During the past few decades, it has been one of the hottest research subjects in materials chemistry and its cutting-edge fields to explore new bio-inspired strategies for the generation of materials with unique structural specialty and complexity. This lecture will present our recent advances on bio-inspired synthesis of a family of bio-based structural materials with designed micro-/nano-

scale structure and tunable surface chemistry and the macroscopic scale assemblies of the bio-based building blocks like cellulose nanofibers and other biomass particles with surface nanocrystallization. Especially, we will report our recent advances on how to realize the production of sustainable structural materials spanning all length scales, such as synthetic nacre, nacre-inspired structural material, cellulose nanofiber plates, regenerated isotropic wood, soft wood, and deformable bioceramics. These sustainable bio-based structural materials prepared by bio-inspired manufacturing are emerging as a new material system, which holds the key to advance a global sustainability goal.

Keywords: Five keywords [Times New Roman, 12pt Bold, comma separated, centred]

Topical Sessions =》 12. Nano-bio Analysis,Nanobioimgaing and Diagnostics

最终交流类型: Invited

Single Molecule Protein Sequencing based on Nanopores

龙亿涛
NanJing University

Protein is the main component of organisms and the main bearer of life activities. The function of proteins in life activities is closely related to the amino acid sequence. In view of the current lack of amplification approaches for protein sequencing, a highly sensitive sensing technology is under urgent demand to read the amino acid sequence and post-translational modification information of a single protein with high throughput, accuracy and speed. In response to the above challenges, a new method for single-molecule protein sequencing based on nanopore was proposed.1,2 Utilizing the nanopore single-molecule interface, a three-dimensional confinement environment enhanced by its internal physical-chemical synergy from the level of a single chemical group has been precisely constructed. This confinement environment can regulate weak interactions between the target molecule and the sensing groups of the interface, capture and manipulate a single peptide, so as to acquire the information including the molecule length, amino acid composition and post-translational modification and position of a single protein molecule.3 Furthermore, combined with the weak current measuring instrument and the rapid quantitative method of big data developed by our group independently,4,5 a strategy to reveal the molecular evolution of complex systems was developed, realizing the precise identification of peptides with single amino acid differences.6 Attributed to the single-molecule and label-free characteristics of nanopore technology, the interaction of enzyme reactions can be "intrinsically" reflected without introducing additional interference. Our findings have shown broad application prospects in biological single-molecule analysis, single-molecule weak interaction research, and protein single-molecule sequencing, opening up a new direction for nanopore single-molecule spatiotemporal omics.

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Keyword: single biomolecule interface, protein sequencing, nanopores, single molecule sensing,

最终交流类型: Oral

Microarray chip based high-throughput screening of NfL self-assembling peptide for non-invasive diagnosis of Alzheimer's disease

王子华
福建医科大学

Alzheimer's disease (AD) starts decades before cognitive symptoms develop. Easily accessible and cost-effective biomarkers that accurately reflect AD pathology are essential for both diagnosis and therapeutics of AD. Neurofilament light chain (NfL) levels in blood and cerebrospinal fluid (CSF) are increased in AD more than a decade before the expected onset, thus providing one of the most promising blood biomarkers for diagnosis of AD. The clinical practice of single molecule array (Simoa) technology is limited by the high costs and difficulties in synchronous detection of multi-targets. Herein, we developed a microarray chip-based high-throughput screening method, and screened a novel self-assembling peptide targeting NfL. Through directly “imprinting” and further analyzing the sequences, morphology and affinity of the identified self-assembling peptides, the Pep-NfL peptide nanosheet with high binding affinity toward NfL (KD = 1.39×10^{-9} mol/L), high specificity, and low cost was characterized. The superior binding ability of Pep-NfL was confirmed in AD mouse models and cell lines. In the clinical diagnostic groups, the Pep-NfL peptide nanosheet could discriminate patients with AD ($P< 0.001$, $n= 37$), mild cognitive impairment (MCI) ($P< 0.05$, $n= 26$), and control groups ($n= 30$). In comparison to Simoa and ELISA, Pep-NfL platform offers advantages of faster detection time, detection sensitivity, cheaper and simplicity. Our data provide a new insight into the establishment of innovative high-throughput screening system and efficient strategy of screening self-assembling peptides for blood-based diagnosis of AD. The findings hold great potential more efficient and sensitive detection toward the blood-based diagnosis of AD using self-assembling peptides toward NfL and meanwhile provides novel insights into the novel high-throughput screening strategy of self-assembling peptides. This SPR biosensor platform holds high promise for the point-of-care diagnosis and monitoring of disease progression. This simple high-throughput screening strategy can quickly identify self-assembled peptides suitable for the development of various biomedical diagnostic materials.

Keyword: Self-assembly peptide, Imprinting, Neurofilament light chain, Blood biomarker, Alzheimer’s disease, Early diagnosis

最终交流类型:

Acupuncture Needle-Based Transistor Neuroprobe for in Vivo Monitoring of Neurotransmitter

李玉桃
湖北中医药大学

Chemical communication via neurotransmitters is central to brain functions. Nevertheless, in vivo real-time monitoring of neurotransmitters released in the brain, especially the electrochemically inactive molecules, remains a great challenge. In this work, a novel needle FET microsensor based on an acupuncture needle is proposed, which was demonstrated to be capable of real-time monitoring dopamine molecule as well as neuropeptide Y in vivo. The FET microstructure was fabricated by successively wrapping an insulating layer and a gold layer on the top of the needle, where the needle and the Au served as the source and drain, respectively. After assembling reduced graphene oxide (RGO) between the source and drain electrodes, the specific aptamer was immobilized on the RGO, making this needle-FET biosensor highly selective and sensitive to real-time monitor neurotransmitters released from rat brain, even in a Parkinson’s diseases model. Furthermore, the needle-FET biosensor was applied to detect a variety of targets including hormones, proteins, and nucleic acid, and further proved to be capable of real-time monitoring of neuropeptide Y in vivo. By constructing a FET sensing interface on an acupuncture needle and implanting the sensor in a rat’s brain for in vivo detection, this work provides a new sight in the FET domain and further expands the species of real-time in vivo detection. The needle-

shaped FET microsensor holds follow merits: (1) Diversity: the sensor can be used to detect a variety of targets including small molecules, proteins, and nucleic acid. (2) Portability: the single needle FET device is movable and portable, and can be easily moved or inserted into cells or any part of the living body for detection. (3) Toughness: The needle is tough enough so that in vivo detection can be realized and damage is minimized. (4) Re-generation: due to its simple structure and easy-to-fabrication, it can be re-generated by grinding it hundreds of times, which is economical and affordable. This will possibly facilitate the development of interdisciplinary research areas across analytical chemistry and life science.

Keyword: Acupuncture needle, Field effect transistor, Neurotransmitter, Real-time, In vivo

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最终交流类型: Invited

Long-Term Fluorescence Imaging Analysis and Targeted Detection of Eye Disease

何耀
苏州大学

Fluorescein angiography (FA) is a standard imaging modality for evaluating vascular abnormalities in eye diseases, which is recognized as the major cause of vision loss. Long-term and real-time fluorescein angiography is of great importance in preclinical research, nevertheless remaining big challenges up to present. On the other hand, Infectious keratitis that would lead to corneal opacities is one globally major cause of vision impairment and blindness. Whereas the pathogens have been proved to include bacteria, fungi, viruses and protozoa, proper diagnosis (i.e., infections are definitively confirmed and causative organisms are identified) is critical to initiate aggressive treatment. The prevailing diagnostic techniques are currently Gram stain and culture, typically time-consuming, hours to days, and tedious in manipulation. Nevertheless, infectious keratitis recommended as a medical emergency usually implies an acute and rapid disease progression (e.g., Staphylococcus aureus (S. aureus)-induced keratitis can even cause the loss of vision within days as the complete destruction of corneal stroma is induced), and hence time is absent in this sight-threating disease. Consequently, a substantial room is reserved for developing novel strategies, those are suitable for rapid, non-invasive, and sensitive diagnosis of infectious keratitis. In this presentation, we introduce new kinds of nanoprobes featuring high fluorescence intensity (photoluminescence quantum yield, robust photostability, begin biocompatibility, good water

dispersibility as well as small size. Furthermore, the nanoprobes are employed for long-term immunofluorescent cell imaging, imaging and treatment of ocular neovascularization, imaging and photoactive killing of Gram-negative and Gram-positive bacteria. Typically, we show that long-term fluorescence imaging of vessels is enabled through a kind of fluorescent photostable probes, which feature strong fluorescence, robust photostability, lengthened blood residency and negligible toxicity. In particular, the presented nanoprobes are capable of imaging retinal capillaries in ~10 min, which is around 10-fold longer than that (~1 min) of fluorescein sodium (FS, known as the most widely used contrast agents for FA in clinic). Based on rational surface modification of the probes, targeted fluorescence detection of neovascularization could be readily realized. On the hand other, we further introduce a new kind of SiNPs-based nanotheranostic agents for bacterial keratitis prepared through modifying fluorescent SiNPs with vancomycin (Van) molecules (SiNPs-Van). Notably, the glycopeptide antibiotic of Van is capable of forming a strong five-hydrogen bond with the D-Ala-D-Ala dipeptide on the cell wall of Gram-positive bacteria (e.g., S. aureus), enabling it to prevent bacteria infection-relative eye diseases.

Keyword: Fluorescein angiography, Nanoprobes, Real-time, Long-term fluorescence imaging, Targeted detection, Bacteria infection

最终交流类型: Invited

Optical imaging probes for in vivo biomedical applications

李凯
Southern University of Science and Technology, China

The continuous or real-time tracking of biological processes using biocompatible contrast agents over a certain period of time is vital for precise diagnosis and treatment, such as monitoring tissue regeneration after stem cell transplantation, understanding the genesis, development, invasion and metastasis of cancer and so on. Recently, fluorescence imaging and photoacoustic imaging have attracted great attention, enjoying the advantage of high resolution and sensitivity. To acquire desired functional information, researchers have been dedicated to exploring novel contrast agents based on molecular engineering. For instance, it is generally considered that the large absorption coefficient at long wavelength and high nonradiative nature of contrast agents are two dominant factors to yield strong photoacoustic signals. Guided by a molecular designing mechanism, we have designed a series of semiconducting polymers with large absorption coefficient in the near-infrared (NIR) I and II regions. In addition, we have demonstrated their exciting performance in stem cell tracking, tumor detection and treatment, and precise nanoparticle delivery.[1-3] On the other hand, we also discovered that NIR light can facilitate the precise and efficient delivery of photoacoustic nanoparticles to specific tumor tissues via a transient vascular barrier opening process, which opening a new door in nanoparticle-based delivery system.[4] In this talk, the speaker will introduce recent progresses of exploring advanced fluorescence and photoacoustic nanoprobes and their biomedical application in his lab.

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Keyword: optical probe, fluorescence, photoacoustic, cell tracking

最终交流类型: Invited

Nanoparticle-assembled coacervate for biomedical applications

边黎明
华南理工大学

A key challenge for the effective treatment of gastrointestinal diseases including inflammatory bowel disease is to develop an orally administered drug delivery system capable of prolonged retention in the gastrointestinal tract. Herein we report a bioadhesive liquid coacervate based on hydrogen bonding-driven nanoparticle assembly. Free from electrostatic interactions, our fluid nanoparticle-assembled coacervate demonstrates significant pH- and salt-independent structural stability and forms a physically adhesive coating on a large surface area of intestinal tract with an extended residence time of more than 2 days to mediate the sustained release of preloaded water-soluble small molecule drugs in vivo. The orally administered drug-laden nanoparticle-assembled coacervate significantly mitigates the symptoms of inflammatory bowel disease, restores the diversity of gut microbiota, reduces systemic drug exposure, and improves the therapeutic efficacy in a rat acute colitis model compared with the oral administration of the same amount of drug in solution form. We suggest that the nanoparticle-assembled coacervate provides a promising drug delivery platform for management and treatment of numerous gastrointestinal diseases where controlled drug release with extended residence time is desired. Developing a generalizable delivery system for mediating the multimode release kinetics of diverse macromolecular drugs of varying attributes is highly desired for treating various diseases. We utilized a vacuolated coacervate, in which a dense coacervate matrix functions as a molecularly crowded barrier to regulate the release rate of macromolecules preloaded in the vacuoles. The transient disruption of the coacervate matrix by ultrasound can open the vacuoles to trigger burst release of macromolecular cargoes both in vitro and in vivo, while the liquidity of the nanoparticle-assembled coacervate (named NPA coacervate hereafter) enables the coacervate matrix to be quickly recovered in seconds upon pausing ultrasound, restoring long-term linear release of macromolecules segregated within the vacuoles. Considering the liquid and water-immiscible nature of coacervates, we believe that the concept of a “vacuolated coacervate-based macromolecular reservoir” to regulate macromolecular release kinetics can be highly instrumental in the treatment of diverse diseases.

Keyword: coacervate, nanoparticle, drug delivery

最终交流类型: Invited

Nature Biomedical Engineering--discovery and technology for improving human health

王丽倩
SpringerNature

Abstract:

This talk will give an overview of Nature BiomedicalEngineering including the coverage of the fields, editorial values, and peer-reviewprocesses. Further information on what we are looking for, and how we declinemanuscripts, together with some practical tips for writing accessibility willbe discussed.

Short biography:

Liqian conducted research in DNA nanotechnology and bioelectronics at Oak Ridge National Laboratory in Tennessee, and then at the Shanghai Institute of Applied Physics. Most recently, she developed a molecular electromechanical system based on field-effect-transistor biosensors at Fudan University in Shanghai. Liqian obtained a PhD in materials science from the University of Rome Tor Vergata in April 2016, after developing electronic devices leveraging DNA self-assembly. Liqian joined Nature Biomedical Engineering in August 2022, where she championing the contents of imaging, diagnostics and devices, and handling manuscripts in broad discipline of biomedical engineering.

Journal information:

Launched in January 2017, Nature Biomedical Engineering is an online-only monthly journal publishing original research, reviews and commentary of high significance to the biomedical engineering community, including bench scientists interested in devising materials, methods, technologies or therapies to understand or combat disease, engineers designing or optimizing medical devices and procedures, and clinicians leveraging research outputs in biomedical engineering to assess patient health or deliver therapy across a variety of clinical settings and healthcare contexts.

Straddling the life sciences, the physical sciences and engineering, Nature Biomedical Engineering aims to bring together the most important advances from the broad discipline of biomedical engineering, enhancing their visibility through opinion and news articles, and providing overviews of the state of the art in each field. The journal's scope includes materials, therapies and devices that facilitate the understanding of human disease, or lead to improvements in human health or healthcare.

Like all the other Nature-branded titles, Nature Biomedical Engineering has no external editorial board. Instead, all editorial decisions are made by a dedicated team of professional editors.

Keyword: Biomedical Engineering

最终交流类型: Oral

Dynamic Interference Nanolithography Integrated with Machine Learning for Predictive Stem Cell Fate Mapping

阳乐涛

同济大学

Nanostructures of the extracellular matrix (ECM) plays a crucial role in regulating stem cell fates. Harvesting the “outside-in” signaling between nanostructures and stem cells has thus been a highly pursued strategy in the field of regenerative medicine. However, the

systematic analysis of nano-bio interfaces has been critically restricted by a lack of creating combinatorial nanoarrays that recapitulate the complexity of natural ECM nanostructures. Additionally, how to analyze a large number of non-linear alteration of ECM structures for predictive stem cell fate mapping represents another major challenge in the field of nanobiotechnology.

To address these challenges, my research in the past has focused on the development of advanced nanolithography and big data analytics for the discovery of fundamental rules lying behind the nanostructure-based stem cell fate control. Specifically, in this presentation I will focus on the development of a dynamic interference lithography (DIL) that successfully generated one of the most comprehensive combinatorial micro/nano arrays, with sizes spanning 4 orders of magnitudes (from sub-100 nm to over 10 μm), and covering both common (e.g., dots, lines, grids) and unconventional hierarchical micro/nano structures were produced on a single centimeter-scale substrate (Yang et al. Research 2022). Remarkably, these large-scale combinatorial micro/nano arrays can be generated within a few minutes using DIL. Furthermore, by integrating machine learning-based big data analytics, the nanoarray-based high throughput cell screening platform was successfully applied for the quantitative, systematic, and predictive evaluation of biophysical cues in stem cell behavior control and cellular reprogramming (Yang et al. ACS Nano 2022). A platform like this can be broadly applied to investigate many different types of cell-material interactions and has not been lacking so far. Cell-specific biomaterial design for enhancing phenotypes of patient-derived induced pluripotent stem cells, will also be demonstrated using our screening platform in this presentation.

Keyword: Nanolithography; Cell mapping; High throughput screening; Stem cell; Machine learning

最终交流类型: Invited

Design of Magnetic-Optical Nanoprobes for Precise Imaging in vivo

宋国胜

Hunan University, China

In the field of biomedical imaging, in vivo imaging technologies play an increasingly important role in early disease diagnosis, drug screening, and treatment evaluation, making it an important research direction in chemical metrology. In order to obtain a more realistic understanding of disease mechanisms and treatment processes, it is urgent to develop advanced in vivo imaging technologies for real-time, dynamic, whole-body, long-term, and holistic studies of pathological processes at the in vivo level. However, there are many challenges involved in imaging research at the in vivo level, such as the inability of most imaging signals to penetrate thick biological tissues (such as bone and muscle), low concentrations of biomarkers involved in biological events, and extremely complex microenvironments within the body. To address these issues, (1) we have developed highly sensitive alloy magnetic particle probes and proposed a new method of magnetic susceptibility modulation for MRI imaging. (2) We have developed a significantly enhanced long-lived luminescence imaging strategy based on electron transfers and achieved long-lived luminescence imaging of free-moving animals for the first time. (3) We have developed a new technology for in situ monitoring of magnetic-optical multimodal functional imaging in vivo, providing a powerful tool for studying the dynamic evolution of the tumor immune microenvironment and evaluating early treatment efficacy.

Song, G*.; Zhang X.* et al. Electron Transfer based Ultra-bright Organic Afterglow Nanoprobe for Accurate Molecular Imaging in Mice Nature Biomedical Engineering 2023 in press

Song, G*.; Rao, J.* et al. FeCo nanoparticles as ultrasensitive magnetic-particle-imaging tracers with photothermal and magnetothermal properties. Nature Biomedical Engineering 2020,4, 325.

Yue R.; Song, G.* et al; Dual key co-activated nanoplatform for switchable MRI monitoring accurate ferroptosis-based synergistic therapy, Chem, 2022, 8: 1956

Guan G; Song, G.* et al; Ternary Alloy PtWMn as a Mn Nanoreservoir for High-field MRI Monitoring and Highly Selective Ferroptosis Therapy. Angew. Chem. Int. Ed. 2022, 61: e2021

Zhang X*.; Song, G.* et al ; “Four-In-One” Design of a Hemicyanine-Based Modular Scaffold for High-Contrast Activatable Molecular Afterglow Imaging, JACS, 2023, 145: 5134

Keyword: Precise Imaging, Nanoprobes, MRI, luminescence imaging

最终交流类型: Invited

Building Cu ion activity center for Catalytic Anti-Biofilm

周云龙
国科温州研究院

Biofilms are often associated with human bacterial infections, and the natural tolerance of biofilms antibiotics challenges clinical enterprise. According to the National Institutes of Health of the USA (NIH), bacterial biofilms are associated with over 80% of chronic bacterial infections. Currently, strategies to treat biofilm infections include physical debridement and chemotherapy. However, neither physical nor chemical treatment can effectively kill bacteria or inhibit the adhesion of bacterial debris, thereby resulting in poor prevention of bacterial biofilm formation on the surface of the wound or other areas.10−11 Therefore, an ideal strategy to inhibit the formation of bacteria biofilm should be able to strongly inhibit bacterial adhesion and effectively kill bacteria. Recently, Fenton-like nanocatalysts, an emerging antimicrobial strategy, have exhibited plenty of advantages (e.g., broad-band antimicrobial ability, low toxicity, and lack of resistance) in anti-biofilm therapy. However, the catalytic performance of Fenton-like type nanocatalysts is largely dependent on the oxidation states of catalytic centers and biofilm microenvironment.

Bacteria use intense respiration during mass reproduction, producing numerous bacterial extracellular electrons. Therefore, it is feasible to build a microbial fuel-like self-powered system that ideally facilitates the extraction of charges and the fast charge conversion between different oxidation states of the active center to exert ROS production and elimination. Here, we self-organized Cu ion with graphene oxide-Bacteria composite via cation-π interaction to self-activate the bacterial extracellular electrons, which initialize the self-powered Fenton-like cascade reaction, dynamically inhibiting biofilm formation in situ. Specifically, the non-conductive water-soluble graphene oxide was in situ reduced to conductive reduced graphene oxide by absorbed bacteria and finally produced an electrochemical bioactive nanocomposite. Then, Cu2+"stapling" bioactive nanocomposite in situ through cation–π interaction between Cu2+ and BrGO. Among them, the formation process of bioactive nanocomposite not only consumes the highly expressed GSH in the biofilm but also increases the local electron density to assist in the reduction of Cu2+. The fast conversion of Cu2+ /Cu+redox coupled with BrGO-Cu facilitates the whole Fenton-like process. Moreover, the BrGO with redox activity can provide extracellular electrons to oxygen to supply H2O2, further providing continuous power for the reaction process. In addition, BrGO-Cu dynamically responds to the microenvironment of live bacteria to enhance the anti-biofilm therapeutic effect by Fenton-like cascade catalysis and restrict bacterial resistance both in vitro and in vivo.

Keyword: Antibacterial biofilm; Bacterial extracellular electrons; Cu ion;

最终交流类型: Keynote

An acid degradable linker that rapidly hydrolyzes in the endosome enhances the delivery of lipid nanoparticle/mRNA complexes in vivo

Niren Murthy
University of California at Berkeley

Acid degradable linkages (ADLs) have the potential to significantly impact the field of drug delivery and have been intensely investigated. ADLs can target the mildly acidic pH of tumors, endosomes and sites of inflammation, and have been used to engineer endosomal disruption in a variety of gene carriers, trigger drug release in endocytosed antibody/polymer conjugates, and trigger drug release in tumors. These pioneering studies have demonstrated the great potential of ADLs and their numerous potential applications.

Although ADLs have great promise, a key limitation of existing ADLs is their inability to rapidly hydrolyze at the pHs of 6.0-6.8. Developing ADLs that rapidly hydrolyze at mildly acidic pHs is challenging because of their instability, and performing multi-step organic synthesis or aqueous solution chemistry with them is challenging. ADLs that are compatible with aqueous solution chemistry have wide applications because the vast majority of drug delivery vehicles, ranging from lipid nanoparticles (LNPs) to antibody drug conjugates, are formed or synthesized in aqueous solutions. ADLs currently hydrolyze on the timescale of days at the pHs of 6.0-6.8, and delivery vehicles made with them are consequently trafficked to lysosomes and degraded there. In addition, delivery vehicles made with current ADLs are also inefficient at targeting tumors or sites of inflammation. ADLs are also challenging to use for generating antibody drug conjugates because they hydrolyze too slowly in the lysosome to generate therapeutic concentrations of the drug.

In this presentation we present a new ADL based on an acetal, which rapidly hydrolyzes at endosomal pHs but has exceptional stability at pH 7.4. The acetal linker has a hydrolysis half-life of days at pH 7.4 and can be conveniently synthesized and incorporated into delivery vehicles. However, it hydrolyzes with a $t_{1/2}$ of less than 15 minutes at pH 6.0 and rapidly degrades in endosomes. We show here that the acetal linker can generate acid degradable analogs of lipids used in LNP formulation and can significantly improve the transfection efficiency of lipid nanoparticle/mRNA complexes in cells and in mice. LNP/mRNA complexes containing acid degradable lipids were able to deliver mRNA efficiently to either the liver, lung or spleen of mice and also to HSPCs in vitro and with significantly higher efficiency than conventional LNPs. The acetal linker has the potential to solve the instability problems associated with using unstable ADLs and has numerous applications in drug delivery.

Keyword: Lipid nanoparticles, mRNA delivery

最终交流类型：Invited

Needle-free delivery of immunotherapeutic antibodies

陈倩
Soochow University，China

Recent studies in cancer immunotherapy have demonstrated great therapeutic responses by educating and awakening patients' own immune system to attack cancer. Immune checkpoint blockade represented by anti-CTLA4 and anti-PD1/PDL1 has brought new hope to cancer patients, and achieved amazing results in various solid tumors. However, protein drugs especially antibodies usually have large molecular sizes and complex structures, and they are fragile in complex physiological environments. Moreover, antibodies could hardly penetrate various biological barriers such as mucosal barriers and skin barriers. Thus, immune checkpoint blocking antibodies are mainly administered intravenously, which not only limits their clinical application, but also causes immune-related side effects in normal tissues. In recent years, we developed several platforms based on chitosan or modified chitosan for pulmonary, topical or oral delivery of macromolecular drugs.

Firstly, we developed an inhaled chitosan-immunotherapeutic antibody complex for immunotherapy for lung cancer treatment. In this system, chitosan is used as a delivery vector of anti-programmed cell death protein ligand 1 (aPD-L1) to achieve efficient transmucosal delivery. In addition, we have found that chitosan can trigger immune responses by activating cyclic-di-GMP-AMP synthase (cGAS)-stimulator of interferon genes (STING) pathway. Then, we found that fluorocarbon modified chitosan (FCS) could act as an innovative transmucosal carrier for effective oral delivery of immune checkpoint antibodies. FCS could promote the transmucosal delivery of the protein drugs by inducing temporary rearrangement of tight junctions between intestinal epithelial cells. Under the dose of five times the conventional intravenous delivery, the FCS-based oral delivery of anti-programed cell dealth 1 (anti-PD1) could achieve therapeutic effects comparable to that achieved with i.v. injection, with significantly reduced immune related side effects. Inspired that these nanocomplex could facilitate the transmucosal or transdermal delivery of various proteins including antibodies for immunotherapy, we further systematically studied the effectiveness, safety and mechanism of chitosan-based platforms and explored its potential to deliver various macromolecular drugs.

Keyword: immunotherapy, needle-free, antibodies

最终交流类型: Oral

Regulation of biological fate of nanomaterials by the chiral-mediated protein corona

Didar Baimanov
Institute of High Energy Physics, CAS

Chirality has a key role in the synthesis of biomolecules and the development of life. It is well known that most biomolecules are chiral and attain stereospecific interactions in different biological processes attracting interest on the “chiral self-sorting” principle. However, from a biomedical aspect, chiral nanomaterials are still rarely explored or understood, and those that are used usually obtain their chirality from chiral molecules. These chiral surface modifications usually have the leading role in regulating biological processes mediated by protein corona, consequently covering up and/or emphasizing the stereoselectivity. Therefore, we studied how chirality mediates the formation of stereoselective coronal fingerprints that in turn leads to a varied *in vivo* tissue distribution and *in vitro* cellular recognition of mirrored nanoparticles. Herein, we developed a novel *in situ* “Fishing” method allowing us to determine the dynamic evolution of protein corona, and isolate soft/hard coronas on chiral nanoparticles. We observed the formation of several simultaneous corona layers due to altered binding affinities with nanoparticles and/or neighboring proteins. We concluded that re-modeling and dynamic evolution of coronal composition, *i.e.*, dysopsonins and opsonins, at the nano–bio interface is the key to regulating the varied biodistribution and recognition of chiral nanoparticles. Additionally, to determine the influence of surface chirality on the function of coronal proteins, we performed a model study with chital gold nanoparticles. Interestingly, we observed that functionality of lipoproteins, *i.e.*, apolipoprotein AI and E, altered on mirrored nanoparticles acting as dysopsonin or opsonin. Thus, we believe that understanding chirality translation from mirrored nanoparticles to biomolecules in vivo could greatly improve the targeting efficacy of nanomedicine. Taken together, these findings might partially explain the nature of chirality-mediated biological processes. Our study aims to lay a foundation for elucidating the routes and reasons for chirality-dependent tissue and cell targeting to deepen understanding the nature of stereoselectivity.

Keyword: protein corona, chiral nanoparticles, stereoselective fingerprint, nano-bio interface, biodistribution

最终交流类型: Invited

Publishing with Wiley Chemistry Journals

金娟

Wiley, China

In this talk, firstly I will give a brief introduction to Wiley chemistry journals including Angewandte Chemie, a journal of the German Chemical Society (GDCh) and journals published on behalf of Chemistry Europe and Asian Chemical Editorial Society (ACES). I will focus on some recent developments at Angewandte Chemie, including preprints, faster speed, authors' choice, open access, advisory editors, appeal policy, new author profile, and so on. We believe that such developments would make Angewandte Chemie an inclusive home of excellent chemistry. From the introduction, you would know better the history, scope and requirements of our Wiley chemistry journals and the transfer cascade among them, which will help your papers to be published in the most suitable journals.

Then I will introduce the Wiley chemistry team in China and the WeChat platform. Currently, there are several chemistry editors and journal publishing managers based in Shanghai and Beijing, China. Wileychem, the official platform for Wiley chemistry journals in China, was launched in June 2021 and has attracted more and more followers. Via Wileychem, you would read summary highlights of recently exciting papers published in Wiley chemistry journals, interviews of active chemists, important news at Wiley and Wiley chemistry journals, interesting chemistry stories and so on. All of you are very welcome to follow and contribute content to Wileychem.

In the end, I will bring up some tips on writing and submitting papers from the aspect of an in-house editor. I will show how we pre-screen a submission, including duplication submission and plagiarism detection. I will then explain how we read a submission, decide to send a submission out for peer review and choose reviewers. I will also explain how we make a decision and give some suggestions on revision or rejection. More importantly, I will talk about some ethical issues, like the responsibilities of authors, reviewers, and editors.

Keyword: Angewandte Chemie; Chemistry Journals; Writing Skills

最终交流类型: Invited

Nanorepair Medicine

倪大龙
上海交通大学

Organ injury, such as acute kidney injury, ischemic stroke, and osteoarthritis, often results in complications that can be life-threatening or even fatal. There exist many types of organ injury, such as acute kidney injury, ischemic stroke, spinal cord injury, among several others. These injuries sometimes share similar disease characteristics such as activated inflammatory microenvironment and oxidative stress. Despite some similarities in pathogenesis, each organ injury type has their own unique underlying pathological processes that are intricate and not well-understood. These complexities may therefore cause difficulties in clinical treatment applications, resulting in low therapeutic efficacy and poor patient outcome. Given the limitations, recent efforts have been devoted to developing effective detection, prevention, and treatment methods, most of which are based on the use of nanomaterials with novel chemical compositions and tunable physicochemical properties.

Recently, many nanomaterials have emerged as promising repair agents for various organ injuries. Our lab focuses on the field of nanomaterial-based repair medicine and (abbreviated as “nanorepair medicine”) by synthesizing new nanostructures and synergetic strategies for repairing acute liver/kidney/lung injury, inflammatory bowel disease, osteoarthritis/osteoporosis, etc., and revealing their repairing mechanism in vivo. Our lab has proposed “Nanorepair Medicine” as a branch of nanomedicine, which is an emerging cross-disciplinary field that intends to explore the applicability of nanomaterials for the repair of organ injuries. Nanorepair medicine encompasses three interrelated research emphases: detection, prevention, and treatment of organ injuries using nanomaterials. We will briefly introduce our studies on repairing acute liver/kidney injury, inflammatory bowel disease, and osteoarthritis/osteoporosis. We then give some examples of applying different strategies to repair organ injury, including scavenging reactive oxygen species (ROS) directly, scavenging ROS combined with gene therapy, and regulating immune microenvironment of injured organs. Finally, we offer our perspectives on current challenges as well as expectations for future advancements of nanomedicine designed for organ injury repair.

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Keyword: Nanomaterials, reactive oxygen species, organ injury

最终交流类型: Invited

Separation Strategy, Photoluminescence Mechanism and Bio-Imaging Analysis of Units-Emitting Carbon Dots

夏云生
安徽师范大学

Carbon dots (C-dots) are an emerging carbon material with size below to 10 nm. In addition to small size and compact structure, C-dots possess multiple appealing properties including metal-free composition, highly bright and wavelength tunable fluorescence, as well as excellent biocompatibility. So, they have attracted considerable attention in the fields of biomedicine, photo- and electro- catalysis, optoelectronic devices, and so on. To date, great achievements have been made in C-dots fabrication and application. In contrast, understanding the relationship between their composition/structure and property, for example the photoluminescence mechanism, bio-toxicity origin and catalytic active-site, cannot obviously follow the pace. One of primary obstacles is lack of effective means for C-dots' separation and purification. As a result, the characterization data from inadequately purified samples would inevitably cause inaccurate and even false conclusions, resulting in significant barriers to revealing their true nature.

Here, we present a combination separation strategy: First, the crude C-dots products are extracted for coarse separation; then, fine separation is conducted by using preparative thin layer chromatography for adequate purification. On this basis, we propose a "unit-emitting" photoluminescence mechanism for C-dots emission based on experiments and theoretical calculations: each C-dot surface contains multiple conjugated polyaromatic rings with a consistent structure as emitting units. Due to strong brightness of single particle photoluminescence, anti-photobleaching, high signal-to-noise ratio and selectivity, as well as instant signal response and output, the unit-emitting C-dots have great advantages for real-time and dynamic bio-imaging applications.

Keywords: Carbon Dots, Emitting-Units, Photoluminescence Mechanism, Bio-Imaging

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最终交流类型：Invited

Hypoxia-Responsive Host-guest Drug Delivery System

郭东升
南开大学

A host-guest drug delivery system (HGDDS) refers to a complex formed by an artificial receptor and a therapeutic agent which can dissociate at the lesion site and release the loaded cargo. Macrocyclic receptors including cyclodextrin, calixarene, cucurbituril, and pillararene, have been widely used as drug carriers to construct HGDDSs. They own the precise molecular weights, well-defined structures, exact drug loading pattern and quantifiable binding constants, which provide a theoretical feasibility to construct DDSs with the good batch-to-batch reproducibility. However, from the viewpoint of practical application of HGDDSs, a macrocyclic carrier is expected to meet the following demands: 1) high binding affinity for therapeutic agent with selectivity to biologically coexisting interferents, to prevent off-target leaking; 2) broad-spectrum encapsulation capability to make it appealing in personalized medicine, where the same carrier could be utilized in delivering different drugs alone or in combination; 3) stimuli-responsiveness to fulfil the controlled release targeting the assigned lesion.

Calixarene, representing the third generation of supramolecular hosts, is one kind of macrocycle comprising phenolic units linked by methylene groups at positions 2 and 6. Significantly, it is highly modifiable, making it an ideal receptor for tailored binding. Using calixarene as the core framework, we developed a series of azocalixarenes to construct hypoxia-responsive HGDDSs. Azocalixarenes possess deepened cavities, which helps to obtain high binding affinities towards therapeutic agents. The azo group can be specifically reduced under hypoxic microenvironments, a salient feature of many diseases, which confers the HGDDS with hypoxia-triggered release due to the remarkable decrease in affinities following reduction. The fast release kinetics further facilitates the efficient accumulation of drugs at the lesion site. These azocalixarene-based HGDDSs have been applied in diagnosis and treatment of several diseases including tumor, bacterial infection, kidney injury, and inflammation.

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Keyword: drug delivery, hypoxia, supramolecular chemistry, host-guest recognition, calixarene

最终交流类型: Invited

Intracellular polymerization and self-assembly for supramolecular approach to control cellular fate

Ja-Hyoung Ryu
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Cancer is a leading cause of death worldwide. The endeavor efforts to cure the cancer have been made to develop cytotoxic chemotherapy, targeted chemotherapy, to immunotherapy. However, the cytotoxic chemotherapy has severe side effects to kill healthy normal cells, and targeted chemotherapy which inhibits specific cancer proteins has a drug resistance problem, and immunotherapy is only applicable for limited patient. Therefore, it is highly demanded to develop a new paradigm of cancer therapy. Our research team has focused the efforts on the development of new cancer therapy using supramolecular approach through molecular design based on the knowledge of supramolecular chemistry. The polymerization-induced artificial assembly of synthetic building units inside a living cell and the interaction of these assembly with the cellular components have rarely been studied, but are emerging as an intriguing strategy to control cellular fate. Recently, we developed intra-mitochondrial polymerization induced self-assembly (Mito-PISA) strategy for constructing polymeric structures by ROS-dissipative system. Targeting mitochondria, the vital organelle for cell survival, has been recognized as an efficient strategy in different therapeutic techniques by disturbing the normal function. Recently, we reported that intra-mitochondrial assembly induced the dysfunction of mitochondria by disrupting the membrane, resulting in the selective apoptosis of cancer cells. In addition, we described a mitochondria-targeting biomineralization system that favorably can induce silicification and consequent apoptosis of various cancer cells. Herein, we report that the in situ disulfide polymerization inside mitochondria is based on both large accumulation of monomers (increased local concentration for polymerization) and high ROS environment (chemical fuel for disulfide reaction). During the polymerization in a mitochondrial reducing environment, the autocatalytic process enables the continuous generation of ROS and the construction of bulky structures for mitochondrial dysfunction. This in-situ polymerization shows great potential for anticancer treatment against various cancer cell lines including drug resistant cancer cell. To the best of our knowledge, this is the first example showing intracellular polymerization to cause mitochondrial dysfunction and these findings can provide a new insight into intracellular polymerization and assembly for the regulation of cellular functions and a therapeutic approach and new targeting platform for the biomedical community.

Keyword: Supramolecular therapy, self-assembly, intracellular polymerization

最终交流类型: Invited

Nanocatalytic immunotherapy

胡萍
上海硅酸盐研究所

The burden of cancer incidence and mortality is rapidly growing worldwide, which reflects both aging and growth of the population, presents great demand for new technologies for effective treatment. Immunotherapy, in which the patient's own immune system is trained to recognize and destroy tumor cells, has shown great promise in treating patients with the primary tumor and metastatic tumors. Unfortunately, The immune system is largely counteracted by their immunesuppression function of most solid tumors.

In recent years, our group attempted to reactivate the anti-tumor immune effect and reverse tumor immune suppression by specific catalytic reaction of nanomaterials response to tumor microenvironment. For example, i) a nanocatalytic medicine (MSN-Ru^{2+}/Fe^{2+}, MRF) is constructed to induce oxidative damage in the mtDNA of tumor cells by Fenton reaction. Such an oxidative mtDNA is able to escape from the tumor cells and acts as an immunogenic damage-associated molecular pattern to M1-polarize tumor-associated macrophages (TAMs), resulting in the reactivated immunoresponse of macrophages against cancer cells. ii) Nanocatalytic bacteria disintegration by Fenton reaction in a magneto-thermal environment, and reverses immunosuppression of colorectal cancer. iii) A mild magnetocaloric regulation approach using a magnetogenetic nanoplatform MNPs@PEI-FA/pDNA (MPFD), which is synthesized by loading a heat-inducible plasmid DNA (HSP70-IL-2-EGFP) on polyethyleneimine (PEI)- and folic acid (FA)-modified $ZnCoFe_2O_4$@$ZnMnFe_2O_4$ magnetic nanoparticles (MNPs) was proposed, to promote the proliferation and activation of tumor-infiltrating NK cells under magnetic manipulation without limitation of penetration depth for orthotopic liver cancer immunotherapy. Based on these findings, nanocatalytic immunotherapy presents a greatly desirable prospect in the solid tumor immunotherapy in clinics.

Keyword: solid tumor；nanocatalytic immunotherapy；innate immune，chemical reaction.

最终交流类型：Invited

Biofuel cell self-powered electrochemical biosensor for disease warning and treating

朱俊杰
南京大学

Biofuel cell self-powered biosensor (BFC-SPB) represents an external-energy-equipment-free sensing system which is capable of continuously providing precious quantitative analytical information of various analytes according to the change in the output of BFC.[1] Recently, we focused on designing novel BFC-SPBs to realize the efficient disease early warning and timely treating. We developed the first ultra-sensitive self-powered cytosensor for the detection of acute leukemia CCRF-CEM cells, pioneering the application of BFC-SPB in cancer diagnosis. [2] To further multiply the detection target and improve the reliability, we also succeeded in constructing a self-powered system which could quantify two types of cancer-related biomarkers (miR-21 and miR-141).[3] And then, we developed a highly integrated self-powered sensing system by combining the BFC-SPB and the membrane separation technology. This sensing system could separate and detect the exosomes and host cancer cells in a damage-free and time-saving approach, which was beneficial for the disclosure of the growth state or even more detailed biology information of tumor. [4] To advance the application of BFC-SPB in disease treatment, we have devised a high-compact and self-sustained theranostic platform which possessed triple cascaded “diagnosis-therapy- therapeutic evaluation” functions. The presented platform hints a sustainable cross-link between BFC and advanced theranostic, further offering guidance towards adjusting the preclinical medication to achieve preferable personalized medicine at an economical cost.[5] Considering that the above BFC-SPB has not realized the efficient therapy in vivo, we designed a self-powered and drug-free diabetic wound healing patch, based on the enzyme protection strategies we have proposed.[6] This self-powered patch could synergistically regulate the local hyperglycemia, break the limitations of insufficient ROS caused by low H2O2 levels, and realize precise sterilization. Thus, it could significantly accelerated chronic wound healing in vivo. It is believed that our research on BFC-SPB will provide a new approach for disease warning and precisely regulating.

Keyword: Biofuel cell, Self-powered, Electrochemical biosensor, Disease warning, Therapy

最终交流类型: Invited

Afterglow Bioapplication by Utilization of Triplet Excited States of Organic Materials

李倩倩
Wuhan University

Organic room temperature phosphorescence materials with ultralong lifetime possess the remarkable advantage in bioimaging for elimination of background noise by characteristic time scale. However, most of RTP luminogens need to be excited by the harmful UV lamp, and exhibit green or yellow emission with shallow tissue penetration, constraining the in vivo bioimaging for further application in clinical diagnosis and pathological study. Recently, the much safer excitation process by sunlight and mobile phone flashlight is realized by organic luminogens with various electronic pull-push systems. Moreover, the bright red RTP emission with lifetime up to 344 ms is achieved by optimizing molecular geometry and electronic property. Especially, the mobile phone flashlight excited red afterglow imaging of lymph nodes in living mice has been realized for the first time, affording a safe and conventional approach to achieve the afterglow imaging of living mice with deep issue penetration and high signal-to-noise ratios. Moreover, we demonstrated a phosphorescence imaging method by organic nanoparticles to detect early tumor metastasis progress with microenvironmental changes, putting the detection period ahead to the formation of secondary tumors. In the orthotopic and simulated hematological tumor metastasis models, the microenvironmental changes could be recognized by phosphorescence imaging at Day 3, after tumor implantation in liver or intravenous injection of cancer cells. It was far ahead those of other reported imaging methods with at least 7 day later, providing a sensitive and convenient method to monitor tumor metastases at the early stage.

Keyword: afterglow bioimaging, room temperature phosphorescence, organic materials, nanoparticle

最终交流类型: Keynote

Robust Homooligomeric Self-Assembly of RNA Tiles: From Design to In Vivo Assembly

Yossi Weizmann
Ben-Gurion University of the Negev

Homooligomerization, the self-assembly of a single chemical species into larger structures, is a prevalent strategy in biological systems. However, designing artificial homooligomeric systems with the structural diversity and complexity comparable to those found in nature has proven challenging. In this study, we introduce a robust and versatile self-assembly system based on RNA tiles folded from a single-strand of RNA, which can be generated both in vitro and in living cells. Leveraging advances in structural DNA and RNA nanotechnology, nucleic acids offer an ideal platform for designing homooligomeric structures. However, previous composite structures made from different types of single strands posed challenges in maintaining accurate stoichiometry and integrity. To address this, we employ a natural linear RNA motif, the kissing loop (KL), and engineer a branched, three-helix motif known as the branched kissing loop (bKL). This modification enhances the bKL's versatility, enabling the creation of diverse homooligomeric structures.

One of the key highlights of this work is the cotranscriptional folding and assembly of bKL-based tiles during RNA synthesis. This feature not only allows efficient folding but also suggests the potential for in vivo self-assembly of RNA tiles into target structures. To demonstrate this compatibility, we integrate bKL-based tiles with RNA aptamers and a tRNA scaffold, enabling their stable expression in living cells. Overall, our findings showcase the robustness and potential of RNA tiles as a self-assembly system. By utilizing single-stranded RNAs, which can be readily produced by cells, we pave the way for large-scale production of artificial structures and their potential application in various fields, including nanobiotechnology, Imaging, and synthetic biology.

Keyword: Self-Assembly; DNA Nanotechnology, RNA

最终交流类型: Invited

Ultrasensitive biorecognition through bio-responsive self-assembling biomolecules and multifunctional nanointerface

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东南大学生物科学与医学工程学院，数字医学工程全国重点实验室

The ultrasensitive biorecognition for the early diagnosis / monitoring of some important disease like cancers has attracted much attention in the relevant fields, especially as a hot topic in the areas involving in patient care and treatments. In this study, we have explored the possibility of the application of some biomolecular probes combining with the bio-responsive

self-assembly nano-scaled agents in targeting bio-recognition and high-sensitive biosensing / bioimaging of the diseased locations. Especially, we have developed some novel strategies for the rapid imaging and highly sensitive recognition of the targeted biomolecules and cancer cells / exosomes by combining the active agents and functionalized nanointerfaces for multiscale theranostics. Our observations demonstrate that the in situ self-assembly of the specific biomolecules with the nano-probes could provide a multifunctional interface for the rapid identification and precise imaging of cancer cells / exosomes, with a broad detection range and low detection limit. It is evident that different types of cancer cells or bacteria could be readily distinguished on the bio-responsive spectra-electrochemical nano-interfaces, which have the promising application to be adopted as a significant way to detect various kinds of mutant cells / tissues or related exosomes in vivo and advance the clinic diagnosis and treatment of some important diseases like cancers. Moreover, some ultrasensitive and intelligently multi-functional nanoscale biomarkers based on the in vivo bio-responsive self-assembly of bio-synthetic nanoclusters through utilizing the peculiarities of the microenvironment and relevant redox homeostasis from cancer cells or bacteria have been also explored for the real-time multi-scale monitoring and multi-modality / or panoramic imaging of cancer cells and relevant exosomes as well as affected tissues for precise theranostics.

Keyword: precise theranostics bio-responsive multifunctional nanointerface

最终交流类型: Keynote

Novel Synthetic Techniques for Catalyst Design

Il-Doo Kim
KAIST,Korea

Electrocatalysts play a crucial role in the fields of sensors, energy, and the environment. Research on the synthesis and application of catalysts with various shapes, sizes, and compositions is currently underway. Our research team is actively engaged in the synthesis of single-atom catalysts, bimetallic, high-entropy alloy, and polyelemental alloy catalysts, as well as the development of sensors and Li-air batteries. Particularly, we have been conducting interesting research on catalyst design using the Joule heating process and photo-induced optical sintering process for novel catalysts design. The Joule heating process is a technique for producing multi-metal catalysts-decorated conducting carbon fibers. The photo-induced process utilizes a xenon flash lamp to rapidly produce multi-metal catalysts within a few tens of milliseconds. Another interesting catalyst design technique that has recently received significant attention is the exsolution catalyst synthesis method. This technique involves the exsolving of elements doped within the lattice of oxide support to the surface of a material via a reduction heat treatment process. The catalyst is strongly anchored to the oxide support, providing excellent durability. In this presentation, I will also introduce the exsolution process as a new catalyst synthesis method. In this presentation, I will discuss and introduce our new catalyst synthesis techniques and methods for designing high-efficiency chemical sensors through catalyst design.

Keyword: Sensor, Catalyst, Thermal Shock Synthesis

最终交流类型: Oral

Nanoprobes for Bacterial Optical Imaging and Therapy

王后禹
苏州大学

The reporter focuses on the sensor/probe design for capturing/targeting different bacteria to achieve imaging analysis and treatment of different bacteria [1-5]. The authors proposed the first "bacterial probe swallowing" imaging strategy, which uses bacterial-specific transporter proteins to transport glucose polymer-modified probes into the bacterial cell interior. Unlike conventional probes targeting the bacterial cell wall, the payload of the probe entering the bacterial cell interior is relatively higher than that of the probe targeting the bacterial cell wall, resulting in a high imaging sensitivity that can detect different bacteria at concentrations as low as ~10^5 CFU at the in vivo level, which is about two orders of magnitude more sensitive than most bacterial contrast agents. In terms of in vivo therapeutics, most of the currently reported bacterial nanodrug delivery systems are still loaded on the bacterial surface, and in addition to the relatively low drug loading, bacterial surface modification of nanomaterials may negatively affect the function or activity of bacteria. Based on the strategy of "bacterial swallowing probe", the reporters have developed the "Trojan" bacterial nano-drug delivery system, which can effectively target deep tumor tissues in vivo through the specific colonization and penetration ability of bacteria, and realize the deep tumor tissue treatment. The work will contribute to the development of a new approach to deep tumor therapy.

Keyword: bacteria, nanoprobe, imaging, therapy

最终交流类型: Invited

Interaction between Carbon Nanotube and Pulmonary Surfactant Monolayer: Role of Aggregation State and Contaminant Presence

胡国庆
浙江大学

With the increasing use of carbon nanotubes (CNTs), the potential impact on human health, particularly in the respiratory tract, is becoming an area of increased focus. The tiny dimensions of CNTs allow them to infiltrate the deep recesses of the lung where they inevitably interact with the pulmonary surfactant (PS) monolayer, potentially disrupting the biophysical properties of the monolayer.

Our primary investigation revolves around exploring the regulation of these interactions by the aggregation state of the CNTs using coarse-grained molecular dynamics simulations. We found that, compared to their dispersed counterparts, aggregated CNTs induce more significant structural perturbations in the PS monolayer during both compression and expansion stages. The increased lipid perturbation around the CNTs is attributed to their increased diameter, initial interaction angle, and irregular configurations when aggregated. This disturbance promotes pore formation on the PS monolayer under high surface tension conditions, resulting in inhibition of the biophysical function of the PS monolayer. Consequently, aggregated CNTs become difficult to remove from the monolayer. These findings suggest that aggregated CNTs pose a potentially higher risk of respiratory nanotoxicity compared to dispersed CNTs.

Our secondary work, which complements the primary work, focuses on the interaction of CNTs with the PS monolayer in the presence of other contaminants, such as benzo[a]pyrene (BaPs). Using passive dosing and fluorescence techniques, we demonstrate the partial solubilization of BaPs adsorbed on CNTs by PS in a simulated alveolar fluid. Furthermore, molecular dynamics simulations help to elucidate the interaction dynamics between BaPs, CNTs and PS. We identify two opposing effects of PS on CNT toxicity - on the one hand, corona formation by PS reduces CNT toxicity by decreasing their hydrophobicity and aspect ratio. Conversely, the interaction with PS increases the bioaccessibility of BaP, potentially enhancing the inhalation toxicity of CNTs.

Keyword: carbon nanotube, pulmonary surfactant, molecular dynamics simulation, aggregation, contaminant

最终交流类型：Invited

Tumor Microenvironment-mediated Nanoplatform for Cancer Theranostics

程亮
苏州大学

Cancer therapy has become a worldwide problem and hot topic, and every year lots of people will suffer from various kinds of cancer. With the development of nanotechnology and novel functional nanomaterials, some new type of cancer therapy methods has been developed successfully, such as phototherapy, sonodynamic therapy. Tumor microenvironment (TME), which consists tumor cells, many other types of cells, cytokines, small molecules, and abnormal blood vessels, is considered a complex internal environment for the occurrence and development of tumors. In recent years, great progress has been made to regulate these various micro-environmental hallmarks such as hypoxia, acidic pH, high H2O2, and GSH levels, vascular malformations and so on. Utilizing the unique physical and chemical properties, various kinds of inorganic nanomaterials have been used for cancer therapy [1-6]. Herein, I will briefly introduce functional transition metal complex nanomaterials (for example, transition-metal dichalcogenides, transition metal carbides, transition metal oxides, and metal coordination nanocomplex) for cancer imaging and therapy. Then, I will talk about some methods to tune the TME and enhance cancer therapy. Last, I will give some information about the clearance behavior of inorganic biomaterials for cancer theranostics. Therefore, our work highlights the promise of functional inorganic nanomaterials for biomedical applications.

Keyword: Bioactive materials, metalloimmunotherapy, tumor microenvironment, sonodynamic therapy, toxicity

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最终交流类型：Invited

Aggregation based skin decontamination agent for uranium

第五娟
苏州大学

Efficient skin decontamination technique is indispensable to mitigate the external contamination of radionuclides for people in case of nuclear accidents. Current decontamination products show limited decontamination efficiency and transcutaneous uptake inhibition ability, as well as lack of real-time monitor of decontamination effect, which may lead to the overuse of cleaning products and produce large volume waste solution. Herein, a bidentate ligand 3-hydroxypyridin-2(1H)-one (3, 2-HOPO) were attached to the surface of the carbon quantum dots (CQDs) to obtain the nano composite of CQD-3, 2-HOPO. Taken the advantage of effective uranyl chelation by 3, 2-HOPO ligands, the CQD-3, 2-HOPO material could rapidly and selectively complex with uranyl ions, resulting in sufficient removal of uranyl from contaminated skin. Meanwhile, this new material with a pristine size of 2 - 4 nm could rapidly aggregate to 300 - 500 nm or even micron level after the complexation of uranyl, which is beneficial in preventing the transcutaneous uptake of uranyl. Moreover, the fluorescence intensity of the CQD-3, 2-HOPO decreases with the increase of uranyl concentration, which enables the detection of decontamination efficiency in real-time. In conclusion, the nanocomposite of CQD-3, 2-HOPO features high uranyl decontamination efficiency, sufficient inhibition of transcutaneous uptake, as well as real-time display of the decontamination progress, rendering it a new generation of radionuclide decontamination agent.

Keyword: Skin decontamination, Uranyl, Nanomaterial

最终交流类型：Oral

Molecular Targeting Nanomaterials

李洋

中国科学院深圳先进技术研究院

Currently, the clinical approved nanomedicines are mainly the delivery systems such as nano-carriers. To develop the nanomedicine that specifically targeting the biomolecules for disease treatment is still a challenge. Such molecular targeting nanomaterials should be studied like small molecule chemical drugs, which clearly evaluates their molecule-targets and reveals their binding sites with a purpose to disclose the potential biological/immunological/pharmacological mechanisms. Therefore, the development of molecular targeting nanomaterials should be focused on exploring their intrinsic and specific biological properties, which could easily pave the way for future clinical translation. Such molecular targeting nanomaterials, in parallel with nano-carriers drugs, could be called as nano “core” drugs.

We have discovered two nanomaterials that could specifically/selectively target biomolecules for disease treatments, black phosphorus (BP) and CuInP2S6 (CIPS) nanosheet.

BP could be used as DNA checkpoint inhibitor to specifically target and inactivate the PLK1 kinase, which consequently causes centrosome dysfunction, mitotic catastrophe, and ultimately leads to cell apoptosis. Thus, BP could be used as a potential anti-tumor drug. CIPS could selectively target the RBD region of SARS-CoV-2 spike protein. Such interaction caused a denaturation of the secondary structure of RBD and occupied the relevant binding sites of RBD-ACE2, thereby inhibiting the infection of SARS-CoV-2 in host cells and inducing the subsequent immunological effects. Thus, CIPS could be used as a potential anti-SARS-CoV-2 nano-drug. These studies reveal that nanomaterials could have specifically/selectively intracellular or extracellular molecular targets, which clarifies the feasibility of molecular targeting nanomaterials and provides the fundamental strategies for future studies towards this direction.

Keyword: Molecular targets, nano-molecule interface analysis, nano "core" drug

最终交流类型: Oral

Optical nanosensors for non-invasive monitoring of neural activities

刘佳男
中国科学院脑科学与智能技术卓越创新中心

Extracellular potassium concentration affects the membrane potential of neurons. Indeed, alterations of potassium levels can be related to neurological disorders, such as epilepsy and Alzheimer’s disease, and, therefore, selectively detecting extracellular potassium would allow the monitoring of disease. However, currently available optical reporters are not capable of detecting small changes in potassium. Furthermore, they are susceptible to interference from sodium ions. We developed a highly sensitive and specific potassium nanosensor that can monitor potassium changes in the brain of freely moving mice undergoing epileptic seizures. An optical potassium indicator is embedded in mesoporous silica nanoparticles, which are shielded by an ultrathin layer of a potassium-permeable membrane, which prevents diffusion of other cations and allows the specific capturing of potassium ions. The shielded nanosensor enables the spatial mapping of potassium ion release in the hippocampus of freely moving mice.

Furthermore, we developed a highly sensitive and selective nanosensor for near-infrared (NIR) K+ imaging in living cells and animals. The nanosensor is constructed by encapsulating upconversion nanoparticles (UCNPs) and a commercial K+ indicator in the hollow cavity of mesoporous silica nanoparticles, followed by coating a K+-selective filter membrane. The membrane adsorbs K+ from the medium and filters out interfering cations. The UCNPs convert NIR to ultraviolet light, which excites the K+ indicator, thus allowing the detection of the fluctuations of K+ concentration in cultured cells and intact mouse brains

We also developed a near-infrared (NIR)-excited nongenetic voltage nanosensor that achieves stable recording of neuronal membrane potential in intact animals. The emission intensity of the nanosensor can report the membrane potential. Using the nanosensor, we monitor not only electrically evoked changes in the membrane potential of cultured cells but also sensory responses of neurons in intact zebrafish and brain state-modulated subthreshold activities of cortical neurons in intact mice.

Keyword: Nanosensor, Near-infrared imaging, Neuronal activities, Brain science

最终交流类型: Invited

Biomedical used optical functional materials

丁丹
南开大学

We aim to integrate both the advantages of AIEgens and afterglow luminescent materials by design and synthesis of afterglow luminescent AIE nanoparticles (termed afterglow luminescent AIE dots). By rational design, the resultant afterglow luminescent AIE dots with hydrodynamic diameters of around 120 nm can emit luminescence more than 1 day after single white light excitation for 5 min. The luminescence that the afterglow luminescent AIE dots emit has a peak centered at 670 nm and possess a big emission tail above 800 nm. It is found that the afterglow luminescent AIE dots are capable of penetrating tissue for about 1 cm. The afterglow luminescent AIE dots were then applied for tumor detection in vivo. 4T1 cancer cells were used to establish the tumor-bearing mouse model. After injection of afterglow luminescent AIE dots into tumor-bearing mice, the dots are enriched in the tumor mass by EPR effect. As the lifetime of mouse autofluorescence is at nanosecond level, it is facile to differentiate the long-lasting afterglow luminescence from the mouse autofluorescence. Therefore, the tumor tissues are able to be detect in a rather high-contrast manner. It is also found that the emission of afterglow luminescent AIE dots can be easily quenched in the normal tissues, such as liver and spleen. As the nanomaterials are prone to accumulation in these organs, as compared to currently available fluorescent nanoparticles and afterglow luminescent nanoparticles, high tumor-to-normal organ signal ratios are realized. The afterglow luminescent AIE dots were then applied for image-guided cancer surgery. Thanks to the long-lasting afterglow luminescence, the afterglow luminescent AIE dots can help the surgeon detect the micro-sized tumors and residue tumors during the surgery. Furthermore, the afterglow luminescent AIE dots are also able to differentiate tumor and inflammation in vivo owing to the different pH values in these two tissues.

Keyword: aggregation-induced emission, afterglow imaging, in vivo bioimaging, nanoprobe, biomedicine

最终交流类型: Oral

NIR-II Imaging-Guided Tumor Therapy: From Nanotheranostics to Drug-Free Therapeutics

姜鹏
武汉大学

Near-infrared-II (NIR-II: 1000-1700 nm) fluorescence imaging has great promise for tumor imaging-guided tumor therapy due to its deep-tissue penetration, high imaging resolution, and low autofluorescence. In recent years, we have developed a series of NIR-II imaging-guided tumor therapy strategies: (1) A one-step method to synthesize water- soluble NIR-II Ag2S quantum dots (QDs) with tunable emissions has been developed;[1] (2) A highly efficient GSH-responsive “turn-on” NIR-II fluorescent Fenton nanocatalyst was fabricated based on MnO2 nanosheet and Ag2S QDs for multimodal imaging-guided photothermal/chemodynamic synergistic cancer therapy;[2] (3) A series of tumor microenvironment regulation (elevating H2O2 levels, relieving hypoxia, etc.) strategies was designed to enhance the therapeutic effect of nanotheranostics;[3, 4] (4) A near-infrared-II fluorescent nanocatalyst has been fabricated for enhancing CAR T cell therapy against solid tumor by immune reprogramming, and a CAR T cell membrane-camouflaging strategy was developed to improve the tumor targeting ability of the nanocatalyst;[5] (5) A drug-free tumor therapy strategy, defined as “Triboelectric Immunotherapy”, was invented to directly damage tumor cells and recruit immune cells by applying pulsed direct-current (DC) generated from a small size fabric DC triboelectric nanogenerator (DC-TENG), which avoids the risk of drug-related side effects, toxicity, adverse reactions, drug dependence, drug resistance, etc.[6]

Keyword: NIR-II Imaging; Tumor Therapy; CAR T cell Therapy; Tumor Microenvironment; Triboelectric Immunotherapy

最终交流类型: Oral

In vivo dynamic NIR-IIb sO2 imaging assessing the cancer metabolism predicts response to immunotherapy

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National Center for Nanoscience and Technology, China

In vivo quantitative assessment of oxyhemoglobin saturation (sO2) status in tumor-associated vessels could provide insights into cancer metabolism and behavior. Here, we developed the next generation of in vivo noninvasive sO2 imaging to dynamic visualize the sO2 landscape of mouse head and tumor, based on photoluminescence bio-imaging in near-infrared-IIb (NIR-IIb; 1500-1700 nm) window. Real-time dynamic sO2 imaging with high frame rate (33 Hz) revealed the cerebral arteries and veins through intact mouse scalp/skull, consistently with the hemodynamics analysis result. Utilizing our noninvasive sO2 imaging, the tumor-associated vessel sO2 (TAV-sO2) levels of various cancer models were evaluated. A positive correlation relationship between the TAV-sO2 levels and the basal oxygen consumption rate of corresponding cancer cells at the early-stages of tumorigenesis, suggested a cancer cells modulated tumor metabolic microenvironment. We also found that a positive therapeutic response to the checkpoint blockade cancer immunotherapy could lead to a dramatic decrease of the TAV-sO2 levels. Two-plex dynamic NIR-IIb imaging was then achieved to simultaneously glean tumor vessels sO2 imaging and PD-L1 molecular imaging, allowing a more accurate prediction of immunotherapy response.

Keyword: NIR-II bioimaging, oxyhemoglobin saturation, cancer metabolism, immunotherapy

最终交流类型: Oral

Single-Molecule Electrochemical Imaging Resolves the Midpoint Potentials of Individual Fluorophores

卢晋
国家纳米科学中心

Electron transfer is a fundamental process in all living systems that governs various energy-conversion pathways. At the molecular level, each electron transfer step only spans up

to a few nanometers, from one donor molecule to an acceptor in its vicinity. Resolving and imaging such electron transfer activities at the nanoscale has drawn much attention recently.

Here, we proposed a strategy by introducing the redox-responsive fluorescent molecules that participate in the electron transfer process. These fluorescent molecules switch between the fluorescent and nonfluorescent states by losing or gaining electrons. We therefore can detect the redox process by monitoring the on-off switch of the fluorescent signals at the single-molecule level.

We first introduced a porous conducting oxide layer to temporarily adsorb the free fluorescent probes or hinder their diffusion. We next tested a series of fluorescent probes with enhanced brightness and excellent photostability. Our finding indicated the ATTO and Alexa Fluor dyes underwent reversible redox process, and the emissive state of each fluorophore is modulated by electrochemical potential. Our data showed that the number of emitting single molecules follows a sigmoid function during a potential scan. It allows us to optically determine the formal redox potential of each dye and produce spatial maps of midpoint potential to quantify the spatial heterogeneity of electron-transfer processes.

We further studied how the redox behaviors of single fluorescent probes are modulated by redox mediators. We observed each redox-responsive fluorescent probe to have a significantly shifted redox potential. It implies that dye reduction is highly coupled to the electrochemistry of nearby mediators in solution, and the quantitative analysis indicates that this process follows an electrocatalytic (EC’) reaction mechanism. It implies the possibility that we can “indirectly” image any electrochemical process of interest and resolve their spatiotemporal dynamics with single molecule sensitivity.

Keyword: redox-active fluorescent probes, redox mediators, electrocatalytic mechanism, phenazine methosulfate, riboflavin

最终交流类型: Invited

Interface-Engineered Field Effect Transistor Biosensors

袁荃
湖南大学

Field-effect transistor (FET) biosensors with intrinsic signal amplification capability could directly convert trace biomolecule information into a readable electrical signal, endowing its high sensitivity characteristic. The sensing principle of FET biosensors relies on the change in charge carriers at the biosensing interface upon the recognition of charged

target biomolecules. Yet, in practical biological environments such as saliva with relatively high ionic strength, the biosensing interface and charged biomolecules would be severely screened by oppositely charged ions through electrostatic interaction, thus weakening the interaction between FET biosensors and target biomolecules. To address these limitations, we developed a series of interface engineered FET biosensors to efficiently identify target biomolecules. We developed the recognition molecules orientation and structure regulating strategy to shorten the length occupied by recognition molecules on the electrode surface and narrow the distance between targets and sensing interfaces. Then, we validate an integrated urinalysis device that is composed of an indium gallium zinc oxide field-effect transistor (IGZO FET) biosensor array, a device control unit and an Internet terminal to afford directly analysis of five bladder tumor-associated proteins in untreated urine samples. With the assistance of machine-learning algorithm, our device could identify bladder cancer with an accuracy of 95.0%, distinguishing cancer stages with an overall accuracy of 90.0% and assessing bladder cancer recurrence after surgical treatment. The non-invasive urinalysis device defines a robust technology for remote healthcare and personalized medicine.

Keyword: field effect transistor, Debye screening effect, biosensing, interfacial engineering, point-of-care testing

最终交流类型: Invited

Glucose Oxidase-Instructed Antitumor Therapy

黄鹏

Shenzhen University

Glucose oxidase (GOx) has aroused great research interest in the context of cancer treatment due to its inherent biocompatibility and biodegradability, and its unique catalytic properties against β-D-glucose. GOx can effectively catalyze the oxidation of glucose into gluconic acid and hydrogen peroxide. This process depletes oxygen levels, resulting in elevated acidity, hypoxia and oxidative stress in the tumor microenvironment. All of these changes can be readily harnessed to develop a multimodal synergistic cancer therapy by combining GOx with other therapeutic approaches.

In this talk, we will highlight our recent efforts on systematic design and construction of functionally specific GOx-based nanomaterials and present representative paradigms for effectively treatment of cancer. Specifically, our work is mainly launched in three aspects: (1) developing multimodal synergistic therapy by combining GOx with other therapeutic

approaches, often oriented by the cascade reactions triggered by GOx and other agents; (2) enhancing the catalytic activity of GOx by rational design of nanomaterials that can adjust the acidity, temperature and O2 levels of tumor tissues; (3) developing the immobilization methods to improve the stability and histocompatibility of GOx without compromising the enzyme activity. Finally, we will discuss the challenges and perspectives of the clinical translation of GOx-based nanomedicine for cancer treatment.

Keyword: Glucose oxidase, antitumor therapy, starvation therapy, synergistic therapy, nanomedicine.

最终交流类型: Oral

Metal-Organic Framework-based Biohybrid Nanoassemblies for NIR-II imaging guided synergistic therapy

贺良灿
哈尔滨工业大学

Nanotechnology has made remarkable progress in manipulating nanoparticles (NPs) with precise control over their properties. This work presents a novel DNA-mediated assembly strategy to enhance the localization of erbium-based nanoparticles (ErNPs) on bimetal-organic framework (CPM) nanohybrids (ECPM) at tumor sites, leading to improved imaging and therapeutic efficacy. The ECPM nanohybrids exhibit a virus-like structure, with CPM as the core and ErNPs as the outer layer. The surface of ECPM is modified with pH-responsive i-motif DNA strands, which undergo quadruplex structure formation in the acidic tumor microenvironment. This self-assembly process triggers the formation of NP clusters within the tumor region. The ErNPs within these clusters emit visible photons upon excitation, which are harnessed by porphyrin ligands in CPM for NIR-induced photodynamic therapy. Importantly, the integration of CPM does not compromise the down-converted NIR-II emission, enabling dual imaging and therapeutic capabilities. One of the challenges in cancer therapy is the presence of GSH, which can reduce the effectiveness of ROS-mediated therapies. To address this, the CPM component in ECPM can deplete intracellular GSH levels, enhancing oxidative stress for improved photodynamic therapy. The responsive self-assembly of ECPM enables selective accumulation within tumors, resulting in enhanced NIR-II imaging and therapeutic effects compared to dispersed ECPM systems. In summary, the DNA-mediated assembly strategy utilizing ECPM nanohybrids holds promise for improving tumor localization, imaging, and therapeutic outcomes. The pH-responsive self-assembly of ECPM allows for selective tumor accumulation, while the integration of CPM enables dual imaging and therapeutic functionalities. These findings showcase the potential of nanomaterial assembly strategies for advanced applications in nanomedicine.

Keyword: DNA nanotechnology, biohybrid nanoassemblies, nanoreactor, NIR II imaging, theranostics

最终交流类型:

Tracking the orientation dynamic of RNA origami self-assembly by atomic force microscopy and neural networks

Yonghui Zhang
Aarhus University

Ribonucleic acid plays an essential role in biological functions, such as regulating gene expression, protein production and so on. Therefore, RNA nanotechnology receives more and more attention recently for its potential to organize RNA-based nanodevices or develop new strategies for targeted delivery or storage methods. However, due to its single-strand structure that makes RNA a fragile molecule, few publications focused on RNA manipulation and programmable designs. In this work, it was the first time to report that RNA origami worked as a building block to construct two-dimensional arrays. By simply shortening or grafting a single strand, molecular flexibility was able to be tuned and grow into different conformational patterns, which was driven by intermolecular interaction. During the self-assembly process, two main types of interaction were clarified. In the initial landing process, origami molecules had landing angle preference and primarily matched the three main orientations of the mica lattice structure, where molecules were largely attracted by an inorganic interface. After landing on the surface, individual molecules were witnessed to move, rotate, or lineup, which was driven by intermolecular force from neighboring new RNA origami molecules, intermolecular force dominated. Therefore, the whole population had to adjust the position to minimize energy where the three most intensive peaks started to shift and then merge into one or two strong peaks instead. These results demonstrated that the RNA origami can be programmable and self-assemble into 2D patterns, setting the platform for developing RNA-based nanotechnology and exploring the potential possibility for novel medical applications.

Keyword: RNA origami, self-assembly, atomic force microscopy, neural network

最终交流类型: Oral

Single-Particle Study Based on Solid-State Nanonet and Nanochannel

翟月明
武汉大学

Nanopore detection has attracted widespread attention due to its advantages such as high sensitivity, label-free detection, and strong universality, and has become a highly promising technique for single-particle and single-molecule detection. Nanoparticles (biological nanoparticles, synthetic nanoparticles) are widely distributed in fields such as biomedical science, energy catalysis, and sensing detection. Their unique properties and functions are determined by their size, morphology, charge, and surface chemical properties. Therefore, the development of technologies for single-particle characterization and manipulation is of great significance for both basic research and practical applications. The speaker will introduce the advantages of using nanonet and long nanochannel for single-particle analysis, specifically discussing the way for the analysis of individual protein molecule and inorganic nanoparticle.

By transforming photo-induced silicon nitride nanopores into nanonet structure, a stable and effective solid-state nanonet protein capture platform was constructed, and the capture of single protein molecule was studied based on electrophoresis and electroosmotic flow. Additionally, a long single micrometer-long uniform through nanochannel is fabricated in the silicon wafer, which is employed for shape-based nanoparticle distinguishing.

Keyword: nanopore sensing, single nanoparticle

最终交流类型: Invited

Enhancing the Performance of Smart DNA Hydrogels via Active, Rapid and High-Degree Swelling-Shrinkage Cycles

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Smart hydrogels that can respond to specific external stimuli and undergo volume changes or hydrogel-to-solution transitions have shown great potential in various applications, including biosensing, drug delivery, soft robotics, and artificial organs. In particular, the introduction of functional DNA units leads to the formation of smart DNA hydrogels with programmable response to various types of stimuli, such as pH changes, metal ions, ligands, nucleic acids and proteins. However, due to the 3D polymeric network, the response of these

hydrogels to biomacromolecular targets is usually slow, severely limiting their practical applications. Herein, inspired by the respiratory system of organisms, we demonstrate an active strategy to accelerate mass transport between the hydrogel matrix and external solutions, and to enhance the responsiveness of these hydrogels to biomacromolecular targets, through the fast and high-degree “swelling–shrinkage” cycles of hydrogels stimulated by dynamic temperature changes or intermittent light illumination. First, hierarchically structured poly(N-isopropylacrylamide) (pNIPAM)–DNA hydrogels composed of free water containing interconnected macroporous channels and densely crosslinked functional DNA-tethered pNIPAM networks between the channels were constructed via typical cryostructurization processes. Dynamic temperature changes or intermittent light irradiation can induce rapid and reversible shrinking/swelling cycles with high-volume changes of the hydrogel matrix, driving the formation of dynamic water flow between the hydrogel matrix and surrounding solution, resulting in faster uptake of external biomacromolecular substances and the expulsion of endogenous substances, thus promoting the functional properties of hydrogel systems. As demonstrated by different model DNA-based catalytic systems, significantly enhanced catalytic efficiencies of up to 2 to 4 times are achieved. Moreover, the active mass transfer strategy can significantly improve the efficiency of these smart DNA hydrogels in the extraction of different types of biotargets, including DNA, proteins and exosomes. These hydrogel systems with enhanced substance transport and transformation properties are promising in future biosensing and therapeutic applications.

Keyword: DNA hydrogels, Biosensing, Functional nucleic acids, Cryogels, Catalysis

最终交流类型: Invited

Constructing Chiral Nanoprobes and Biological Effect

徐丽广
江南大学

Viruses not only pose severe threats to public health, but also influence the development of society1. In this lecture, we will report 4±0.5 nm copper (I) sulfide nanoparticles (NPs) with 46 mdeg chiroptical property at 530 nm were synthesized to selectively cleavage Hepatitis B virus core antigen (HBcAg) and effectively blocked HBV assembly and prevented Hepatitis B virus infection both in vitro and in vivo under near infrared light at 808 nm2. Experimental analysis showed that the chiral copper (I) sulfide NPs specific bound with the functional domain from phenylalanine23 (F23) to leucine30 (L30) from HBcAg primary sequence and the cutting site was between amino acid residues F24 and proline25 (P25). Under excitation at 808 nm, the intracellular HBcAg concentration was reduced by 95 %, and in Hepatitis B virus transgenic mice, the levels of Hepatitis B virus surface antigen and Hepatitis B virus DNA were decreased by 93 % and 86 %, respectively. Together, this finding provides a good candidate strategy and a new insight for the development of antivirus, such as severe acute respiratory syndrome corona-virus 2 (SARS-CoV-2), influenza virus, human immunodeficiency virus and Ebola virus.

Keywords: Chirality, Copper (I) Sulfide Nanoparticles, Photoinduced Treatment, Ultrasmall Scale.

最终交流类型: Oral

Programmable engineering nano-bio interfaces for highly sensitive liquid biopsies

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Nanjing University of Posts and Telecommunications

Nano-biology interfaces are critical to many intelligent nanomedicine designs for diagnostic and therapeutic biomedical applications. However, the progress is often obscured by the lack of understanding of the functional interaction between biological matters, as well as the boundary conditions, thus limiting the effect of nanomedicine for disease management. Here, we report a programmable engineering strategy in two-dimensional transition metal nanosheets (2D material) that leverages the interface interaction between biomasses for measuring circulating biomarkers - exosomes. We found that 2D surface modulates the binding affinity of the 2D material towards biomolecules. Surface engineering in 2D MoS2 thus enables generation and fine-tuning of biomass interaction to maximize detection outcomes. Compared with the untrained MoS2 platform, the programmable engineered 2D substrate offers enhanced sensitivity and specificity to multiple targets. Through exosomal protein and microRNA marker profiling, we identified a signature of combined markers for cancer detection. By implementing an engineered 2D MoS2 platform on a self-powered microfluidic device for the assessment of drug treatment, we show that the treatment prognosis and side effect on cancer can be identified accurately.

Keyword: nano-bio interfaces, liquid biopsies, 2D material, MoS2, exosome

最终交流类型：Oral

Mimicking Extracellular Matrix Patterns with Maskless Microstructuration for Probing Cellular Responses in Health and Disease

Anne-Kathrine Kure Larsen
Aarhus University

The abstract summarizes our work on fabricating microstructures for the investigation of extracellular matrix mimicking patterns on cell responses and a proof-of-concept study on aSyn aggregation in Parkinsons' disease models.

Keyword: Microstructures, Extracellular Matrix Mimicking, Mask-less, Neurodegeneration, Mechanotransduction

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最终交流类型：Oral

DNA-Programmed Tuning of the Growth and Enzyme-Like Activity of Bimetallic Nanozyme and Its Biosensing Applications

鲁娜
Shanghai University of Engineering Science

Nanozymes, which combine the merits of both nanomaterials and natural enzymes, have aroused tremendous attention as new representatives of artificial enzyme mimics. However, it still remains to be a great challenge to rationally engineer the morphologies and surface properties of nanostructures that lead to the desired enzyme-like activities. Here, we report a DNA-programming seed-growth strategy to mediate the growth of platinum nanoparticles (PtNPs) on gold bipyramids (AuBPs) for the synthesis of bimetallic nanozyme. We find that the preparation of bimetallic nanozyme is in a sequence-dependent manner, and the encoding of polyT sequence allows the successful formation of bimetallic nanohybrids with greatly enhanced peroxidase-like activity. We further observe that the morphologies and optical properties of T15-mediated Au/Pt nanostructures (Au/T15/Pt) change over the reaction time, and the nanozymatic activity can be tuned by controlling the experimental conditions. As a concept application, the Au/T15/Pt nanozymes are used to establish a simple, sensitive, and selective colorimetric assay for determination of ascorbic acid (AA), alkaline phosphatase (ALP), and the inhibitor sodium vanadate (Na3VO4), demonstrating excellent analytical

performance. This work provides a new avenue to rational design of bimetallic nanozymes for biosensing applications.

Keyword: DNA, bimetallic nanozyme, peroxidase-like, colorimetric detection, alkaline phosphatase, inhibitor

最终交流类型: Invited

Construction of Various Non-enzymatic Autocatalytic DNA Machineries for Amplified Intracellular Imaging

王富安
Wuhan University, China

The construction of robust, modular and compact DNA machinery facilitates us to build more intelligent and ingenious sensing strategies in complex biological systems. The performance of conventional DNA amplifier machines is always impeded by their limited in-depth amplification efficiency or miscellaneously enzymatic requirements. Herein, we constructed a series of entropy-driven autocatalytic DNA circuit for the amplified FRET transduction of microRNA targets. The autocatalytic DNA machinery involves an autonomous cross-invasion of two different amplification molules, where the reciprocal reinforcement of the autocatalytic hybridization process accelerates the entire reaction procedure and promotes the generation of an amplified FRET readout, as systematically explored by various experimental studies and computer-aided reaction simulations. Moreover, by integrating with an auxiliary hairpin probe, the DNA amplifier can be executed as a general sensing platform for analyzing miR-21 in vitro and in vivo, originating from inherent reaction accelerations and multiple-guaranteed recognitions. The autocatalytic DNA machinery provides a versatile, robust, amplified and selective platform for the detection of DNA and a universal module for analyzing miRNAs in living cells. It introduces major advances over the conventional DNA circuit systems and provides a legendary analytical tool in DNA nanotechnology, thus holding great potential in clinical diagnosis and assessment.

Keyword: DNAzyme, microRNA, biosensing, Amplification, DNA machine

最终交流类型: Oral

Chiral nanoprobe fabrication and their life analysis

孙茂忠

Jiangnan university

In the rapidly expanding fields of nanoscience and nanotechnology, there is considerable interest in chiral nanomaterials, which are endowed with unusually strong circular dichroism. The principles of organization underlying chiral nanomaterials and generalize the recent advances in the main strategies used to fabricate these nanoparticles for bioscience applications was proposed. The creation of chirality from nanoscale building blocks has been investigated both experimentally and theoretically, and the tunability of chirality using external fields, such as light and magnetic fields, has allowed the optical activity of these materials to be controlled and their properties understood. Therefore, the specific recognition and potential applications of chiral materials in life analysis are discussed. The effects of the chirality of nanostructures on biological systems have been exploited to sense and cut molecules, for therapeutic applications, and so on.

Keyword: chiral; NLRP3; amyloid-β; senescence; Alzheimer’s disease

最终交流类型：Invited

Polymeric carriers for nucleic acid delivery

田华雨
厦门大学

mRNA drugs have shown great socio-economic benefits and broad clinical application potentials, and development of efficient mRNA delivery systems is the key to mRNA drug research and commercialization. Polymeric carriers have unique advantages in the field of drug delivery and are expected to break through the foreign patent barriers of existing lipid nanoparticle delivery systems. Cationic polymers can carry nucleic acids, proteins and other types of drugs, hold a wide range of applications in gene detection, gene therapy, nucleic acid vaccines, anti-tumor combination therapy and biomanufacturing. Beginning from the problems encountered in the practical application of polymer carriers, our group has developed a series of strategies for polymer design, synthesis and carrier assemble, realizing the application of polymer nanocarriers in tumor nucleic acid diagnosis, gene therapy, tumor and influenza nucleic acid vaccines and other fields. Some of our research results have completed preclinical proof-of-concept, the key materials for biomanufacturing have achieved large-scale production and in vitro gene transfection reagents have been commercialized.

Keyword: polymeric carriers, nucleic acid delivery, tumor vaccine, gene therapy, anti-tumor combination therapy

最终交流类型: Invited

Catalytic Biomaterials

陈雨
上海大学

Catalytic therapy can concurrently enhance therapeutic efficacy and decrease side effects by converting less toxic or nontoxic endogenous substances into various highly toxic reactive species (e.g., toxic radicals) to induce cell apoptosis/necrosis, which has been exploited to combat different types of diseases. As material science and nanotechnology evolve for application in disease therapies, a variety of catalytic biomaterials and nanomedicines have been elaborately designed and synthesized to mediate catalytic reactions and/or enhance the corresponding catalytic treatment efficacy. Delivery carriers loaded with anti-cancer drugs will be distributed throughout the blood, and the loaded drugs have high cytotoxicity, which makes it easy to cause serious side effects on normal tissues and organs. In order to solve this key scientific problem, we innovatively combine the "catalytic performance" of inorganic biomaterials with "disease diagnosis and treatment", do not use chemotherapy drugs, and only use the "catalytic reaction" triggered by catalysis biomaterials to treat diseases. It is used in the design and control of equipment, performance optimization, biological effect regulation, and research on the diagnosis and treatment of major diseases such as malignant tumors of "disease microenvironment response" or/and "field response" of "catalysis biomaterials". Focus on the "catalytic function" of biomaterials; reasonably design and prepare "disease microenvironment response" or/and "external field excitation response."

Keyword: catalytic biomaterials，tumor microenvironment，external field response，diagnosis and treatment

最终交流类型: Invited

Development and application of protease-dependent protein targeted degradation technology

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中国科学院杭州医学所

The strategy of targeting protein degradation (TPD) is gaining prominence as a novel approach in the field of drug development. Nevertheless, all TPD technologies currently depend on either the ubiquitin-proteasome system or the lysosome system. The application of the TPD technique is not feasible in membranous organelles, such as mitochondria, due to the lack of aforementioned protein degradation machinery. The majority of proteins within mitochondria undergo degradation via AAA + proteases. We introduced small molecules to induce conformational changes in the target proteins, which were then degraded by protease LONP1. We then devised a general mitochondrial protein-targeted degradation technique (MTPTAC). By employing the AAA + protease degradation system, we have effectively accomplished targeted degradation of the mitochondrial protein POLRMT, alongside a novel cancer biomarker LRPPRC. The bi-functional POLRMT-degradator has the ability to selectively hinder the synthesis of tumor mitochondria while leaving the biological functions of existing mitochondria in normal tissue cells unaffected. This presents a unique approach to tumor therapy that focuses on targeting mitochondrial metabolism. The LRPPRC protein was selectively degraded through the administration of a commercially available, established pharmaceutical agent. This intervention effectively depleted tumor stem cells and concurrently arrested the cell cycle by suppressing the expression of CDK6 protein. The co-administration of LRPPRC degrader and CDK4/6 inhibitor has demonstrated significant efficacy in overcoming resistance to CDK4/6 inhibitor treatment. In conclusion, the protein-targeted degradation technology we have developed, which relies on the AAA+ protease system, holds significant potential for application in cancer-targeted therapy.

Keyword: targeted protein degradation; mitochondria; protease; targeted therapy; CDK4/6 inhibitor

最终交流类型:

Nanomaterials induced Endothelial Leakiness

David Leong
National University of Singapore

Many nanobioimaging probes depend on escaping from the blood vessels to exert their designed functions at the specific locations. The single first step of crossing the endothelial barrier is critical. While exit of nanomaterials from blood vessels are certain, the “how” answers are hotly debated and elusive. Here, we are proposing that certain nanomaterials are capable of inducing endothelial leakiness (NanoEL), even in the absence of tumors based on our initial surreptitious discovery (Setyawati et al. Nature Comms 2013). We will share in a

few studies the characteristics of NanoEL, nanotoxic implications of unbridled NanoEL (Peng et al. Nature Nanotech 2019) and also opportunities if we have a better understanding of NanoEL (Setyawati et al. Nature Comms 2023).

Keyword: Endothelial Leakiness, EPR, Nanoprobes

最终交流类型: Invited

Reversible Protein Crystallization by Controlling External Factors

Mingdong Dong
Aarhus University

Amyloid self-assembly is a fascinating and intricate phenomenon that holds significant relevance in both the context of degenerative human disorders and materials science. These self-assembled structures include amyloid fibers, particles, and crystals, with crystal amyloids exhibiting exceptional stability from an energetic standpoint. Despite the potential advantages of crystal amyloids, achieving precise control over amyloid assembly and mastering the ability to reversibly manipulate the crystallization process remain formidable challenges.

To address these challenges, this comprehensive study sets out to explore the reversible formation of macroscopic amyloid crystals by systematically investigating the effects of crucial factors such as temperature, pH, ionic strength, and solvents. By unraveling the intricate interplay of these variables, the research aims to shed light on the underlying mechanisms that govern the formation and dissolution of amyloid crystals.

In the quest for a deeper understanding, cutting-edge in situ microscopy techniques will be employed to capture the dynamic process of amyloid disassembly at the molecular level. The real-time visualization of these intricate structural changes promises to offer unprecedented insights into the kinetics and thermodynamics of amyloid self-assembly.

Furthermore, the observation of reversibility in amyloid self-assembly under the influence of external stimuli presents valuable opportunities for gaining a more comprehensive understanding of amyloid formation. These findings emphasize the crucial role played by external factors in shaping the crystal formation process. Understanding the relationship between environmental factors and the structural organization of amyloids not only enriches our knowledge of self-assembly processes but also paves the way for the development of innovative biomaterial design strategies.

Keyword: Crystallization, Biomaterial Design, Amyloid self-assembly

最终交流类型: Invited

Publishing - Present and Future

Oliveira José
Wiley

A highly competitive research environment with increasingly limited research funding has created a “Publish or Perish” attitude among scientists who are judged on the quantity rather than quality of their research articles. This presentation provides a brief overview of current trends and challenges in scientific publishing and peer review, some ethical considerations, how publishers and authors interact and influence each other, and how the publishing arena is being transformed.

Keyword: Publishing, Peer Review, Ethics

最终交流类型:

Life in a Bubble - EV-based Assays Enabling Personalized Diagnosis

Tony Hu
Tulane University

Diagnostics for infectious and malignant diseases often exhibit poor specificity/sensitivity, hindering early detection and treatment evaluation, but development of improved assays is limited by several challenges, including absence of disease-specific factors, low biomarker concentrations, and interfering factors. We have employed an array of sensitive analytic technology platforms to identify key host-pathogen interactions that influence pathogenesis and applies this information to identify diagnostic and predictive biomarkers that can be applied for personalized medicine to improve patient outcomes. We reported the development and validation of several nanotechnoloy-based assays platforms that can be used to quantify protein and nucleic acid changes in EV-associated protein biomarkers, and which have the capacity to target EVs derived from specific cell populations, including EVs derived from Mtb-infected phagocytes and other cell populations involved in granuloma formation. Candidate biomarkers identified in this study will be analyzed using these platforms and correlated with changes in specific granuloma and systemic cell populations.

Keyword: Extracellular vesicles (EV), Proteomics, Nanotechnologies, Cancer, Infectious diseases

Topical Sessions =》 13. Nanobiotechnology and Nanomedicine

最终交流类型: Oral

Smart nanorobots for on-target tumor vessel infarction

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Like normal organs, tumors need to establish a blood supply to satisfy their demand for oxygen and nutrients and accomplish other metabolic functions. However, tumor vessels display considerable variation in the patterning and properties, as well as in their responses to vessel targeted therapy. Based on the potential vulnerabilities that could be targeted in vascular system, we developed several nanorobotic drugs to selectively infarct tumor vessels or modulate microenvironmental components to achieve safe and effective antitumor therapy. For achieving targeted tumor vessel occlusion, we have constructed an autonomous, tubular DNA nanorobots capable of specifically binding to the tumor vascular endothelium and presenting the coagulation protease thrombin to locally induce tumor infarction and necrosis. The DNA nanorobots inhibited mammary tumor growth and led to sustained regression of primary melanomas and metastases, without observable thrombotic side effects in both mice and Bama miniature pigs. We also developed the intelligent polymer nanodrugs to combine the infarction therapy and other therapeutic methods in one nanoplatform, dramatically reducing tumor recurrence rate compared with single infarction therapy. With this seminal work in the development of intelligent anticancer therapeutics, it may be asserted that ‘swallowing the doctor’ may not be too far away.

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Keyword: intelligent nanodrug, tumor vessel, targeted drug delivery, tumor therapy

最终交流类型：Oral

A transistor-like pH-sensitive nanodetergent for selective cancer therapy

Menghua Xiong
华南理工大学

Plasma membrane rupture (PMR) induced cell death commonly bypasses the intracellular signaling pathways of target cells and ignores their drug-resistance spectrum and metabolic heterogeneity, opening up a promising strategy for the treatment of drug-resistant pathogen infection and cancer. Membranolytic molecules (MMs), such as host defence proteins/peptides and cationic polymers, often have a common amphiphilic structure including cationic and hydrophobic moieties. The cationic residues exert a strong electrostatic attraction to the negatively charged cell membrane of bacterial and cancer cells, followed by the insertion of the hydrophobic regions into phospholipid bilayers, inducing a detergent-like membranolytic effect. However, the amphiphilic structure is also the main culprit for their high toxicity against normal tissues/cells. Thus, the key for the application of MMs is to achieve high selectivity towards target cells, while minimizing their toxicity to normal tissue cells. The delicate balance of structural and physicochemical parameters of the amphiphilic structure, such as cationicity (net charge), hydrophobicity, amphipathicity and structural propensity, has enabled the development of MMs with high selectivity towards pathogens due to the large differences in the structure and composition of cell membranes between pathogenic microorganisms and mammalian cells.

Here, we report the design of “proton transistor” nanodetergents (pTNTs) that can convert the subtle pH perturbation signals of tumour tissues into sharp transition signals of membranolytic activity for selective cancer therapy. Our top-performing pTNT, P(C6-Bn20), can achieve a >32-fold change in cytotoxicity with a 0.1 pH input signal. At physiological pH, P(C6-Bn20) self-assembles into neutral nanoparticles with inactive membranolytic blocks (MBs) shielded by PEG shells, exhibiting low toxicity. At tumour acidity, a sharp transition in its protonation state induces a morphological transformation and an activation of the MBs, and the cation-π interaction facilitates the insertion of benzyl groups-containing hydrophobic domains into the cell membranes, resulting in potent membranolytic activity. P(C6-Bn20) is well tolerated in mice and shows high anti-tumour efficacy in various mouse tumour models.

Keyword: Nanodetergent, selective cancer therapy, pH sensitive

最终交流类型: Oral

Living Assembly of Nanomedicine and Stem Cells for Spine and Spinal Cord Regeneration

Letao Yang
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Injuries and degeneration of the spine and spinal cord can result in devastating conditions with severe pain and impairment of motor functions. Organoids and spheroids 3D-assembled from stem cells can secret trophic factors and differentiate into various types of functional cells, thus holding excellent potential for tissue engineering. Nevertheless, how to effectively control stem cell fates in 3D and in vivo remains critical hurdles to be addressed.

In this presentation, I will introduce my work on the living assembly of nanomedicine and stem cells for enhancing spine and spinal cord regeneration. To overcome the diffusion barriers, drug-loaded and extracellular matrix (ECM) protein-functionalized 1D and 2D self-therapeutic nanomaterials were used for guiding the assembly of stem cells into

3D spheroids and organoids with controlled neurogenesis (Nature Communications 2018, Biomaterials 2019, Advanced Materials 2020, Science Advances 2021), as well as chondrogenesis (National Science Review 2022, Advanced Materials 2023) required for spinal cord and spine regeneration, respectively. We have termed this strategy as synthetic matrix assisted and rapidly templated (SMART) assembly. Implantation of these 2D and 3D stem cell hybrid assemblies with varying forms of nanomedicine resulted in new populations of neurons after hemisection spinal cord injury (SCI) in mice. With additional therapeutic functionalities (e.g., scavenging of reactive oxygen species, or ROS) SMART spheroids were further explored for guiding chondrogenesis and the treatment of intervertebral disc degeneration. Most importantly, with these efforts now we are able to realize robust functional recovery and pain reduction after spine and spinal cord injuries.

In summary, we developed to a strategy for the living assembly of nanomedicine and stem cells for treating spine and spinal cord injuries. By working with clinicians, we will further advance this SMART assembly-based therapeutic strategy by addressing the vascularization barriers associated with organoid for spine and spinal cord regeneration.

Keyword: Stem cells, Spinal cord injury, Spine, Living assembly, Tissue engineering

最终交流类型: Oral

Multifunctional polymers synergize with innate immunity to improve anti-tumor treatment

Zhiyue Zhang
山东大学

Tumor immunotherapy is an approach to clear tumors by regulating the body's immune system and enhancing the innate or adaptive immune response to exert an anti-tumor immune response. Intrinsic immunotherapy has attracted much attention because of its outstanding therapeutic effects and long-lasting therapeutic effects such as immune memory. However, tumor-only immunotherapy is often limited in its clinical research and application due to inter-individual patient differences, cytokine storm, and immune escape. Tumor microenvironment stimulus-responsive polymers are a series of novel polymers that use the unique physiological conditions of the tumor microenvironment as a stimulus for responsive structural or physicochemical property changes, and have the advantages of high biocompatibility, good stability, in vivo degradable metabolism, and easy modification. The combination of stimuli-responsive polymers with tumor immunotherapy is expected to be a

new strategy in tumor therapy. The polymers are structured and modified based on the physiological properties of TME to selectively release immunotherapeutic drugs under TME, thereby modulating the conversion of immunosuppressive effects to stimulatory response factors at the tumor site. In this paper, we introduce the application of multi-stimulus-responsive polymers in tumor immunotherapy and discuss their advantages and challenges in tumor immunotherapy with the aim of providing a reference for the application of stimulus-responsive polymers in tumor immunotherapy.

We report a GSH-activatable IMQ-conjugated c-RGD-modified nanoimmunomodulator (cN@SS-IMQ) that induces greater immune activation within tumors while limiting extra-tumoralstimulation. cN@SS-IMQ was prepared via the self-assembly of c-RGD-modified amphiphilic block copolymers composed of a hydrophilic stealth polymer, poly(N,Ndimethyl acrylamide) (pDMA), and a hydrophobic IMQligated poly(2-((2-hydroxyethyl) disulfanyl) ethyl methacrylate-IMQ) (pIMQ (SS)). This system was further engineered for tumor targeting ability and enhanced stability in blood upon systemic administration by the introduction of c-RGD and a high quantity of poly(DMA). The lethal side effects of the systemic administration of IMQ were eliminated by blocking the C4 amine moiety with polymeric carriers. Once it entered the tumor, high concentrations of GSH facilitated the release of native IMQ and thus promoted the maturation of dendritic cells (DCs) for further enhancement of T lymphocyte infiltration against tumors. These observations show the broad versatility of GSH-responsive monomerbased precursors in safe systemic cancer immunotherapy.

Keyword: Glutathione-Responsiveness, Imidazoquinolines, Immunotherapy, Systemic Administration, Toll-Like Receptors

最终交流类型: Invited

Selection of new DNA aptamers for drug delivery

Juewen Liu
University of Waterloo

Aptamers are single-stranded DNA oligonucleotides that can selective bind to target analytes. They have been shown to be of great interest for targeting certain cells and tissues for drug delivery and imaging applications. This talk will discuss ocular drug delivery using aptamers for the treatment of dry eye disease. While liposomes have been a popular vehicle for treatment of ocular diseases including DED, most do not have a specific targeting mechanism. While cationic materials may increase the retention time, they may also exert toxicity. Therefore, formulations that can increase the retention time is needed. Cornea is the major barrier to drug delivery to eye, which results in low bioavailability and poor efficacy of topical eye treatment. While various methods have been developed to increase the retention time of drugs, an effective active targeting method is still lacking. We selected cornea-targeting aptamers using tissue-SELEX on pig cornea. The top two abundant aptamers, Cornea-S1 and Cornra-S2, were confirmed to bind to pig cornea and human corneal epithelial cells with Kd values of 361 nM and 174 nM, respectively. The Cornea-S1 or Cornea-S2 increased the retention time by up to 24 hours, fasten the cellular uptake by 15 minutes. Cyclosporine A (CsA), a hydrophobic endecapeptide molecule, is an FDA-approved ocular drug for dry eye disease (DED). CsA functions as an immunosuppressive agent to reduce inflammation and interfere with tear production. However, CsA possesses low solubility in aqueous solutions, which makes it difficult to deliver it safely and effectively into the eyes. The efficacy of cyclosporine A (CsA)-loaded liposomes in human corneal epithelial cells (HCECs) with dry eye conditions compared to the non-aptamer liposomes. When CsA was encapsulated in aptamer-conjugated liposomes, 10 times less CsA was needed to achieve similar anti-inflammation and tight junction modulation as CsA free drug. These suggested aptamer-functionalized liposomes were more efficient as nanocarriers. Such aptamers obtained from cornea-SELEX can serve as a general ligand for ocular drug delivery.

Keyword: aptamers, drug delivery, cornea, SELEX, dry eye disease

最终交流类型：Keynote

Nanozymes: definition, units, activity, selectivity and new applications

Juewen Liu
University of Waterloo

Since the emergence of nanozyme as a term in the literature, this term has been used to describe various catalysts from immobilized inorganic metal complexes, immobilized enzymes to inorganic nanoparticles. In this talk, the history of nanozyme is described in detail and they can be largely separated into two types. The type 2 nanozymes, which rely on the surface catalytic properties of inorganic nanomaterials, are the dominating type in the past decade. The definition of nanozyme has been evolving and a function-based definition based on the same substrate and product as enzymes is able to cover most currently claimed

nanozymes, although they may have different mechanisms compared to their enzyme counterparts. A broader definition can inspire application-based research to replace enzymes with nanomaterials for analytical, environmental and biomedical applications. Comparison with enzymes also requires a clear definition and a nanozyme unit, and four ways of nanozyme unit definitions are described. More and more current work has been devoted to understanding catalytic mechanisms of nanozymes, which provides a basis for further rational engineering of active sites.[1] This talk will also cover some of our work on improving the activity of nanozymes and thoughts to improve the selectivity. For example, molecularly imprinted polymer technology allowed excellent selectivity of nanozymes. Finally, some new applications of nanozymes will be discussed. For example, hydrophilic bare Fe3O4 nanoaggregates allowed efficient removal of the most common microplastics including high-density polyethylene, polypropylene, polyvinyl chloride, polystyrene, and polyethylene terephthalate. Full extraction was achieved using Fe3O4 at 1% of the mass of microplastics. Hydrogen bonding is the main force for the adsorption of Fe3O4. Unlike the more commonly used hydrophobically modified Fe3O4 nanoparticles, the bare Fe3O4 benefitted from the peroxidase-like activity of its exposed surface, enabling further catalytic degradation of microplastics with nearly 100% efficiency and easy recovery of the Fe3O4.[2]

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Keyword: nanozymes, enzyme mimics, peroxidase, iron oxide, microplastics

最终交流类型: Invited

Neuronal Differentiation of Stem Cells Regulatated by Nanostructure Mediated Electric Signals for Neurodegenerative Disease Therapy

Hong Liu
山东大学

Stem cell therapy is a promising treatment approach for neurodegenerative diseases and other disease. However, directly regulation of stem cell differentiation especially in vivo is still one of the greatest obstacles for stem cell therapy.

The conventional approach for inducing or accelerating directly differentiation is building bio-microenvironment of the stem cells with some biomolecules as growth factors. However, the biomolecules, including proteins, enzymes, and RNAs, are of expensive and easily to be degraded in vivo or out control to diffused into other tissues, which brings great difficulties for practical stem cell therap. Fortunately, some receptors with related to physical signals on the surface of extracellular matrix of stem cells provided a great opportunity to regulate stem cell fate by material cues or physical signals derived from materials. Compared with bio or chemical signals, material cues can be applied quantificationally and timely on the cells which are derived from interaction of the external physical field and internal nanostructured materials. Among all the physical fields, localized electric filed with wireless mode should be most promising approach to stimulate stem cells in vitro or in vivo. However, for the conventional electric stimulation approach, external electric signal generator and a pair of conductive wires are essential to providing a electric pulse current to a conductive substrate and realizing electric stimulation on the stem cells seed on the surface of the substrate. To overcome this problem, recent years, we proposed a new concept in bio-materials-physics interdisciplinary research, regulation of stem cell fate by nanostructure mediated physical signals, and great progress in this area have achieved. In this talk, we will introduce the principal, progress, and prospective of this topic by introducing recent works in our group. The important part of this talk are the evidences that wireless electric signals generated on piezoelectric or conductive nanomaterials driven by ultrasound or alternating magnetic field can realize the promotion of neuronal differentiation of neural stem cells and mesenchymal stem cells in vitro, and demonstrated stem cell therapy of the neurodegenerative disease based on the animal experiments.

Keyword: Stem cell, Nanostructure, Neuronal differentiation, Electric signal, Neurodegenerative disease therapy

最终交流类型: Invited

In Situ Remote Control of Nanomaterials for Regenerative Immunomodulation and Cancer Therapy

Heemin Kang
Korea University

Cells continuously interact with native nanostructured extracellular matrix at the molecular level. Developing remotely controllable nanobiomaterials can present bioactive

ligands or deliver functional molecules as a nanomedicine to regulate or understand dynamic nanoscale cell-nanomaterial interactions. In this talk, I will demonstrate the design of nanoengineered biomaterials that can be remotely controlled by various tissue-penetrative stimuli, such as magnetic field, light, self-assembly, or their combinations.

Magnetic field can control the motion of magnetic nanomaterials, such as reversibly controlling RGD ligand nano-sliding, nano-blocking, nano-stretching, and nano-coupling, to regulate the focal adhesion-mediated mechanosensing and resultant differentiation of stem cells. Near-infrared light that can activate photonic nanomaterials enabling photoisomerzation or visible light mediate reversible swelling and deswelling of liganded supramolecular self-assembly, respectively, and delivering the loaded molecules to regulate the adhesion-mediated pro-regenerative and anti-inflammatory polarization of macrophages. Furthermore, molecules/ions can reversibly induce *in situ* self-assembly of biofunctional nanomaterials.

I will also introduce a few recent cancer therapies for which this kind of remote-control strategies can be potentially applied via magnetic field, light, and ultrasound enabling cancer therapy and imaging using mechanical stimuli, 1-D nanomaterials, in situ self-assembly, and ferroptosis. These approaches can present benefits for safe patient-tailorable therapies without drug resistance that arises from conventional chemotherapy.

Keywords: *In situ* control, remote control, nanomedicine, regenerative immunomodulation, cancer therapy

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最终交流类型：Invited

Dynamic DNA nanotechnology enables ultrasensitive detection of nucleic acids and proteins in clinical samples

李峰
四川大学

Nucleic acids and proteins are important biomarkers for disease diagnosis and prognosis. However, many clinically important nucleic acids and proteins exist in trace concentrations in clinical samples. Detection of trace levels of biomarkers in clinical samples against high concentrations of interfering molecules has long been an analytical challenge. Facing this challenge, a primary goal of molecular diagnosis is the rational design of molecular probes with enhanced analytical performances for clinical uses. In this talk, I will introduce our recent effort to harness dynamic DNA nanotechnology and fundamental chemical thermodynamics to guide the rational design of molecular probes. Specifically, we have developed a set of new tools capable of precise measurement and control of key thermodynamic properties of molecular probes. The combined theoretical and experimental approaches also revealed key thermodynamic parameters determining the analytical performance of molecular probes. Guided by thermodynamic models, we further developed a panel of ultrasensitive DNA hybridization probes for the discrimination of low abundant single nucleotide variants (SNVs) in complicated clinical samples, such as human serum. With these tools, we have successfully achieved sensitive detection of circulating tumor SNVs in 108 lung cancer patients. We have also developed a panel of ultrasensitive DNA probes for detecting trace levels of protein biomarkers, such as cancer biomarkers and anti-SARS-CoV-2 antibodies, which enabled the monitoring of seroconversion in 85 kidney transplant recipients subject to COVID-19 vaccination. Clinical validation using serum samples collected from the general population (n = 197), demonstrates that our assay for ultrasensitive protein detection has 100% sensitivity and 98.5% specificity. With ultrahigh sensitivity, our technology enables the quantitative analysis of serum anti-SARS-CoV-2 levels in vaccinated kidney transplant recipients who are shown to produce “undetectable” anti-SARS-CoV-2 using standard immunoassay. Because of the high sensitivity and simplicity, we anticipate that the ultrasensitive tools enabled by dynamic DNA nanotechnology will find wide applications for clinical uses in both centralized laboratories and point-of-care settings.

Keyword: DNA nanotechnology; Clinical diagnostics; bio analysis

最终交流类型: Oral

Responsive organic nanoagents for cancer immunotherapy

Jingchao Li
Donghua University

Inducing immunogenic cell death (ICD) by sonodynamic therapy (SDT) is promising for cancer immunotherapy, which however is inefficient due to oxygen depletion that compromises SDT effect and mediates recruitment of immunosuppressive myeloid-derived suppressor cells (MDSCs). The fabrication of sono-activatable semiconducting polymer nanopartners (SPNTi) to simultaneously augment ICD and alleviate MDSCs for immunotherapy is reported. A sonodynamic semiconducting polymer, hydrophobic hypoxia-responsive tirapazamine (TPZ)-conjugate, and MDSC-targeting drug (ibrutinib) are encapsulated inside such SPNTi with surface shell of a singlet oxygen (1O2)-cleavable amphiphilic polymer. TPZ and ibrutinib serve as drug partners to enlarge immunotherapeutic effect. Upon sono-activation, SPNTi generate 1O2 to break 1O2-cleavable polymers for in-situ liberations of TPZ-conjugate and ibrutinib in tumor sites, and oxygen is consumed to create severer hypoxic tumor microenvironment, in which, TPZ-conjugate is activated for augmenting ICD action, while ibrutinib alleviates MDSCs for promoting antitumor immunological effect. In a bilateral tumor mouse model, SPNTi-mediated sono-activatable immunotherapy results in growth restraints of primary and distant tumors and noteworthy precaution of tumor metastases. This study thus provides a sono-activatable immunotherapeutic strategy with high precision and safety for cancer via overcoming post-treatment hypoxia and targeting MDSCs. Such a therapeutic strategy has shown significant advantages for cancer treatments in terms of both precise drug delivery and amplified therapeutic effect. The sono-activatable nanosystem could achieve in-situ specific deliveries of drugs into tumor sites upon activation mediated by US, enabling more precise drug delivery compared to traditional and tumor microenvironment-activatable drug delivery nanosystems. Overall, we report a sono-activatable immunotherapeutic strategy with high precision and efficacy. This study thus presents the first sono-activatable nanoplatform that allows US-triggered on-demand releases of two drugs to achieve ICD augmentation and

MDSC alleviation simultaneously. In consideration of the satisfying tissue penetration depth of US, this sono-activatable immunotherapeutic strategy should be available for treatment of deep-seated orthotopic tumor models, which will be explored in future works.

Keyword: Myeloid-derived suppressor cells, immunotherapy, sono-activation, semiconducting polymer nanoparticles, immunogenic cell death

最终交流类型: Oral

Rational Design of Lipid-based Nanoparticles for Organ Selective mRNA Delivery

刘帅
College of Pharmaceutical Sciences

mRNA therapeutics have shown various utilities for the COVID-19 vaccines, CRISPR/Cas gene editing, and diverse human diseases. However, vectors are required for mRNA function, since these nucleic acids encounter difficulty in entering the targeted organs, tissues, and cells. Therefore, targeted, efficacious, and safe mRNA delivery have remained challenging, hindering the advancement and clinical translation of mRNA drugs. Lipid nanoparticles (LNPs) have been regarded as the most successful non-viral mRNA carriers for the clinical translation. Thus far, most LNPs only mediate mRNA expression in the hepatocytes, and extrahepatic delivery remains to be solved. To solve this problem, we designed a novel ionizable phospholipid (iPhos) library, and the formulated iPLNPs enabled organ selective (liver, lung, or spleen) mRNA delivery and CRISPR/Cas gene editing in vivo. The structure-activity relationships revealed that iPhos chemical structure, especially alkyl length, could control in vivo efficacy and organ selectivity. Additionally, iPhos lipids synergistically functioned with various helper lipids to formulate multi-component lipid nanoparticles (iPLNPs) for selective organ targeting. Zwitterionic, ionizable cationic, and permanently cationic helper lipids enabled selective protein expression in spleen, liver, and lungs (respectively) following intravenous mRNA delivery. For the delivery and application requirement to other specific organs (e.g. lymph nodes), in pursuit of other mRNA carrier types might provide a way forward. Polymers represent a promising therapeutic vehicle class for gene delivery outside the liver but are hampered by low efficacy in vivo. We proposed a facile phospholipidation and post-modification methodology to introduce zwitterions into cationic polymers. Ultimately, the zwitterionic polymers mediated efficacious and safe mRNA expression specifically in the lymph nodes and spleens, demonstrating great

immunotherapy potential. This strategy has extended the utility of polymer family for precise gene therapy, providing an insight of new nucleic acid vector development besides LNPs. All above research achievements about lipid-based nanoparticle delivery systems show substantial translation potential.

Keyword: Lipid nanoparticles, mRNA delivery, Organ selectivity, Zwitterionic polymers, Precise gene therapy

最终交流类型: Oral

Assembled nanodrug inhibit uveal melanoma growth and metastasis by targeting dysregulation of m6A modification

Hao Tian
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Uveal melanoma (UM) is the most common primary intraocular malignancy in adults, characterized by high invasion and lack of effective treatment options. Our previous studies have demonstrated dysregulation of m6A modification in UM. The level of m6A in UM cell was much lower than that in normal cells, and the expression of m6A demethylase FTO was significantly upregulated in UM cell. These findings suggested that dysregulation of m6A modification played a significant role in the pathogenesis and progression of UM[1,2]. In this study, we found that meclofenamic acid (MA), an inhibitor of m6A demethylase FTO, could effectively suppressed the proliferation and migration of UM cells. However, due to its hydrophobicity, in vivo application of this drug posed challenges. As an endogenous molecular, DNA has high biocapacity and low immunogenicity, Besides, some research had used DNA to deliver drugs by chemical modification. Thereby, without affecting the active site, MA was linked to the phosphorothiolated DNA backbone (PSDNA) via a disulfide bond to construct a MA loaded spherical nucleic acid (SNAMA). Agarose gel electrophoresis confirmed the successful linkage of DNA-MA, TEM showed the SNAMA is homodisperse with 15 nm diameter, DSL revealed a relatively narrow distribution of nanoparticle size. SNAMA presented relatively stability in serum, and the fluorescence image showed a good cell uptake rate of SNAMA. CCK-8 demonstrates a higher anti-tumor efficiency in SNAMA than MA, and IC50 was decreased about 4-fold. Additionally, the m6A dot blot presented a restored m6A modification in UM cells after SNAMA treatment, which means the active site of MA were not destroyed. Further, the SNAMA also showed significant efficacy in both orthotopic tumor models and liver metastasis models that it could significantly inhibit tumor

growth, as well as enhancing the immune microenvironment within the tumor area. In summary, this study constructed a nanomedicine delivery system that provided a new strategy for the treatment of UM and other malignancy by targeting dysregulation of m6A modification.

Keyword: Uveal melanoma, Spherical nucleic acid, m6A modification, Nanomedicine, Liver metastasis

最终交流类型: Invited

Tumor microenvironment-responsive nanoparticle enhance radiosensitivity in triple-negative breast cancer through enzyme-like activity

潘越
Sun Yat-Sen University, China

Breast cancer is the primary global cancer. Radiotherapy is vital in its treatment, but has drawbacks in tumor therapy. For instance, solid tumors' hypoxic environment lowers reactive oxygen species (ROS) production, reducing radiosensitivity and treatment effectiveness. Higher radiation doses harm surrounding normal tissues. Hence, enhancing tumor cell radiosensitivity is crucial for improving breast cancer radiotherapy efficacy. To address these limitations, we developed a tumor microenvironment-responsive nanoparticle (FeS2@Pt) that combines high atomic number element Pt with catalase-like activity (CAT) onto the peroxidase-like (POD) pyrite-based (FeS2) nanoparticle. We also modified the nanoparticle with the targeting molecule hyaluronic acid (HA) to allow for targeted delivery to tumor cells. This targeted nanoparticle (FeS2@Pt-HA) can be taken up by breast cancer cells through endocytosis mediated by the CD44 receptor, and its high atomic number element Pt allows for increased deposition of radiation energy in breast cancer. Additionally, it catalyzes excessive hydrogen peroxide (H2O2) in the tumor microenvironment to produce oxygen (O2) and hydroxyl free radicals (•OH), increasing the production of ROS and improving lipid peroxidation levels in breast cancer cells. This leads to increased DNA damage and radiosensitization of breast cancer cells through both endogenous and exogenous mechanisms. Furthermore, FeS2@Pt-HA induces apoptosis and ferroptosis of breast cancer cells after radiotherapy, resulting in their death. Our results show that tumor microenvironment responsive nanoparticle FeS2@Pt-HA can combine the intrinsic nature of high-Z element and the advantages of nanozyme to kill breast cancer with radiotherapy at

both cellular and animal levels, providing a promising approach for the development of nanozymes for radiotherapy sensitization of breast cancer.

Keyword: tumor microenvironment, responsive nanoparticle, radiotherapy, enzyme-like activity, triple-negative breast cancer

最终交流类型: Invited

Modulating Bio-Nano Interaction with A Superior Class of Antifouling Polymers

Changkui Fu
The University of Queensland

Poly(ethylene glycol) (PEG) has been used as a standard antifouling polymer for decades. However, increasing evidence has shown the limitations of PEG, especially its apparent immunogenicity. The PEG immunogenicity has significantly compromised its function as a safe stealth material and has been indicated as a possible cause for anaphylactic reactions to pegylated therapeutics such as mRNA-based vaccines for COVID-19. Although PEG is always regarded as a hydrophilic polymer, it is actually amphiphilic. The hydrophobicity of PEG due to the ethylene backbone or terminal group contributes to its interaction with protein molecules, facilitating the formation of protein corona to some extent of pegylated nanoparticles that would alter their circulation and biodistribution behavior. The emerging limitations of PEG have driven the development of alternative antifouling polymers for use in various biomedical fields. Driven by the highly hydrophilic nature of sulfoxide structures, sulfoxide polymers demonstrate exceptional hydrophilicity and have emerged as promising polymeric materials for biological applications. The talk will present our research on investigating the potential of sulfoxide polymers as a new class of antifouling polymers. I will talk about how sulfoxide polymers can modulate the interaction between material surfaces and biological systems, and their potential applications in constructing antifouling surfaces and advanced nanomedicines with prolonged circulation and improved targeting and accumulation within diseased tissue.

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Keyword: Antifouling Polymer, Bio-Nano Interaction, Nanomedicine, Surface Coating, Immunogenicity

最终交流类型: Invited

Modular and adaptive self-assembling dendrimers for biomedical applications

Ling PENG
CNRS

The application of nanotechnology is widely expected to bring breakthrough in medicine for disease treatment and diagnosis. Dendrimers are ideal materials for elaborating nanomedicine by virtue of their well-defined structure, multivalent cooperativity and nanosize per se. We have recently established modular and adaptive self-assembling dendrimer nanosystems [1] for the delivery of imaging agents [2] , anticancer drugs [3] and nucleic acid therapeutics [4] for cancer detection and treatment. Remarkably, these dendrimer nanosystems are able to exploit the in situ tumor-secreted extracellular vesicles for effective delivery and deep penetration in tumor tissue, while overcoming tumor heterogeneity and dynamic evolution.[3] Our findings offer a fresh perspective for exploiting the advantageous features of supramolecular dendrimers to reach the ultimate goal of nanomedicine

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Keyword: dendrimer, nanovector, drug delivery, nucleic acid delivery, bioimaging

最终交流类型: Invited

Amphiphilic dendrimer nanovectors for nucleic acid delivery

Ling PENG
Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, Aix-Marseille University

Nucleic acid therapeutics is becoming a new drug modality for treating various diseases, offering the unique opportunity to target "undruggable" targets, respond rapidly to evolving pathogens, and treat diseases at the genetic level for precision medicine.[1] However, nucleic acid therapeutics are unstable and have poor bioavailability, requiring delivery vectors to protect them and safely deliver them to the site of action to achieve the desired therapeutic effect.[2] Dendrimers, by virtue of the precisely controllable structure and cooperative multivalence, represent precision delivery vectors. We have constructed a series of amphiphilic dendrimers as nanovectors for nucleic acid delivery. These vectors are lipid/dendron conjugates, able to harness the delivery advantages of both lipid and polymeric vectors, the two most advanced nonviral vectors, while exploiting the nanosized structure for nanotechnology-based targeted delivery.[3] We will present our recent results on molecular engineering of amphiphilic dendrimers as smart and adaptive vectors to deliver various nucleic acid molecules to overcome their innate flaws and fulfill their therapeutic potentials in cancer treatment.[4]

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Keyword: dendrimer, nanovector, nucleic acid delivery, lipid/dendirmer conjugates, non-viral vector

最终交流类型: Oral

Nanoadjuvants: From Nanocarriers to Immunomodulators.

Jie Tang
The University of Queensland

Adjuvants play a critical role in enhancing the efficacy of vaccines by inducing stronger immune responses against antigens. However, the lack of adjuvants capable of eliciting potent cellular immunity remains a major challenge for the development of vaccines against cancer and infections. In this study, we aimed to design a next-generation Nanoadjuvant platform technology using surface engineered silica-based nanoparticles to not only act as nanocarriers for antigen delivery but also as immunomodulators to enhance vaccine efficacy.

In Nature, innate immune cells such as dendritic cells (DCs) undergo pyroptosis upon pathogen infection. Current studies mainly focus on inducing pyroptosis in cancer cells for tumour inhibition. There are few reports using DC pyroptosis-mediated protective immunity, which is important to design advanced adjuvants for vaccines.

Our research team synthesized sodium-stabilized dendritic mesoporous aluminosilicate nanoparticles (Na-^{IV}Al-DMSN) and investigated their ability to induce dendritic cell (DC) pyroptosis-mediated protective immunity. We made two key innovations: (1) Firstly, we synthesized Na-^{IV}Al-DMSN, a new material, using a simple chemical reaction between aluminate and silicate. This material possesses framework-stabilized sodium that can exchange protons, a large mesopore of ~ 30 nm, and a uniform particle size of ~ 240 nm. A PCT Patent has been filed, indicating the novelty and significance of our innovation. (2) Second, we have elucidated the structure-function relationship of Na-^{IV}Al-DMSN, which induces H^+/Na^+ exchange in acidic lysosomes, leading to lysosome rupture and K^+ efflux. This mimics the process by which natural viral infections occur, where pyroptosis is triggered in antigen presenting cells, eliciting protective immunity.

Our designed nanoadjuvants demonstrated excellent antigen loading capabilities and induced enhanced T-cell responses and innate immunity in a prophylactic colorectal cancer mouse model. The use of mesoporous aluminosilicates as DC modulators and the underlying structure-function mechanism are novel in materials science and nanomedicine. Overall, this study provides a promising next-generation nanoadjuvant platform for vaccine applications that could contribute to the development of effective cancer and infection vaccines.

Keyword: Adjuvants, Mesoporous silica nanoparticles, Nanovaccine, Pyroptosis

最终交流类型: Oral

Nanomedicine for Improving Cancer Immunotherapy

Yuanzeng Min
中国科学技术大学

Conventional treatments for cancer today include surgery, chemotherapy, radiotherapy, and a multidisciplinary combination of these treatments. The traditional paradigm of these therapies is to eliminate cancer by interfering with the growth and survival of tumor cells. Unfortunately, cancers often escape with the help of acquired mutations and cancer stem cells, leading to recurrence and thus limiting the efficacy of these treatments. Cancer immunotherapy, especially immune checkpoint blockades (ICBs), has revolutionized cancer treatment options by reactivating the host immune system, but significant challenges that limit the broader effectiveness of current immunotherapy remain to be addressed. Certain "cold" tumors (immunosuppressive phenotypes), such as pancreatic cancer, glioblastoma, ovarian cancer, prostate cancer, etc., have a very low response rate to ICBs due to their

inherent low immunogenicity. In addition, many patients who initially respond to ICBs lack a sustained response due to T-cell exhaustion. The increasing understanding of the immune system, the molecular mechanisms of the carcinogenic process and the identification of neoantigens have brought attention to the recognition and development of personalized therapeutic strategies to enhance the immune response, eradicate these cancer cells, and revitalize the anti-tumor effects with the help of memory cells when the cancer recurs.

First, we constructed an intelligent nanotherapeutic platform that responds to tumor acidic niches to provide a novel approach for drug design and use. Specifically, the stimulus-responsive nanoplatform retains its invisibility in normal physiological tissues, but can be activated to trigger the release of loaded drugs when homing into the tumor microenvironment. With a wide range of drug candidates, such as R848, Loxoribine, MK1775, Capecitabine, Simvastatin and NLG919, as model drugs, we verified that by combining the high permeability and retention effect (EPR) of nanoparticles with tumor site-specific local drug release, this delivery strategy improved off-target toxicity and anti-tumor efficacy. Given the complex mechanisms of cancer immune evasion, we also developed combination therapies that simultaneously targeted different stages of the cancer immune cycle. For example, the immunogenic cell death characteristics of traditional chemotherapy drugs, photothermal agents and ferroptosis inducers delivered by nanoplatform could not only directly kill tumor cells, but also initiate in situ vaccination from tumor-associated antigens released from dying tumor cells. Moreover, the use of tumor inhibitory cytokines, chemokines, TLR agonists, STING agonists, IDO inhibitors, immune checkpoint inhibitors, and cell cycle checkpoints can promote antigen presentation and immune cell activation. Our multifunctional nano-delivery system combined therapeutic agents with different mechanisms of action to overcome drug resistance caused by tumor heterogeneity, reverse the tumor immunosuppressive microenvironment, burst a powerful and durable anti-tumor response, and avoid tumor recurrence and metastasis. Finally, yet importantly, we treat cancer cells with ultra-high doses of various chemotherapy drugs in vitro to artificially enrich the diversity and specificity of neoantigens. Based on proteomic analysis, we confirmed that in vitro chemotherapy-induced nanovaccines prepared from cell lysates contain multiple neoantigens and DAMPs, exhibit comprehensive antigenicity and adjuvant properties, and provide a simple and promising nanotechnology-based strategy for the generation of autologous tumor cell vaccines.

In summary, we use nanomedicine strategies to improve the responses of cancer immunotherapy.

Keyword: Cancer nanoimmunotherapy, Clinical translation, Nanovaccine, Photothermal therapy, Responsive nanotherapeutic platform

最终交流类型: Oral

Self-Adaptive Nanomedicine for Cancer Treatment

Xiangdong Xue
上海交通大学

Due to the superb structural controllability, versatility, and tumor targeting, nanomedicines have been widely used in the diagnosis and treatment of various cancers. Although thousands of nanomedicines, such as liposome-, micelle-, and polymeric nanoparticle-based nanomedicines, etc., have been developed, only a handful have been approved for clinical use. Moreover, the majority of nanomaterials only improve the safety of pharmaceuticals and reduce the frequency of administration, without significantly enhancing their efficacy. The complex synthesis of the building blocks not only consumes a lot of labor force and resources, but also introduces organic solvent residues and extra chemicals, such as coupling agents and catalysts. For each and every chemical intervention, the biosafety of the corresponding solvent/chemical residues must be carefully evaluated, thereby substantially increasing the costs associated with the "bench-to-bed" translation. Complex biological barriers also considerably reduce the efficacy of drug delivery, and it is difficult for nanomedicines to simultaneously overcome the barriers because of inherent contradictions. Positively charged nanomedicines, for instance, are conducive to cellular uptake but susceptible to opsonization, which shortens the blood circulation time; if the nanomedicines were designed with negatively charged surfaces to prevent opsonization, their cellular uptake would be reduced. The stable nanomedicines can securely store cargoes but may not be able to release them effectively; while the loosened nanostructure may be conducive to complete drug release, blood sheer force and protein adhesion are detrimental to the nanostructure's maintenance in the bloodstream. Therefore, it would be beneficial to develop an easy-to-manufacture but comprehensive solution with a high drug-loading capacity that can overcome various biological barriers in order to deliver therapeutic and imaging agents efficiently.

Herein, we construct high drug-loading nanomedicines that can generate adaptive changes in structure, image signals, surface properties and other aspects in different biological microenvironments so that they can efficiently cross biological barriers, accurately deliver drugs or imaging agents to target cells, and achieve efficient and accurate tumor treatment and diagnosis effects. Our strategy can extensively improve drug loading, tumor targeting, and delivery efficiency, which would surely provide a new paradigm for developing nanomedicine with effective therapeutic and precision imaging properties.

Keyword: Drug delivery, cancer therapy, nanomedicine, biological barrier, imaging

最终交流类型: Oral

Mechanochemical bond scission for the activation of drugs

Shuaidong Huo
厦门大学

Pharmaceutical drug therapy is often hindered by issues caused by poor drug selectivity, including unwanted side effects and drug resistance. Spatial and temporal control over drug activation in response to stimuli is a promising strategy to reduce and circumvent these problems. Here we use ultrasound to activate drugs from inactive macromolecules or nano-assemblies through the controlled scission of mechanochemically labile bonds, providing the possibility to achieve precise regulation of drug activity. Using sono-mechanochemistry, we achieved the selective breaking of weak covalent bonds or non-covalent bonds by constructing different strategies and, for the first time, realized the precise activation of small-molecule chemotherapeutic drugs in polymers or nanostructures1. Subsequently, the selective regulation of protein structure and properties by ultrasonic mechanical force2 and the dynamic regulation of metal ion-based DNA base pair hybridization3 were realized. In view of the shortcomings of traditional polymer synthesis steps, such as cumbersome steps and long response time to ultrasonic mechanical force, we cross-integrated nanostructure and mechanochemistry, further designed and constructed a nanodimer that responds to ultrasonic mechanical force realizing ultrasound-controlled drug release and activation4. With this US method, the tissue penetration depth is easily regulated by varying frequency and energy through exposure time. Moreover, medically established HIFU was shown to promote mechanochemistry, again underlining the potential of mechanochemically controlled drug activation with tissue penetration depths in the centimeter range. These results offer a promising approach that can be tailored to the diverse molecular structures of modern pharmaceuticals. With this approach, we conceived of a potential future pharmacotherapy that might avoid systemic side effects and may be tunable to medical demands and clinically established techniques with spatiotemporal resolution. Relevant studies have further verified the advantages and potential of mechanochemistry in regulating drug activity, laid a theoretical foundation for customizing force-responsive drug activation systems, and provided a new strategy for precise drug therapy.

Keyword: Drug activation, Mechanochemistry, Ultrasound, Bond scission, Nanosystems

最终交流类型: Oral

Suppression of Bacteria and Viruses: The Potential of Carbonized Nanodots and Nanogels Derived from Phytochemicals

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National Taiwan Ocean University

Carbon-based nanomaterials such as fullerenes, carbon nanotubes, graphene oxides, and carbon dots hold potential in fighting bacterial and viral infections. However, their production methods tend to be intricate and lengthy. Addressing this issue, we've established a single-step, mild pyrolysis technique to create a range of bio-carbon nanomaterials with antimicrobial properties. Our initial strategy centered around generating antibacterial carbon quantum dots through the single-step pyrolysis of a biogenic mix of spermine and dopamine. The resulting polymeric carbon quantum dots exhibited notable antibacterial properties and showed high adhesive capabilities on both glass and polymeric contact lens materials. Moreover, a straightforward single-step dry heating method facilitated the production of carbon quantum dots from curcumin. These dots displayed robust antiviral activity against enterovirus 71 via various mechanisms. We've also crafted a single-step procedure for fabricating carbonized nanogels using biogenic quercetin and lysine. Serving as bifunctional agents, these nanogels demonstrated both antibacterial and antioxidant capabilities, thereby presenting a potential solution for treating topical bacterial keratitis. Furthermore, we exploited the thermal transformation of basic amino acids to create bio-carbonized nanogels, which inhibit drug-resistant bacteria, biopolymer-producing bacteria, and clinical isolates through multiple mechanisms. In conclusion, our study paves the way for developing antimicrobial carbonized nanomaterials. These materials provide a sustainable means to counter bacterial and viral infections in clinical settings.

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Keyword: carbonized nanomaterials, mild pyrolysis, biogenic amines, flavonoids, infectious diseases

最终交流类型：Invited

Nano Physical Pharmaceutics: the essential study for promoting in vitro/vivo performance of nanomedicine

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The clinic application of nanomedicine remains limited although tremendous intelligent nano-based delivery systems have been reported all these years. Benefited form closely interact with clinic MDs and carefully analysis of web of science, we thought that the big “bottle-neck” of nanomedicne, that is, the inconsistency between the exciting *in vitro* performance and disappoint *in vivo* behaviors was mainly attributed to the lack of physical chemistry properties study. To be more specific, the characterization of nanomedicine usually undergoes in the static solution, failing to take the impact of *in vivo* dynamic blood circulation, protein adsorption, complex interactions with cells and tissues into consideration.

Recently, we aim to tackle the development bottleneck of nanomedicine by proposing to study the physicochemical properties of nano-formulations, namely, the Nano Physical Pharmaceutics. Herein, the effects of surface chain dynamics, the kinetic properties of micelles and nanogels on their *in vitro/vivo* therapeutic index were systematically investigated. Then relations between physical chemistry parameters and *in vivo* performance were carefully proposed. Take polymeric micelles as an example, we have prepared a series of micelles with poly(*n*-butyl methyacrylate)$_x$-*b*-poly(*N*-acryloylmorpholine)$_y$ (PBMA$_x$-*b*-PNAM$_y$). The stability was determined by the hydrophobic/hydrophilic balance (K), namely, the ratio of hydrophobic core volume Vcore to the hydrophilic shell chain density rshell ($K = V_{core}/p_{shell}$). Microscopically, the hydrophilic PNAM chain segment density (p_{NAM}) lineally increased with the hydrophobic/hydrophilic block length ratio (N_{BMA}/N_{NAM}) because the surface chain area (S_{shell}/N_{agg}) decreases. Such increase of p_{NAM} means that the PNAM chain densely packed inside shell leading to loss of its mobility. This entropic repulsion forced enhanced micelle solubility *in vivo* at the distance smaller than 3 nm, resulting in the increase of micellar escaping effect. In addition, the antibody conjugation and the fundamental *in vitro/vivo* correlations between drug delivery and physicochemical properties of micelles, such as V_{core}, V_{core}/p_{NAM}, p_{NAM}, and S_{shell}/N_{agg} were also carefully investigated. Consequently, the Nano Physical Pharmaceutics will not only be instructive for the design of the nano-based DDS, but also greatly benefit the clinical application of nanomedicines.

Keyword: Nanomedicine, Physical chemistry, Nano physical pharmaceutics, Chain kinetics, in vivo behaviors.

最终交流类型: Oral

Macromolecular Aminoglycoside Targets Neutrophil Extracellular Traps in Treating Severe Sepsis

Dan Shao
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Sepsis is a life-threatening condition caused by systemic infection of the host. Sepsis is a complex, dynamic, non-linear disease that presents a considerable challenge to healthcare systems worldwide due to the complexity and variability of host-bacterial interactions. Despite the tremendous efforts made to sepsis medical care, sepsis remains a huge challenge for healthcare systems around the world and remains the leading cause of ICU deaths. The current treatment for sepsis comprises supportive care and timely administration of antibiotics that aim to control septic lesions. Antibiotics are primary and irreplaceable agents for sepsis treatment, as speedy and accurate control of the causative source of sepsis is critical. Previous studies have rigorously examined the use of immunomodulatory therapies and provided evidence for their wide-ranging beneficial effects against sepsis, particularly with persistent infection control. A deep understanding of the complex interplay between pathogens and host immunity can offer novel therapeutic targets to enable effective and safe management of sepsis.

Disrupted immune homeostasis is driven by the excessive activation of innate immune cells, which recognize danger signals including bacterial toxins, proteins, and nucleic acids from pathogens or damaged cells. Recent efforts aimed at developing more effective sepsis

treatments and drugs have focused on sepsis pathogenesis and its danger signals. Different scavenging strategies to treat sepsis have been adopted because excessive danger signals can cause systemic inflammation. NETs, among these danger signals, play a dual role in sepsis as they serve as a protective mechanism to combat bacterial infections, although excessive NETs can activate a series of inflammatory responses through the TLR signaling pathway, leading to diseases such as thrombosis, systemic lupus erythematosus, and sepsis. Therefore, there is a great interest in targeting the formation and scavenging of NETs to restore immune homeostasis in sepsis.

Encouraged by are fruitfully advantageous as macromolecular drugs in their nanoscale size and multivalence, which may render them prolong blood-circulation time, good biocompatibility, particularly with tailored selectivity and activity. Here, we designed the PEGylation cationic compounds Library (PEG-CCL) that showed promising antibacterial properties in vitro. We compared the ability of PEG-CCL to scavenge danger signals and identified the best-performing PEGylation Aminoglycoside compound (PEG-AGs), which exhibited the highest NETs binding affinities, selectivity, and survival rate, while also having lower toxicity both in vivo and in vitro. PEG-AGs is the first selective targeting polymer with inherent and dual activities that targeted NETs in sepsis and showed promising results as a potential therapeutic drug for septic intervention in clinical settings. These findings provide proof of principle for novel immunomodulatory therapy strategies that target NETs in sepsis.

Keyword: Macromolecular Aminoglycoside, Sepsis, Danger signals, Bioactive materials, Neutrophil Extracellular Traps.

最终交流类型：Invited

Metal-Phenolic Network (MPN) biomaterials for cancer therapy

代云路
澳门大学

Metal-phenolic networks (MPN), which make use of the coordination between metal ions and phenolic molecules, have emerged as promising materials for nanomedicine. Compared with other materials, MPNs have several potential advantages, including pH responsiveness, negligible cytotoxicity. Additionally, the phenolic groups in the materials can be functionalized to meet specific applications. We constructed a serious of polyphenol-based nanoplatform for combination cancer immunotherapy. These nanoplatforms were stable

under normal physiological environment and release therapeutic agents in the tumor site. The MPN can enhance anti-tumor immune response by various strategies by exploiting the tumor microenvironment. MPN based nanoplatforms can evoke highly efficacious cancer immunosurveillance while minimizing systemic side effects.

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Keyword: Metal phenolic networks, drug delivery, cancer therapy, nanomedicine

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最终交流类型：Invited

Nanoparticulate Acetone-Based Ketal-Linked Prodrugs

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南开大学

Nanotechnology can enable improved drug delivery, drug screening, and the development of personalized medicine. However, the vast potential of nanomedicine has been hindered by low delivery efficiency and uncontrolled drug delivery. Recently, acid responsiveness has become a frontier and an essential component in developing new medicines and extraordinary drug delivery carriers. Dr. Guo has been engaged in cross-research of functional chemistry and nanomaterials for a long time and has made many innovative achievements in acid-sensitive acetone-based ketal chemistry, iterative evolution and delivery mechanism of nanomedicine, and innovative applications of the prodrug. A new simple and efficient synthetic method for intermediates of acetone-based ketals and two complementary modular construction technologies of acetone-based ketals are established for the first time, which breaks the bottleneck of acetone-based ketal technology. It is the first to construct a nano-drug based on an acetone-based ketal prodrug, and the structure-activity relationship and regulation law are revealed. Moreover, a new concept to achieve in vitro-in vivo correlation of synergistic drug combinations is proposed by utilizing mutual prodrugs with fine-tuning drug release properties. Acetone-based ketal technology is first used to construct new prodrug molecules and long-acting microcrystalline drugs, and the feasibility of acetone prodrug in developing long-acting sustained-release preparations is confirmed. Based on the functional chemistry of acetone-based ketal, Dr. Guo's group will systematically study the adaptation law of prodrug and delivery carrier, build a diverse nanocarrier library and in vivo high-throughput, unbiased screening technology, develop new strategies for the tumor penetration of nanocarriers and promote the innovative development of nanobiology.

Keyword: Drug Delivery; Prodrug; Nanomedicine

最终交流类型: Invited

Normalizing physiological properties of the tumor microenvironment to wake up anti-tumor immunity using drug-free clay nanoparticles

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Cancer treatment efficacy is mostly affected by the tumor microenvironment (TME) complexity where anti-tumor immune cells are severely suppressed, and tumor antigens continue to mutate or lose. Tumor cells may dictate the TME by hijacking immune cells, fibroblasts and stromal cells, and generate the highly pro-tumoral TME with specific physiological properties, such as low pH, hypoxia, high levels of reactive oxygen species (ROS) and metabolites, and chronic inflammation. There is an increasing evidence showing that correcting one of these properties as an adjuvant therapy can essentially benefit the subsequent radiotherapy, chemotherapy and immunotherapy. Therefore, persistent, simultaneous normalization of the TME physiological properties with functional drug-free nanomaterials would be a promising adjuvant therapy, partly inhibiting the tumor growth and promoting the anti-tumor immunity, as demonstrated in our recent investigations.

In this talk, I will introduce our recent research outcomes in the specific aspect. First, we utilized weakly alkaline layered double hydroxide nanoparticles (LDH NPs) to persistently neutralize the excess acid in the TME [1]. Such a persistent neutralization helps effectively block autophagy of tumor cells, specifically induce apoptosis of tumor cells, increase the level of anti-tumor tumor-associated macrophage (M1) and T cells, but decrease the number of pro-tumoral immune cells, such as MDSCs, M2 and Treg cells (Figure 1, left) [1,2]. Overall, the tumor growth was largely inhibited and the anti-tumor immunity was promoted to some degree. Secondly, we functionalized LDH NPs to specifically alleviate hypoxia and deplete lactate in the TME simultaneously [3]. This was achieved by peroxidizing LDH NPs (LDH/MgO2 NPs) for O2 self-supply and co-loading catalase (pcCAT) and lactate oxidase (pcLOX) to reduce the level of H2O2 and lactate in the TME. In such a way, a few reactions occurred, including neutralizing the excess acidity, reducing the ROS level, supplying an essential amount of O2 and oxidizing lactate in the TME (Figure 1, right). These reactions altogether induced cancer cell apoptosis, significantly inhibited primary and distant tumor growth, and moreover transformed the immunosuppressive TME into immunostimulant “hot” one in the mouse model.

Collectively, the functional drug-free LDH NPs are a good immunomodulator and adjuvant to normalize the TME physiology, and successfully ‘awaken’ and promote the host innate and adaptive immune systems against tumors.

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Keyword: Tumor microenvironment, layered double hydroxide nanoparticles, anti-acidity, hypoxia relief, lactate depletion.

最终交流类型: Oral

Tailoring Nanomaterials for Site-Specific Bioimaging and Targeted Therapy

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The tumor microenvironment (TME) has its unique internal physiological characters, such as acidity, hypoxia, and overexpressed glutathione, etc. By taking advantages of these distinct features, the contrast agents or drug molecules could be encapsulated into well-designed nanomaterials, and then selectively activated in the target area, thereby greatly improving the imaging accuracy and antitumor effect. In view of the differences between the TME and normal tissue environment, we have developed a variety of strategies (extracellular vesicle-mediated bioorthogonal strategy, pH-responsive DNA self-assembly strategy, and charge regulation strategy, etc.) to optimize the tissue tropism of nanocarriers and therapeutic agents. Results showed that the therapeutic agents could be selectively activated in tumor tissues, hence remarkably maximizing the therapeutic effect and minimizing undesired systemic toxicity. Meanwhile, in vivo fluorescence imaging and controlled drug release were also achieved at the tumor site. Beyond that, we reported a general strategy that enabled tuning the tropism of polymersomes for liver- and spleen-selective delivery. In this study, we provide evidence for organ-selective delivery of polymersome, that the size, surface chargers, and polymer compositions alter in vivo fate of polymersome, thereby enabling organ-selective bioapplications. Overall, this work may open a new frontier for rational design of tissue-specific delivery systems for a variety of preclinical and clinical applications

Keyword: Site-specific, organ targeting, controlled release, theranositc

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最终交流类型: Oral

Universal Se Nanoadjuvant with Multi-functionality for Vaccine Development in Preventing Major Infectious Diseases

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暨南大学

Major infectious diseases such as SARS-CoV-2 and highly pathogenic avain influenza greatly threaten the health of humans, livestock and poultry, while leading to tremendous economic loss. However, the development of safe and effective novel vaccines is always the

big challenge in this field. It was demonstrated that the imbalance of redox metabolism of immune cells would greatly reduce the quality of the induced immunities under vaccination or pathogens infections. Therefore, novel adjuvant with redox regulation, payload carrier and immunopotentiating activities and its vaccines are greatly desired and meaningful for combating virus infection in clinic.

Se as the essential trace element in humans plays pivotal roles in maintaining the biological processes including the immune functions. Herein, we successfully developed Se nanoadjuvant-based SARS-CoV-2 vaccine by selecting spike proteins as the antigen and engineering the surface chemistry of Se nanoparticles. It was found that Se nanoadjuvant could significantly relieve redox stress of immune cells by regulating selenoproteins expressions and effectively enhance the immunological functions. Meanwhile, the nanovaccine could induce robust innate and cellular immunities and trigger durable specific neutralizing antibodies with high titer to highly efficiently inhibiting pseudovirus infection. In addition, by taking full advantage of biomineralization-like property of Se, we also successfully developed Se nanoadjuvant-based live-killed virus vaccines, which could significantly enhance the immunogenicity of the live-killed virus to induce robust cellular and humoral immunities. Our developed Se nanoadjuvant can not only improve the functions of immune cells by regulating redox metabolism, but also trigger multiple Toll-like receptors signalling pathways to activate immune cells while enhancing the cellular uptake of antigens. Se nanoadjuvant is broadly suitable for developing protein, DNA, and live-killed virus-based vaccines to combat major infectious diseases.

Keyword: vaccine, nanoadjuvant, major infectious disease, Se

最终交流类型: Oral

Macrophage based drug delivery system for combined tumor therapy

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Exploring an effective combination treatment scheme for tumors is an effective means to improve the clinical tumor efficacy. Macrophages, as the most important cell component in the tumor microenvironment, play a crucial role in the occurrence and development of tumors. At the same time, macrophages have the ability of tumor tissue targeting, tumor deep penetration and natural phagocytosis, which makes them have great potential in the design of drug delivery systems. The research group focused on designing novel drug delivery systems based on macrophages: Enhancing tumor chemoimmunotherapy by regulating the activity of macrophages; Designing macrophage membrane or macrophage membrane coated nanoparticles for joint delivery of tumor drugs to improve the effect of combined treatment of tumors; establishing "macrophage nano" delivery syste which was using active macrophages as delivery carriers to achieve drug targeted delivery and cell drug combination therapy. In addition, while focusing on the tumor immune microenvironment, we focused on the role of tumor draining lymph nodes in tumor immunity, and found that regulating the tumor draining lymph node microenvironment can effectively improve the tumor immunotherapy effect, providing a potential means for tumor treatment. The above research results show that macrophages as delivery targets and delivery carriers have good application prospects. At the same time, the strategy of regulating tumor and draining lymph node immune microenvironment is conducive to improving the efficacy of immunotherapy, and has significant transformation potential in the future clinical tumor treatment.

Keyword: Nano drug delivery system，Macrophages，Combined therapy

最终交流类型: Oral

Amphiphilic dendrimer based nanoassemblies as modular and adaptive delivery platform for nucleic acid therapeutics

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Nucleic acid therapeutics offer the unique opportunity to treat various diseases, in particular for “undruggable” diseases, by targeting their genetic blueprints for precision medicine. However, the clinical implementation of nucleic acid therapeutics highly depends on the development of delivery technologies that improve druggability. Among myriad delivery platforms, dendrimers exhibit great promise for nucleic acids delivery by virtue of their precise dendritic structure and unique multivalence property. Recently, amphiphilic dendrimers, marrying the characteristic of dendrimers, self-assembly performance of amphiphilic molecules and the bio-mimicry of lipids, has emerged as particularly appealing delivery platform for nucleic acid therapeutics. Our group has developed a series of amphiphilic dendrimers carrying protein-mimic hydrophilic dendrons and hydrophobic alkyl chains, which capitalize on the delivery advantageous of both dendrimer and lipid vectors to achieve safe and efficient delivery of nucleic acid in various cell lines, including cancer cells, stem cells and primary immune cells, animal model as well. Furthermore, we engineer these dendrimers by varying their structure to customize amphiphilic dendrimers with different size, shape, properties and functions. Such established amphiphilic dendrimer based nanosystems enable to serve as modular and adaptive delivery platform, which can deliver different nucleic acid therapeutics (siRNA and DNA), on-demand and exhibit excellent therapeutic performance both in vitro and in vivo in different disease models. Our studies open a new perspective on the engineering of tailor-made nucleic acids delivery platforms based on dendrimers in precision medicine.

Keyword: nucleic acid therapeutics, amphiphilic dendrimers, modular, adaptive, delivery platform

最终交流类型: Invited

Bioactivated in vivo assembly （BIVA）nanotechnology and biomedical applications

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In order to solve the problem of efficient delivery, bioactivated in vivo assembly (BIVA) nanotechnology based on the concept of enzyme catalytically induced in vivo assembly was proposed to build a modular design of peptide-based polymer delivery platform (as shown in Figure 1). Through experimental verification and molecular dynamics (MD) simulation, the stable conformation of the polymer monomer and the predicted parameters of the residue assembly structure after enzyme digestion (the surface area of the assembly module is %SASA) were obtained, and the three-dimensional conformation of the monomer with β-hairpin as the backbone of the polypeptide was optimized [1]. Different methods of enzyme catalysis were used to realize in-situ nanostructures in vivo, and the biological effects of in-situ assembled nanostructures were obtained through the evaluation of the structure-activity relationship of materials [2]. A new method for quantitative imaging analysis of in vivo assembly efficiency has been developed to optimize in vivo assembly efficiency [3], thereby regulating the metabolic behavior of in vivo assembly structures [4]. Based on BIVA technology, highly sensitive and specific polypeptide nanoprobes for bacterial infection and tumor imaging, variable nanoantibiotics with antibiotic adjuvant effect, and nano-antitumor

drugs with high efficiency in glucose metabolism regulation have been developed, and new ideas and solutions have been proposed for the biomedical application of polymeric materials.

Keyword: bioactivated in vivo assembly nanotechnology; peptide-based polymer; nanomedicine;

最终交流类型: Oral

A nanoscale shape-discovery framework supporting systematic investigations of shape-dependent biological effects

Wei Zhang
UCD

Nowadays it has become inevitable for human beings to be exposed to nanostructures with distinctive complex shapes. Gaining more depth knowledge regarding the nanoscale shape features regulated biological pathways becomes imperative not only for safety purposes, but also for the design of better nanocarriers for medical treatments.

However, a priori rational investigation of such a vast universe of shapes appears to present intractable fundamental and practical challenges. This has limited the useful systematic investigation of their biological interactions and the development of innovative nanoscale shape-dependent therapies. One of the major barriers to figuring out the link between nanoscale shape ensembles and biology is the difficulty to “identify” these irregular nano-shapes. As a basic step to eliminate the barrier shape quantification is required to make meaningful, reportable, and reproducible connections between shape distributions and biological outcomes. However, the major challenge is that in such a vast universe of shape we need to know where to look for interesting biological effects without the impracticalities of guessing or randomly searching a vast unknown shape space.

Here we introduce a concept of biologically relevant inductive nanoscale shape discovery and evaluation that is ideally suited to, and will ultimately become, a vehicle for machine learning discovery. (Figure 1) Combining the reproducibility and tunability of microfluidic flow nanochemistry syntheses, quantitative computational shape analysis, and iterative feedback from biological responses in vitro and in vivo (Figure 2), we show that these challenges can be mastered, allowing shape biology to be explored within accepted scientific and biomedical research paradigms.

Keyword: nanoscale shape, shape identification, microfluidic, tunable synthesis, biological effects

最终交流类型: Invited

NIR-II Fluorescent Probes for in vivo Multiplexed Biodetection

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Fluorescent imaging and sensing with high spatio-temporal resolution and sensitivity allow the direct visualization of dynamic biological interests at different levels of components from the molecules, cells in vitro to the tissues, organs in vivo.Disastrous light attenuation and background autofluorescence in tissue at conventional imaging window of 400-900 nm have limited this technique for in vivo analysis, but they both decrease at progressively longer wavelength. Over the past decade, advances in the development of functional fluorophores operating in the second near-infrared window (NIR-II; 1000–1700 nm) have allowed the investigations of deep anatomical features in vivo with high resolution and sensitivity. However, inhomogeneous signal attenuation due to biological matter hampers the application of multiple-wavelengths NIR-II probes to multiplexed imaging. Here we present lanthanide-doped NIR-II nanoparticles with engineered luminescence lifetimes for in vivo quantitative imaging using time-domain multiplexing. To achieve this, we devise a systematic approach based on controlled energy relay that creates a tunable lifetime range spanning 3 orders-of-magnitude upon a single emission band. We consistently resolve selected lifetimes from the NIR-II nanoparticle probes at depths up to 8 mm in biological tissues, where signal-to-noise ratio derived from intensity measurements drops below 1.5. We demonstrate that robust lifetime coding is independent of tissue penetration depth, and we apply in vivo multiplexing to identify tumour subtypes in living mice. Our results correlate well with standard ex vivo immunohistochemistry assays, suggesting that luminescence lifetime imaging could be used as a minimally invasive approach for disease diagnosis.

Keyword: Rare earth luminescent nanomaterials, NIR, Biomedical analysis

最终交流类型: Invited

Immune Nano-Adaptor and Antibody Delivery

王均

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Antibodies are important therapeutic agents for cancer, and antibodies blocking the negative regulators of T lymphocyte function (known as immune checkpoints) represent the predominant modality of cancer immunotherapy, which have revolutionized the treatment paradigm in oncology over the past few years. Despite remarkable progress, current immunotherapeutic antibodies-based treatments still have many limitations. Combination immunotherapy has recently emerged as a powerful cancer treatment strategy, and extensive clinical efforts are currently underway to examine the efficacy of combining checkpoint inhibitors, but improved efficacy comes at the cost of disabling side effects. As an alternative combination approach, bi/multi-specific antibodies, which contain two or more different antigen-binding sites in one molecule, are now emerging as a growing class of immunotherapies with the potential to further improve clinical efficacy and safety. Inspired by the unique characteristic of bi/multi-specific antibodies, we attempt to construct a nano-platform to conveniently and efficiently bind two or more categories of immunotherapeutic antibodies in clinical or preclinical development and form multivalent nanoantibodies. To achieve this objective, a universal platform was engineered by incorporating anti-IgG Fc antibodies (αFc) or FcγR1, which could specifically react with the conserved Fc fragment of almost all immunotherapeutic antibodies, to the surface of nanoparticles, and multivalent nanoantibodies could be constructed via simple mixing of immunotherapeutic antibodies (e.g., αPD-1 and αPD-L1) with αFc or FcγR1 decorated nanoparticles (named nano-adaptor). By choosing proper antagonistic and/or agonistic antibodies, bi/multi-specific nano-antibodies could activate immune effector cells (e.g., T cells, NK cells, and macrophages) and enhance interaction between effector cells and tumor cells via binding corresponding targets on both cells. Notably, the superiority bi/multi-specific nano-antibodies over the mixture of parental mAbs is validated in T cell, natural killer cell- and macrophage-mediated antitumor immune responses in multiple murine tumor models. Additionally, the versatile nanoplatform we reported here could be extended to the fields of targeted nanomedicine, disease diagnosis, and antibody engineering.

Keyword: Immune checkpoint inhibitor, cancer immunotherapy, bi/multi-specific antibody, nano-adaptor

最终交流类型：Oral

Amphiphilic dendrimer vector for the delivery of siRNA and saRNA in cancer therapy

Jing Wu
CNRS — Aix-Marseille university

Nucleic acid therapeutics are fast becoming an important drug modality for cancer therapy, because they can address undruggable targets and evolving pathogens, and provide precision medicine. [1] In particular, siRNAs are small interfering RNA molecules that can silence oncogenes, and saRNAs are small activating RNA molecules that can activate tumor-suppressor genes for cancer therapy.[1] However, nucleic acid therapeutics are unstable and have poor bioavailability. Therefore, they require delivery vectors to protect them and safely deliver them to the site of action to achieve the desired therapeutic effect.[2] We have developed innovative amphiphilic dendrimer vectors,[3] which are lipid/dendrimer conjugates and able to harness the delivery advantages of lipid and polymeric vectors, the two most advanced nonviral vectors, for nucleic acid delivery.[3] In particular, these dendrimer vectors are very effective for the delivery of both siRNA [4-5] and saRNA [6] in cancer therapy. We will present our recent results on amphiphilic dendrimers for the co-delivery of siRNA and saRNA therapeutics to provide a synergistic effect for more potent anticancer activity in treating pancreatic cancer, for which there is no efficacious treatment.

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Keyword: dendrimer, nucleic acid delivery, siRNA, saRNA, cancer therapy

最终交流类型: Keynote

Cytosolic delivery of biomacromolecules

Xiaohu Gao
University of Washington

Biomacromolecule-based imaging agents and therapeutics such as DNA, RNA, and proteins are often superior in structural and functional diversity compared to small molecules and much easier to design or screen. Despite these fundamental advantages, the power and impact of biomacromolecule -based agents are substantially undermined, because they cannot spontaneously cross the cell membrane. Conventional delivery techniques fail to address this fundamental problem in that the cargos are predominantly delivered inside cells via endocytosis, a remarkably effective cell defense mechanism to prevent intact biomolecules from entering the cytoplasm. Here, we report a unique concept, non-covalent cholesterol tagging, enabling oligonucleotides and virtually any proteins to permeate through the cell membrane, completely bypassing endocytosis. This simple plug-and-play platform greatly expands the biological target space and has the potential to transform basic biology studies and drug discovery.

Keyword: cytosolic delivery, endosome escape, biomacromolecules

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最终交流类型: Invited

Composite Scaffolds of Gelatin, Gold Nanoparticles and Doxorubicin-Encapsulated Thermosensitive Liposomes for Biomedical Applications

Guoping Chen
National Institute for Materials Science

Breast cancer is one of the most commonly diagnosed cancers. Strategies for breast cancer treatment have been widely studied. However, some challenges remain. For example, surgical resection cannot guarantee the complete removal of all cancer cells, and it may result in large resection defects. In recent years, local delivery of photothermal therapy (PTT) agents using photothermal scaffolds has been proposed. Local administration of anticancer drugs has also been reported as an efficient delivery platform. PPT agent- and drug-loaded scaffolds can be implanted during the surgical resection of cancers, therefore constraining the PTT agents and therapeutic drugs in the resected sites to efficiently kill the remaining cancer

cells after surgery. Furthermore, after ablation of cancer cells, the scaffolds can serve as a support to guide the reconstruction of breast tissue.

Therefore, in this study, thermosensitive liposomes loaded with doxorubicin were hybridized with PTT gold nanoparticles, gelatin and polyglutamic acid (PGA) to prepare PTT composite scaffolds for combination of PTT, chemotherapy, and breast tissue engineering. The composite scaffolds had good photothermal conversion and temperature-dependent doxorubicin release properties. Under near-infrared laser irradiation, the composite scaffolds increased the local temperature to not only kill the breast cancer cells in the scaffold but also accelerate the release of doxorubicin to eliminate the breast cancer cells surrounding the scaffolds. In vitro cell culture and in vivo mouse experiments demonstrated the synergistic anti-cancer effects of PTT and chemotherapy under near-infrared laser irradiation. Moreover, after drug release was complete, the composite scaffold supported the proliferation of hMSCs to guide new tissue regeneration. The results suggested that the composite scaffolds provided synergistic photothermal therapy and chemotherapy for breast cancer cell elimination at the early stage and promoted stem cell activities at the late stage.

Acknowledgements: This research was supported by JSPS KAKENHI Grant Number 19H04475 and 21H03830.

Keyword: Composite scaffold, photothermal therapy, chemotherapy, cacer therapy, tissue engineering

最终交流类型: Invited

Sustainable photocatalytic disinfection of pathogenic bacteria by immobilized TiO2-based composite and its mechanism

Yingnan Yang
University of Tsukuba

In this study, an effective visible light-assisted photocatalytic disinfection toward various representative pathogenic bacteria over a highly reusable glue-immobilized P/Ag/Ag2O/Ag3PO4/TiO2 (PAgT) system has been reported. The results showed that the PAgT photocatalyst could rapidly kill all pathogenic bacteria isolated from real water environment, including Gram-positive (+ve) (Enterococcus sp. and Staphylococcus aureus) and Gram-negative (-ve) (Escherichia coli and Salmonella), both in single and mixed bacteria system. Compared to Gram -ve bacterium, the inactivation of Gram +ve bacterium was more

resistant to the photocatalytic treatment, which was mainly ascribed to their thicker peptidoglycan layers in cell walls. In addition, using silicone glue as a binder provided a strong adhesion between the solid matrix and catalyst particles thus making the immobilized PAgT highly reusable. More strikingly, it was found that the enhanced antibacterial performance of immobilized PAgT system was due to a synergistic effect of disinfection mechanism combining the improved photocatalysis on the introduction of heterojunction structure, and the mechanical stress driven from the composite sharp edge morphology. Hence, the present results of the photocatalytic disinfection toward a broad range of pathogenic bacteria, with excellent activity, stability and reusability, reveals the possibility of the developed silicone glue-immobilized PAgT in real water sterilization.

Acknowledgements: This research was supported by JSPS KAKENHI Grant Number 19H04310 and JP18J20620.

Keyword: PAgT disinfection; Gram +ve/-ve pathogenic bacteria; Silicone glue-immobilized photocatalytic system; Synergistic effect on disinfection mechanism; High stability and reusability

最终交流类型: Invited

Polymer-based platinum(lV) prodrugs and their future development directions

肖海华

Institute of Chemistry, CAS, China

Platinum-based drugs have achieved great clinical success, but their toxic side effects and drug resistance limit their further application. To this end, a series of new platinum(IV) prodrugs and their polymer-based delivery systems have been developed. It is generally believed that these delivery systems can deliver platinum(IV) drugs to tumor sites and release platinum(II) specifically in tumor cells, further playing a key anticancer role. However, the distribution, metabolism, cellular uptake, and subcellular organelle distribution of platinum(II) drugs, platinum(IV) prodrugs, and their nanoparticles are significantly different, and their molecular mechanisms could be likely totally different but remains unknown till far. To this end, we propose here a new concept of "Nanomedomics" to explore the differences in the molecular mechanisms of platinum(II) drugs, platinum(IV) prodrugs, and their nanoparticles.

Moreover, as cancer cells are constantly evolving, the treatment modality and therapeutic doses should be dynamically adjusted based on the tumor evolution which results in cancer proliferation, resistance, and metastasis. Therefore, combined multimodal therapeutic methods are necessary to prevent a specific mutation and gradually control the remission of the tumor. Previous studies have demonstrated that multi-functional nanocarriers could deliver a variety of effective anticancer agents, such as chemotherapeutic drugs, drug sensitizers, peptides, proteins, antibodies, and, nucleic acids through physical encapsulation, chemical conjugation, or electrostatic interactions into a single nanomaterial. The unique properties of nanomedicines provide a possible solution to tackle dynamically and constantly evolving tumors. This would change the application of nanomedicines from a current “static treatment” to a “dynamic treatment”, allowing a strategic, purposed and precise treatment of mutating tumors in the future.

Keyword: platinum(lV) prodrugs, nanomedomics, polymer-based delivery systems

最终交流类型: Invited

Advancing Metallomics, Metabolomics, Glycomics and Pathogen Detections using Functional DNA Nanotechnology

Yi Lu
University of Texas at Austin

In comparison to detecting DNA, RNA and proteins, much less is developed to detect metal ions, metabolites, and glycosylated molecules even if they play important roles in human health. Unlike DNA/RNA or protein detections, obtaining sensors that can recognize metal ions, metabolites and glycoRNAs selectively is much more challenging. Similarly, while measuring DNA/RNA/proteins is commonly used to detect pathogens, they cannot tell whether the pathogens are infectious or not, which often result in delayed diagnosis and difficulty to mitigate the spread of the pathogens, including SARS-Cov-2.

To meet these challenges, we have been using in vitro selection to obtain DNAzymes and aptamers, collectively called functional DNAs, which are specific for either a metal ion, metabolite, glycan or infectious pathogen from a large DNA library of up to 1015 sequences and use counter selection to remove interferences from competing targets, such as a noninfectious pathogen. We have converted these functional DNAs into fluorescent, colorimetric and electrochemical sensors by conjugating them with different nanomaterials or device such as upconversion nanoparticles and nanopore.1 These nanosensors have allowed monitoring different metal ions,2 metabolites,3 glycoRNAs4 and infectivity of pathogens5 in the environment, at point of care and in living cells and mice. These advances in metallomics, metabolomics, glycomics and pathogen detections fill a major gap in modern human health and medicine by providing complementary information from genomics and proteomics. Together, they will result in much more accurate diagnosis, understanding and therapy of many diseases, including neurodegenerative diseases, such as Alzheimer diseases and cancers.

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Keyword: Metallomics, Metabolomics, Glycomics, COVID-19, DNAzymes, Aptamers, Nanoparticles, Nanopore

最终交流类型: Oral

COMBINATORIAL SYNTHESIS AND IN VITRO / IN VIVO EVALUTAION OF BISCARBAMATE IONIZABLE LIPIDS FOR LIPID NANOPARTICLE mRNA DELIVERY

Yong Chen
Gent University

mRNA-based drug products hold tremendous potential as vaccines against infectious diseases and cancer, as well as for protein replacement therapy and gene editing. In both cases, the patient's own cellular machinery is utilized as a factory to produce vaccine antigens or other therapeutic proteins. However, the key to successful deployment of mRNA drugs is the delivery of intact mRNA into the cytoplasm of cells where it can be translated by ribosomes into functional proteins. In its unformulated soluble form, mRNA is unable to achieve this goal. However, encapsulation of mRNA into lipid nanoparticles (LNPs) through electrostatic complexation between the phosphate anions of mRNA and the cationic amine(s) of an ionizable lipid can achieve successful cytoplasmic delivery of mRNA. Although ionizable lipids in LNPs have been demonstrated to be crucial for effective encapsulation and transfection of mRNA, the discovery of optimal ionizable lipids that fulfill all required tasks mentioned above remains an empirical process. Currently, the methods for developing ionizable lipids rely on large library screenings, which often involve multiple-step synthesis, iterative column purifications, and result in low overall reaction yields.

We report a novel series of ionizable biscarbamate lipids (IBLs) synthesized using a short, column purification-limited, and robust (> gram scale) method. The IBLs were created by linking dialkyl chains to an ionizable head group through an activated biscarbonate linker, which introduced a reduction-sensitive disulfide bond and a physiologically stable ether bond, respectively. The disulfides in the IBLs could aid in the delivery of intact mRNA in the cytoplasm by cleavage of the disulfide bond due to reductases in endosomes, disulfide exchange with cysteine residues in proteins, and elevated glutathione levels in the cytoplasm.

Keyword: ionizable lipids, lipid nanoparticles, mRNA

最终交流类型: Invited

A LIPID NANOPARTICLE TEMPLATED ANTI-OPIOD VACCINE

Bruno De Geest
Ghent University, Germany

The opioid use disorder epidemic is ravaging society, with high rates of relapse and overdose deaths. Anti-opioid vaccines could reduce long-term opioid (ab)use and the risk of accidental overdose. Current anti-opioid vaccines in pre-clinical development focus on bio-conjugates composed of opioid haptens that are chemically bound to an immunogenic carrier protein in combination with an admixed molecular adjuvant. This approach is sub-optimal on multiple levels: (1) This approach does not co-deliver the hapten-protein conjugate with the molecular adjuvant to antigen presenting cells in lymphoid tissue, although the latter would result in optima immune-induction. (2) Random conjugation of haptens to a carrier is a difficult to reproduce process, hence leading to issues regarding manufacturability. We present an approach inspired by the mRNA lipid nanoparticle (LNP) design that relies on physical entrapment of hapten, immunogen and molecular adjuvant in a single LNP.

These LNP contain: (1) A biologically inactive fentanyl-poly(ethylene glycol)-dialkyl lipid bio-conjugate for multivalent display of fentanyl haptens on the LNP surface. (2) In their interior an ionizable cationic lipid that entraps a CD4 T cell peptide epitope extended by a decaglutamate amino acid sequence to allow for electrostatic complexation with an ionizable lipid. (3) Also in their interior, a lipid-conjugated imidazquinoline TLR7/8 agonist as a moelcular adjuvant. In vivo in mouse models we demonstrate the induction of robust fentanyl-specific antibody responses with the isotype strongly depending on LNP

composition. We demonstrate that serum from immunized mice can sequester fentanyl and preventy it from binding to teh opidoid receptor using an opioid receptor reporter cell assay. Finally we demonstaret that immunized mice show iver a ten-fold reduced latency in responding to a thermal stimulus.

Keyword: anti-opioid vaccine, hapten, lipid nanoparticles

最终交流类型: Invited

Nanotechnologies for skeletal tissues repair

Peter Timashev
Sechenov University

In regenerative medicine, bioequivalents need to be biocompatible. There are different methods to increase the biocompatibility of tissue-engineered constructs, such as using natural biomaterials like collagen or modifying synthetic biomaterials to neutralize their degradation products and enhance their hydrophilicity.

The introduction of biologically active substances with pro-regenerative properties, such as lactoferrin (LF), into the structure of collagen membranes, is a promising strategy. Our research team has developed a technology for producing collagen-lactoferrin matrices with Janus structure providing complete and uniform LF release in 3 days using an electrophoretic co-deposition technique. We later demonstrated their stimulating effect on metabolism, proliferation, and migration in vitro as well as their beneficial effect in vivo.

Cellular component of bioequivalents is no less important. Multipotent mesenchymal stromal cells (MSCs) are the most common cellular component of tissue-engineered constructs due to their unique regenerative potential. They are widely used in three-dimensional bioprinting, as well as for the formation of spheroids, aggregates of cells cultured under non-adhesive conditions. Due to the special microenvironment, gradient of oxygen and nutrients, spheroids represent a unique physiological model for both fundamental and applied research. In particular, they are currently regarded as a promising target for bioprinting. Bioprinting with spheroids ensures rapid and uniform filling of the volume of the construct with cells, which contributes to its better integration.

There is also increasing evidence that the regenerative potential of MSCs is partly due to their paracrine activity, which involves the synthesis of cytokines, chemokines, and extracellular vesicles. In general, the current tissue engineering paradigm implies comprehensive approaches to the creation of bioequivalents, including the use of smart biomaterials and cell secretome, including nanovesicles.

The study was financially supported by the Russian Science Foundation (No 22-75-10120; bioink preparation and characterization) and the Ministry of Science and Higher Education (№075-15-2021-596, cell cultures and nanovesicles).

Keyword: biomaterials, bioprinting, nanovesicles

最终交流类型:

Peculiarities of multipotent mesenchymal stromal cell secretome: cytokines, growth factors and extracellular vesicles

Maria Peshkova
Sechenov University

There is a growing body of evidence that the regenerative potential and therapeutic effect of MSCs are caused not only by their ability to differentiate and replace the damaged tissue areas but also by their paracrine activity. It is determined by the synthesis of cytokines and growth factors, as well as by the release of extracellular vesicles (EVs) - membrane particles transporting biologically active molecules and providing intercellular interactions. However, there is a lack of data on the characteristics of MSCs secretome from different sources. The aim of the study was to compare the MSCs secretome from different sources and under different cultivation conditions, as well as to characterize the proteomic profile of MSCs EVs. MSCs isolated from human bone marrow, umbilical cord, gum, adipose tissue, and placenta were cultured in 2D and 3D conditions, and their immunophenotype was characterized by flow cytometry. The levels of cytokine and growth factor secretion in the cultures were assessed by multiplex analysis. Proteomic analysis was performed via liquid chromatography with tandem mass spectrometry. Human umbilical cord-derived MSCs exhibited higher levels of cytokines and growth factors than MSCs from other sources. Proteomic analysis revealed common patterns in proteomic composition of vesicles obtained from conditioned media and from the extracellular matrix, namely extracellular environment organization, immune, and transport pathways enrichment. However, each type of EVs had a unique differential abundance profile. Thus, it was shown that human umbilical cord-derived MSCs are an optimal source of cytokines, growth factors and extracellular vesicles involved in tissue remodeling and can be used in the development of new therapeutic strategies.

Research was financially supported by the Ministry of Science and Higher Education of the Russian Federation under the grant agreement No. 075-15-2021-596.

Keyword: multipotent mesenchymal stromal cells, extracellular vesicles, cellular spheroids

最终交流类型: Invited

Changes in the structure and secretome profile of mesenchymal stem cells in 2D and 3D culture conditions

Nastasia Kosheleva
Sechenov University

The therapeutic effects of mesenchymal stem cells MSCs are mediated by their ability to secrete paracrine growth factors, cytokines, and extracellular vehicles (EVs). The structural and functional properties of cells depend on their microenvironment and culture conditions.

The aim of this study was to compare the characteristics of MSCs secretome and EVs from different sources and under different culture conditions.

MSCs were isolated from human bone marrow, Wharton's jelly, gingiva, adipose tissue, and placenta and cultured in 2D (monolayer) and 3D (spheroids) culture.

In 2D culture, cells were fibroblast-like and matched the immunophenotype of MSCs. After seven days in 3D culture conditions, MSCs spheroids consisted of several surface layers of elongated, densely packed cells and an inner zone with polygonal cells and an extracellular matrix. Cells in these spheroids had small round shaped mitochondria, well-developed cytoskeleton represented by intermediate filaments of vimentin, and were quantitatively enriched in proteins of mitochondria biogenesis, respiratory chain, extracellular proteins, and cytoskeleton. 2D and 3D cultures of MSCs from the same source exhibited identical prevailing cytokines with some difference in their ratio. Among all the sources Wharton's jelly MSCs demonstrated the highest cytokine levels in the conditioned media, and the secretion was higher in spheroids compared .to monolayers. The obtained EVs exhibited spherical and cup-shaped morphology, the mean size was 80-100 nm. Proteomic analysis revealed extracellular environment organization pathways enrichment in the most monolayer-derived EVs, protein targeting- and translation-related pathways were highlighted in spheroids-derived EVs.

Thus, human Wharton's jelly MSCs are a promising source of paracrine growth factors, cytokines, and regulatory EVs to develop new cell-free therapeutic products.

The research was financially supported by the Ministry of Science and Higher Education of the Russian Federation under grant agreement No. 075-15-2021-596.

Keyword: mesenchymal stem cells, spheroids, secretome, extracellular vesicles

最终交流类型: Invited

Biomedical Application of Emerging NanoAlum Beyond Drug Delivery System

张凌宵
Aarhus University

Magnesium aluminum layered double hydroxides (LDH) is a kind of two-dimensional nanomaterials widely used in biomedical field.[1] As an ideal drug delivery system (DDS), LDH efficiently delivers genes, peptides, proteins and small molecules against major diseases include cancers and neurodegenerative diseases. It is worth noting that LDH has been clinically used as an antigastric drug (Talcid, Bayer) since the 1960s, and our recent study also found that LDH can also be obtained from a commercial aluminum adjuvant (Imject Alum, Thermofisher) by hydrothermal treatment, thus defined as a new type of nano adjuvant (NanoAlum).[2] As DDS, LDH have efficiently deliver antigens or immunomodulators to lymph nodes, spleen and tumors to evoke potent cytotoxic T lymphocyte (CTL) response against solid tumors.[3-8] Besides, LDH with appropriate surface modification also successfully crossed blood-brain barrier and delivered small molecules and genes to relieve the symptom of Alzheimer's disease mice.[9] Beyond DDS, the inherent antacid properties of LDH and the variability of its metal ions allow it to be used directly as drug-free nanoparticles for disease therapy, for example, to effectively remodel the suppressive tumor immune microenvironment (TIME). Our recent study found that peritumoral injection of LDH can neutralize the acidic TIME while supplementing Mg2+, which greatly promotes the recruitment and activation of peripheral CTLs into the tumor to inhibit the growth of solid tumors.[3] Upon LDH is taken up by tumor cells, it can neutralize intracellular acidic lysosomes to block the tumor autophagy pathway, thereby inducing tumor apoptosis.[10] Interestingly, partial replacement of Mg2+ in LDH by nutritional metal ions (M) such as Zn2+ results in nutritional NanoAlum (NanoMAlum) Zn-LDH, which can not only activate anti-tumor immune cells in TIME, but also induce tumor immunogenic death by activating the tumor cGas-STING signaling pathway and down-regulating the expression of tumor immune checkpoints.[11]

Keyword: layered double hydroxides, NanoAlum, drug delivery system, drug-free nanoparticles

最终交流类型: Invited

Transformable nanomedicine for precision cancer imaging and therapy

Yuanpei Li
University of California, Davis, United States

Nanoparticle-based theranostic agents are emerging as a promising paradigm towards personalized nanomedicine for disease- and patient-specific diagnosis and treatment. We have developed a series of highly innovative transformable nano-theranostics that were highly capable to circumvent the sequential biological barriers which had hindered the drug delivery to tumors. These nano-theranostics have intrinsic fluorescence and are able to chelate various metal ions for non-invasive “visualization” of tumor, drug delivery and therapeutic effect by magnetic resonance imaging (MRI) and near infrared fluorescence imaging (NIRFI). Moreover, the synergistic multi-modality therapy (photothermal-, photodynamic-, chemo- and immuno-therapies) with these nano-theranostics were demonstrated to be highly effective with high complete cure rate in a variety of subcutaneous and orthotopic cancer xenograft models. These nano-platforms with powerful delivery efficiency and versatile theranostic functions shows enormous potentials to improve cancer diagnosis and therapy.

Keyword: Transformable nanomedicine, biological barriers, cancer

最终交流类型: Oral

Mapping signal-to-noise ratio in complex solutions of DNA circuits

Alexander Hawes
Newcastle University

As time continuously marches forwards so too does the field of dynamic DNA nanotechnology by utilising the predictability and programmability of Watson-Crick base pairing to create DNA circuits with a wide range of functionality including molecular switches, motors, catalytic cycles, dynamic walkers, computing and memory devices to name just a few. DNA circuits incorporating toehold mediated strand displacement are a widespread tool in the field of molecular computing. Noise can occur in a DNA circuit when a non-target invader with sequence similar but not exact sequence complementarity displaces an incumbent stand from a given gate. Compared to targeted signal mediated reactions, whose kinetics are fairly well understood, the rates of noise mediated reactions involve mismatch kinetics which are difficult to estimate with current simulation software. Consequentially, it is impossible to accurately predict the signal-to-noise ratio (SNR) for a strand displacement circuit. To address this, we map the impact of single and double cytosine mismatches across a ten nucleotide range (six-nucleotide toehold plus initial four-duplex nucleotides) totalling 56 unique invader sequences. We experimentally measure the reaction rates for each sequence and analyse the impact of mismatch quantity and location in non-target pathways. NuPack is utilized to estimate the binding energy of the signal-gate and noise-gate products and compare trends in binding energy against experimentally measured reaction rate constants. This work lays the foundation to understand SNR in complex systems comprised of multiple parallel gates.

Keyword: DNA, DNA nanotechnology, DNA computing, toehold mediated strand displacement, mismatch

最终交流类型: Oral

Ferritin-based targeted delivery of arsenic to diverse leukaemia types confers strong anti-leukaemia therapeutic effects

王昌龙
山东第一医科大学

Trivalent arsenic (As^{III}) is an effective agent for treating patients with acute promyelocytic leukaemia, but its ionic nature leads to several major limitations like low effective concentrations in leukaemia cells and substantial off-target cytotoxicity, which limits its general application to other types of leukaemia. Here, building from our clinical discovery that cancerous cells from patients with different leukaemia forms featured stable and strong expression of CD71, we designed a ferritin-based As nanomedicine, As@Fn, that bound to leukaemia cells with very high affinity, and efficiently delivered cytotoxic AsIII into a large diversity of leukaemia cell lines and patient cells. Moreover, As@Fn exerted strong anti-leukaemia effects in diverse cell-line-derived xenograft models, as well as in a patient-derived xenograft model, in which it consistently outperformed the gold standard, showing its potential as a precision treatment for a variety of leukaemias.

Keyword: Ferritin, Leukemia, Targeted delivery, Arsenic Trioxide

最终交流类型: Oral

Rejuvenation of macrophages by bacteria-targeted transformable peptide nanoagonist for sepsis-caused secondary infection

卿光超
国家纳米科学中心

Secondary infection caused by sepsis frequently lead to organ failure and death. Dysfunctional macrophage is primarily responsible for the insufficient antimicrobial defense in septic patients with immunosuppression, increasing the risk of opportunistic infections. Although there are some progresses in reviving macrophages, simultaneously inhibit bacterial infection and rejuvenate the deactivated macrophages in vivo remains a challenge. Here, a bacteria-targeted transformable peptide nanoagonist (BactTPNa) self-assembled by the peptide that composed of the bacteria-targeted UBI$_{29\text{-}41}$, the cholesteryl hemisuccinate (Chems) modified β-amyloid-derived FFVLK, and the immunoglobulin G derived tuftsin (TKPR) with natural phagocytosis stimulating ability has been proposed to manage the secondary infections through bacterial capture and impaired macrophage' rejuvenation. The results demonstrate that our BactTPNa can effectively bind to the surface of bacteria at the site of infection, and the hidden tuftsin will be everted to the encapsulated bacterial surface by virtue of the self-assembly of FFVLK once the Chems is removed from the skeleton of the peptide by bacterial lipase. After that, the enhanced phagocytosis of macrophages to enveloped bacteria and the subsequent repolarization of macrophages are achieved through the binding of tuftsin and FcγR on bacterial surface and macrophages, respectively, leading to the renovation of impaired local and system immune function to against secondary infection of septic mice. Hence, our BactTPNa-based therapy that combined pathogen control and host immunity restoration is an alternative therapy for sepsis-related secondary infection.

Keyword: Sepsis, Secondary infection, Peptide nanomaterials, Self-assemble, Macrophages, Immunotherapy

最终交流类型: Invited

Self-powered Medical Devices and Electrical Stimulation Therapy

李舟
北京纳米能源与系统研究所

Electrical activity is the basis of human life activities. Regulating electrical activity changes the excited and inhibited states of cells, tissues and organs to treat diseases. Nanogenerators are the new type of energy conversion device that convert low-frequency mechanical energy into electrical energy. In addition, it has gained the attention of researchers because of the flexibility, spinnability, high-output voltage, structural and material diversity . We employed nanogenerators to efficiently convert the mechanical energy of human motion into electrical energy and supply power to electrical stimulation devices and biosensors. Then, we developed self-powered electronic medical devices and medical sensors to carry out more systematic research work. The power generated from the heartbeat can be used to drive the cardiac pacemaker to work for a long time, construct symbiotic cardiac pacemaker, as well as complete the research on improving heart rate and treating arrhythmia in the large animal experiments for the first time. Degradable self-powered electrical stimulation devices are used to regulate the growth direction of nerve cells, enhance intercellular integration and regulation of cardiomyocytes, promote osteoblasts proliferation and differentiation, accelerate skin wound healing. Besides, the devices can be completely absorbed by the body after the disease treatment. There are researches on self-powered cardiovascular biosensors that can realize minimally invasive implantation and have good biocompatibility. These researches focus on self-powered electronic medical devices and electrical stimulation therapy, and have important potential to be transformed into electronic medical devices and medical sensors for clinic treatment.

Keyword: Self-powered; Nanobiotechnology; TENG;

最终交流类型: Invited

Structure Regulation of Fluorescent Probe for Precise Imaging

张晓兵
湖南大学

The efficient acquisition of biochemical information is an important link for human beings to explore the essence of various life phenomena. And the development of high-performance detecting tools for biochemical information provides a significant approach for early diagnosis of diseases and navigation of tumor surgery, thus it has become a research hotspot and difficulty in modern analytical chemistry. Fluorescence imaging technology based on small molecule probes has the advantages of high sensitivity, simple operation, fast response speed, small sample damage and high spatial and temporal resolution, and is a powerful tool for obtaining biochemical information at the cellular and living level. However, due to disadvantages such as easy signal diffusion, limited response specificity, and serious background interference during in vivo imaging, traditional fluorescent probes are difficult to achieve accurate imaging of targets in cells and in vivo. To solve these key scientific problems, we have carried out a series of research work: 1) Based on the orderly assembly mechanism of small molecule probes driven by hydrogen bonds, our group developed a series of novel in situ imaging probes, achieving accurate in situ detecting of target molecules in cells and in vivo; 2) Based on electron-rich anthracene derivatives, our group exploited high-brightness afterglow luminescent materials and constructed a precise imaging method via afterglow luminescence resonance energy transfer, realizing long persistent imaging of conscious and freely moving animals for the first time; 3) Based on systematic study of the "structure-activity" relationship of fluorescent imaging probes, our group proposed a strategy of developing highly selective fluorescent probes through molecular structure regulation, achieving highly specific acquisition of biochemical information in complex biological systems.

Keyword: luorescent molecular probes; Structure regulation; Orderly assembly; Organic afterglow luminescence; Precise imaging

最终交流类型：Oral

Noncanonical Amino Acids Regulate Peptide Assembly into Biomedical Materials

余志林
南开大学

Precise self-assembly of peptides into well-defined nanostructures represents one of the versatile strategies for emulating the structures and functions of proteins and creating advanced biomedical and soft materials. Over the past few years, the reliable sequence-

structure-function relationship for peptides has been broadly demonstrated. This finding inspires the development of the stimulus-responsive sequences to regulate self-assembly of peptides under complicated biological microenvironment. In this context, noncanonical amino acids exhibiting disease biomarker-responsiveness have been designed and incorporated into peptides for in situ formation of biomedical materials in living cells. In this presentation, I will introduce several in situ peptide assembling systems under tumor microenvironment on the basis of stimulus- responsive noncanonical amino acids. The advantages of the in situ assembling systems in drug delivering will be discussed to emphasize the critical role of adaptable morphology of delivery vehicles in overcoming biological barriers and improving drug delivering efficiency. Combining these results with the ligand functions of peptides, the implication of these peptides towards establishing hybrid biomedical materials will also be illustrated.

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Keyword: Peptides; Self-Assembly; Unnatural Amino Acids; Stimulus-Responsive; Drug Delivery

最终交流类型：Keynote

Lipid nanoparticles enabled mRNA therapeutics

Yizhou Dong
Icahn School of Medicine at Mount Sinai

Messenger RNA (mRNA) has shown great promise for broad therapeutic applications. However, the efficient and safe delivery of mRNA remains a key challenge for the clinical use of mRNA-based therapeutics. Lipid and lipid-derived nanoparticles possess unique properties for mRNA delivery. In this talk, I will describe the development of lipid-derived nanoparticles for delivery of multiple types of mRNAs and their potential applications for treating genetic disorders, cancers and infectious diseases.

Keyword: Lipid nanoparticles, mRNA

最终交流类型: Invited

How to write for Nature Reviews journals

Sadra Bakhshandeh
Nature Reviews Bioengineering

This presentation will be a short workshop on how to write for Nature Reviews journals, with a particular focus on Nature Reviews Bioengineering.

Keyword: Scientific publishing

最终交流类型: Keynote

Bacterial and Viral Biosensors with Functional Nucleic Acids and Nanomaterials

Yingfu Li
McMaster University

Rapid detection of bacterial and viral pathogens is vital for preventing infectious disease outbreaks, but current detection methods oftentimes lack the means to detect infectious pathogens in a simple, rapid, and reliable manner at the time and point of need. Functional nucleic acids (such as DNA aptamers and DNAzymes), when combined with nanomaterials, offer the potential to overcome these limitations by acting as key components for point-of-care (POC) biosensors due to their distinctive advantages that include high binding affinities and specificities, excellent chemical stability, ease of synthesis and modification, and compatibility with a variety of signal-amplification and signal-transduction mechanisms. In this presentation, I will discuss the work completed in my laboratory, in collaboration with several other groups at McMaster, towards developing effective biosensors and bioassays that integrate functional nucleic acids with nanomaterials to detect bacterial and viral pathogens, such as E. coli, Salmonella, SARS-CoV-2, porcine epidemic diarrhea virus, directly in water, food or clinical samples.

Keyword: Functional nucleic acids, DNAzymes, aptamers, biosensors, viruses, bacteria

最终交流类型：Oral

Surface Engineered Biohybrid Bacteria as Photo-controlled NO Generator for Tumor Immunological and Gas Combination Therapy

Baizhu Chen
中山大学

The use of bacteria as living vehicles has attracted increasing attentions in tumor therapy field. The combination of traditional functional materials with bacteria for the construction of biohybrid living system dramatically facilitates the antitumor effect. Here, we presented the rationally programmed *Escherichia Coli* MG1655 cells (Ec) coated with black phosphorus (BP) nanoparticles (NPs) to realize the photo-controlled tumor immunological and gas combination therapy [1]. The bacterial cells were genetically engineered to express tumor necrosis factor-related apoptosis-inducing ligand (TRAIL, Ec-T) using the surface display system [2]. The Ec-T cells were associated with BP NPs on their surface to acquire the BP@Ec-T biohybrid living system. The MG1655 cells could transfer the photoelectrons produced by BP NPs after laser irradiation and triggered the reductive metabolism of nitrate to nitric oxide (NO) for the *in situ* release at tumor sites, facilitating the therapeutic efficacy and the polarization of tumor associated macrophages to M1 phenotype. Meanwhile, the generation of reactive oxygen species induced the immunogenic cell death and promote the mature of dendritic cells (DCs) to further improve the antitumor efficacy. Additionally, the living system enhanced the immunological effect by promoting the apoptosis of tumor cells, activating the effect of T lymphocytes and releasing the pro-inflammatory cytokines. The integration of BP NPs, MG1655 cells and TRAIL led to an effective tumor therapy (Fig 1). Our work established an approach for the multifunctional antitumor living combination therapy.

Keyword: Surface Program; Genetically Engineered Bacteria; Photo-controlled NO Generator; Combination treatment; Tumor therapy

最终交流类型：Oral

The development of theranostic nanoplatforms for brain disease and cancer treatment

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Promoting the precise diagnosis and treatment of critical diseases is one of the most important strategic goals in our country’s medical and healthcare field. The reporter’s research work mainly focuses on the development of theranostic biomaterials with controllable properties for the treatment of serious diseases. Based on the interdisciplinary research between materials science, chemistry, biology, and medicine, the reporter has constructed a series of novel micro-nanobiomaterials with well-controlled features to solve current challenges in precision medicine and has achieved several important innovations, which includes (1) the development of blood-brain-barrier (BBB)-crossing nanoplatform to improve the delivery of RNA drug into central nervous system for traumatic brain injury treatment, (2) the fabrication of highly bright and high-contrast imaging nanoprobes to accurately guide the surgery and immunotherapy of tumors, (3) the construction of dynamic biomaterials with tunable properties for on-demand manipulation of the function of therapeutic-related enzymes or cells to promote enzyme- and cell-based therapy. These works are expected to give inspirations for the further development of advanced theranostic platforms via rational material design to boost their performance for precision diagnosis and treatment of critical diseases such as brain diseases and tumors.

Keyword: theranostic nanoplatforms, brain disease, tumor, nanoprobe

最终交流类型: Invited

Nano-neurobiology for treatment of brain diseases

Xue Xue
南开大学

Brain disease is the public health problem that seriously threat to human health. The diagnosis and intervention of major brain diseases are very important content in the field of neurological science and technology in the future. Although brain science research is developing rapidly, there is still a lack of effective diagnosis and treatment methods and clinical medicine. Our research point out that applying novel nanobiomaterials to regulate the homeostasis imbalance of neurobiofilms (including blood-brain barrier membrane and neural cells membrane) is one of the important ways to treat brain diseases. These approaches can not only utilize the superior physical and chemical properties of the material itself, but also interact directly with neurobiofilms, so as to achieve the purpose of regulating the component, structure and distribution of the key regulators on the cell membrane, and ultimately achieve efficient therapy of brain diseases. Our studies also help to reveal the mechanism of brain

diseases, establish diagnostic criteria, discover new biomaterials for interventions, and provide therapeutic targets for brain diseases therapy, providing promising perspectives for neuro-bioeffects exploration of nanobiomaterials.

Keyword: Brain diseases; Neurobiofilms; Nanobiomaterials; Diagnosis and treatment

最终交流类型: Invited

The role of the biochemical and biophysical properties of the microenvironment in the nanomechanical properties of breast cancer cells

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University of Rome "Tor Vergata"
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Keyword: breast cancer, nanoindentation, collagen scaffolds, kappa-carrageenan

最终交流类型: Invited

Size-dependent Nano-bio interactions of Nanoparticles in the Kidneys

杜步婕
华南理工大学

Kidneys, as a major organ for blood filtration and waste elimination, play a key role in the transport and clearance of nanoparticles in vivo. Fundamental understanding nanoparticle-kidney interaction is important for precisely constructing nanoparticles to realize disease-targeting-efficiency maximization and toxicity minimization. Among various physicochemical properties of nanoparticles, size is an essential factor in controlling nanoparticles transport in the kidneys. In this talk, Dr. Bujie Du will present a new size-dependent nano-bio interactions law in the kidneys, which can be summarized as “glomerular barrier behaves as an atomically precise bandpass filter in a sub-nanometer regime”. By systematically studying a series of different-sized renal clearable gold nanoclusters and fluorescent sensors, kidney diseases detection and the strategy to specifically image renal cell carcinoma were illustrated. These discoveries highlight the size precision in the body’s response to nanoparticles and opens a new pathway to develop nanomedicines for precise kidney disease diagnosis and treatment.

Keyword: Size-dependent; Nano-bio interactions; Kidney; Biological effect

最终交流类型: Oral

Strategy and Case Study of Nanodrug Design Based on Tumor Biological Feature

阮静
上海交通大学医学院

Tumor cells are evolved from molecular mutation events under the biological pressure, such as oncogene activation, tumor suppressor gene inactivation, and epigenetic mutation, which occur in some related tumor initiating cells under pressure selection. Exploring the origin and evolution pressure of tumor cells plays a guiding effect in tumor therapy. Different tumors have different origin cells and the pressure environment they are subjected to. Therefore, for different tumor, if the evolution pressure can be rationally used to reverse the molecular mutation of tumor cells, the efficiency of tumor treatment should be improved. Based on the research idea, our research team focused on the ocular melanoma and designed different nanodrug based on this cancer. Strategy 1: Considering the melanoma cell could secret an amount of melanin and the melanin has a strong absorption ability to ultraviolet light, we developed an ultraviolet light-sensitized nano drug. The nano drug could generate amounts of singlet oxygen and reactive oxygen species (ROS) through the ultraviolet light stimulation based on the fluorescence resonance energy transfer, so the ROS could damage the cancer cell and achieve effective treatment on melanoma. Strategy 2: miR-30a-5p was screened and discovered as a kind of tumor suppressive gene on uveal melanoma, based on this biological molecular character of cancer, a nanodrug was designed to efficiently deliver miR-30a-5p mimics through nanocarriers, the nanodrug system not only could protect mimics biological activity under the physiological environment, but also could effectively down-regulate the transcription factor E2F7 expression level, and thus inhibit the cancer cell growth and migration. These two kinds of nano drugs were design based on the biological characteristics of ocular melanoma, they all have advantages of high tumor cell responsive rate, good bioavailability and biosafety, and significant inhibition role on tumor growth.

Keyword: Tumor Biological Feature; evolution pressure; molecular mutation; nanodrug; tumor therapy

最终交流类型:

Functionalized biomimetic hydrogel as a platform for in vitro tissue models

Polina Bikmulina
Sechenov University

Development of novel perspective hydrogels for 3D bioprinting is one of the major challenges in tissue engineering. Here we created hydrogel containing natural polymers, such as fibrin and gelatin, modified with PEG-acrylate to ensure two-step crosslinking and optimal structure. As a cellular bioink component, we used human mesenchymal stromal cell spheroids. With this bioink, the 3D extrusion bioprinting was performed to obtain living structures that has mechanical stability and supports cell adhesion and proliferation. We also performed a detailed analysis of physiological activity of cells during construct maturation. Thus, 3D bioprinting with bioink based on functionalized fibrin-gelatin hydrogel and cellular spheroids provides the microenvironment required for the survivability, maintenance of functional properties and maturation of cells, what is crucial for the full development of in vitro tissue models.

The study was supported by the Russian Science Foundation grant No. 21-15-00349.

Keyword: Hydrogel, fibrin, gelatin, 3D bioprinting, spheroids

最终交流类型: Oral

‘on/off’-switchable crosslinked PTX-nanoformulation with improved precise delivery for NSCLC brain metastases and restrained adverse reaction over nab-PTX

吴昊
西安交通大学

Non-small cell lung cancer (NSCLC) brain metastases present a significant treatment challenge due to limited drug delivery efficiency and severe adverse reactions. In this study,

we address these challenges by designing a ‘on/off’ switchable crosslinked paclitaxel (PTX) nanocarrier, BPM-PD, with novel ultra-pH-sensitive linkages (pH 6.8 to 6.5). BPM-PD demonstrates a distinct ‘on/off’ switchable release of the anti-cancer drug paclitaxel (PTX) in response to the acidic extratumoural microenvironment. The ‘off’ state of BPM-PD@PTX effectively prevents premature drug release in the blood circulation, blood-brain barrier (BBB), and normal brain tissue, surpassing the clinical PTX-nanoformulation (nab-PTX). Meanwhile, the ‘on’ state facilitates precise delivery to NSCLC brain metastases cells, as indicated by the remarkable Pearson's coefficient index (0.77), and enhances tumour penetration distance by over 160 μm. Compared to nab-PTX, BPM-PD@PTX demonstrates improved therapeutic efficacy with a reduced tumour area (only 14.6 %) and extended survival duration, while mitigating adverse reactions (over 83.7%) in aspartate aminotransferase (AST) and alanine aminotransferase (ALT), offering a promising approach for the treatment of NSCLC brain metastases. This research contributes to the field of cancer therapeutics and has significant implications for improving the clinical outcomes of NSCLC patients.

Keyword: NSCLC brain metastases, ultra-pH-sensitive linkages, restrained adverse reaction, switchable crosslinking

最终交流类型: Invited

Targeting oncogenic KRAS with molecular brush-conjugated antisense oligonucleotides

王大力
上海交通大学

The mutant form of the guanosine triphosphatase (GTPase) KRAS is a key driver in human tumors but remains a challenging therapeutic target, making $KRAS^{\mathrm{MUT}}$ cancers a highly unmet clinical need. Here, we report a class of bottlebrush polyethylene glycol (PEG)-conjugated antisense oligonucleotides (ASOs) for potent in vivo KRAS depletion (Figure 1). Owing to their highly branched architecture, these molecular nanoconstructs suppress nearly all side effects associated with DNA-protein interactions and substantially enhance the pharmacological properties of the ASO, such as plasma pharmacokinetics and tumor uptake. Systemic delivery to mice bearing human non-small-cell lung carcinoma xenografts results in a significant reduction in both KRAS levels and tumor growth, and the antitumor performance well exceeds that of current popular ASO paradigms, such as chemically modified oligonucleotides and PEGylation using linear or slightly branched PEG. Importantly, these conjugates relax the requirement on the ASO chemistry, allowing unmodified, natural phosphodiester ASOs to achieve efficacy comparable to that of chemically modified ones. Both the bottlebrush polymer and its ASO conjugates appear to be safe and well-tolerated in mice. Together, these data indicate that the molecular brush-ASO conjugate is a promising therapeutic platform for the treatment of KRAS-driven human cancers and warrant further preclinical and clinical development.

Keyword: NSCLC, KRAS, antisense oligonucleotide, molecular brush, gene regulation

最终交流类型: Invited

Hepatic biotransformation of ultrasmall noble metal nanoparticles

蒋兴垭
华南理工大学

Liver is the central organ for metabolism and detoxification of xenobiotics including many engineered nanoparticles. Biotransformation is a key process involved in liver metabolism and detoxification machinery. This talk will introduce our work in understanding the hepatic glutathione-mediated biotransformation of ultrasmall noble metal nanoparticles, an important class of nanomaterials with widespread application in nanobiotechnology and nanomedicine, and how this hepatic biotransformation process impacts the transport of nanoparticles in vivo. Fundamental understanding of the biotransformation mechanism further allows us to design nanoprobes capable of detecting drug-induced liver injury at such an early stage that liver damage is completely reversible.

Keyword: biotransformation, metal nanoparticle, nanomedicine, physiology

最终交流类型: Oral

Delivery systems for CRISPR/Cas-based cancer therapy

巩长旸
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CRISPR/Cas is the adaptive immune system of bacteria and archaea, which can resist the invading viruses and exogenous DNA. Owing to its simplicity, versatile and low cost, CRISPR/Cas system offers a promising platform for genome editing of mammalian cells. The development of CRISPR/Cas system has rapidly promoted scientific progress in multiple fields such as stem cell engineering, gene and immunotherapy, animal disease model construction, and target screening etc. Although CRISPR/Cas technology has shown promising applications, its in vivo application still faces multiple challenges due to the large coding size of the system, lack of tissue targeting, and the potential off-target effects. In order to address these issues, we have developed a variety of artificial virus for precise and efficient delivery of CRISPR/Cas system in vivo, and have performed a series of studies based on the application of CRISPR/Cas technology in cancer therapy. Compared with traditional virus delivery systems, our artificial virus delivery system has the advantages of precise tumor targeting, high gene loading capacity, low immunogenicity, and scale-up production while maintaining comparable transfection efficiency. Moreover, we have realized genome editing in mouse tumor models utilizing these delivery systems which achieved excellent anti-tumor effect. Thus, artificial virus we developed may serve as gene delivery systems for in vivo application of CRISPR/Cas genome editing system in cancer therapy.

Keyword: CRISPR/Cas; genome editing technology; delivery system; artificial virus; cancer therapy

最终交流类型: Oral

Identification of Antibiotic Resistance in ESKAPE Pathogens through Plasmonic Nanosensors and Machine Learning

鲜于运雷
浙江大学

Antibiotic-resistant ESKAPE pathogens cause nosocomial infections that lead to huge morbidity and mortality worldwide. Rapid identification of antibiotic resistance is vital for the prevention and control of nosocomial infections. However, current techniques like genotype identification and antibiotic susceptibility testing are generally time-consuming and require large-scale equipment. Herein, we develop a rapid, facile, and sensitive technique to determine the antibiotic resistance phenotype among ESKAPE pathogens through plasmonic nanosensors and machine learning. Key to this technique is the plasmonic sensor array that contains gold nanoparticles functionalized with peptides differing in hydrophobicity and surface charge. The plasmonic nanosensors can interact with pathogens to generate bacterial fingerprints that alter the surface plasmon resonance (SPR) spectra of nanoparticles. In

combination with machine learning, it enables the identification of antibiotic resistance among 12 ESKAPE pathogens in less than 20 min with an overall accuracy of 89.74%. This machine-learning-based approach allows for the identification of antibiotic-resistant pathogens from patients and holds great promise as a clinical tool for biomedical diagnosis.

Keyword: gold nanoparticles, bacterial identification, antibiotic resistance, machine learning, biomedical diagnosis

最终交流类型:

Optimized electrospun scaffolds for scaffold-free cell therapies: assessing 3D tissue surrogates and cell interactions

Gilyana Kazakova
Sechenov university

In the realm of scaffold-free cell therapies, there's a quest for developing organotypic three-dimensional (3D) tissue surrogates in vitro, capitalizing on the inherent ability of cells to create tissues with efficiency and sophistication that still remains unmatched by human-made devices.

In this study, we explored the properties of scaffolds obtained by electrospinning thermosensitive polymers Poly-N-isopropylacrylamide/N-tert-butylacrylamide (PNIPAM/nTBA), intended for use in such therapies. These copolymers, having a molecular weight of 223 and 136.6 kDa, were utilized to generate a system based on a multicomponent graft copolymer via a mechanochemical approach and a specialized twin-screw extruder.

We examined the morphology, solution viscosity, porosity, thickness of spun matrices, mechanical properties, as well as hydrophobic-hydrophilic characteristics of the scaffolds. Particular attention was paid to studying the influence of the thermosensitive polymer's weight-average molecular weight on the resultant scaffolds and the role of electroforming parameters on the morphology and mechanical characteristics of the scaffolds.

A critical aspect of this study is the investigation of the interaction between various cell cultures and scaffolds of different thickness and porosity. Our findings provide significant insights into the approaches for optimizing scaffolds for specific cell cultures, thereby offering new possibilities for scaffold-free cell therapies.

This work was supported by the Russian Science Foundation (grant RSF 21-15-00349, https://rscf.ru/project/21-15-00349/).

Keyword: Electrospun nanofiber, thermosensitive polymers, PNIPAM/nTBA, scaffold-free cell therapies, regenerative medicine

最终交流类型: Oral

Self-assembling supramolecular dendrimer nanosystems for tumor imaging

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Centre Interdisciplinaire de Nanoscience de Marseille

Early and accurate tumor detection is key to successful cancer management. However, imaging sensitivity and specificity still constitute major challenges. Application of nanotechnology for elaborating imaging agents has the potential to increase imaging sensitivity, precision and specificity, because nanosized probes possess the ability to carry a large number and different types of imaging reporters while also exhibiting tumor-targeting capabilities via either passive or active tumor targeting. We have recently developed innovative supramolecular dendrimer nanosystems1 for tumor imaging using positron emission tomography (PET)1 and single photon emission computed tomography (SPECT)2. These nanosystems were constructed via self-assembling of amphiphilic dendrimers bearing Ga3+ and In3+ radionuclides respectively, at the dendrimer terminals. They formed uniform and stable nanomicelles, which accumulated readily in tumor lesions. Benefiting from the combined dendrimeric multivalence and EPR-mediated passive tumor targeting, these nanosystems demonstrate superior imaging compared to the clinical reference. In addition, the surface charge of nanoparticle impacted importantly the biodistribution3: slightly positively charged nanoparticle had reduced liver uptake than those negatively charged. Consequently, they constitute promising probes for efficient tumor detection. We are actively investigating the chemistry behind these nanosystems with respect to their size, morphology, surface charge and self-assembly feature to improve biodistribution and imaging specificity.

Keyword: Amphiphilic dendrimer, bioimaging, self-assembly, cancer diagnostic, positron emission tomography

最终交流类型: Invited

Nanomedicine for acute critical illnesses -- physics and engineering to improve safety and efficacy

Jacob Brenner

University of Pennsylvania

Acute critical illnesses are those that can immediately lead to death or permanent organ injury, and these diseases include stroke, sepsis, acute respiratory distress syndrome, and more. A unifying feature of all these diseases is microvascular dysfunction, with capillary leak allowing toxic plasma proteins and leukocytes to infiltrate the parenchyma. To combat this, we develop nanoparticles, primarily liposomes and RNA-LNPs, that bind via targeting moieties to the primary cell types of the microvasculature: capillary endothelial cells and marginated leukocytes. However, in acute critical illnesses, numerous inflammatory pathways can be activated by typical nanoparticles, ranging from complement activation in the plasma to intracellular detection of nanoparticle uptake. We use detailed physics-based models to understand these nanoparticle interactions with the immune system to guide our engineering of improved nanoparticles. With such innovations, we have developed therapeutics for the above acute critical illnesses, though much additional work remains. We will describe both our recently published manuscripts in Nature Nanotechnology, Advanced Materials, and ACS Nano, as well as unpublished work currently under review.

Keyword: nanomedicine, lipid nanoparticle, LNP, RNA, liposome, stroke, sepsis, ARDS

最终交流类型: Oral

Preparation of Microenvironment-Responsive Lipid-like Nanocarriers for Azithromycin and Evaluation of Antibacterial Activity

常进
太原理工大学

Bacterial biofilm is one of the most important factors for multidrug resistant to antibiotics. In recent years, the rapid development of nano-delivery systems has provided new strategies for the treatment of bacterial infections. aiming at the key problems in the treatment of bacterial biofilms, a novel kind of nanoliposome with multiple stimuli responsiveness was designed, termed as AZM-SSLNPs, with the particle size of 180.38±1.94 nm and PDI of 0.29, the Zeta potential is 0.99±0.84 mV and the encapsulation efficiency of AZM is 71.46±0.57%. Afterwards, AZM-SSLNPs electrostatically combined with CA-Tyr to fabricate AZM-SSLNPs@Tyr, with the particle size of 225.45±2.58 nm, PDI of 0.28, the Zeta potential of -15.14±0.62 mV, the adsorption capacity of CA-Tyr of 73.14±0.99%, and the encapsulation

efficiency of AZM of 69.45±1.52%. AZM-SSLNPs@Tyr triggered the immediate release D-Tyr (65.52% release) to damage the matrix of the biofilm with acidic pH stimulus under the simulated bacterial microenvironment. By the introduction of disulfide bonds, the release of AZM was realized thorough GSH combined with Lipase in response to stimuli with 74.46±2.32%, leading to the size and surface charge reversal to facilitate biofilm penetration for killing the bacteria in the biofilm and clearing the surface or the bacterial biofilm of S. aureus formed through multiple responses with 75.44%. In contrast, when AZM alone was used, the residual amount of biofilm was 66.41±1.86%, thus the goal of treating bacterial infections caused by the bacterial biofilm was achieved. In summary, this research developed an effective strategy for the enhanced antibiotic therapy for eradicating biofilm-associated infections.

Keyword: liposome; nano-delivery system; pH/lipase/GSH responsiveness; bacterial biofilm; antibacterial activity

最终交流类型: Invited

Theranostic nanosystems of cancer based on gene recognition

Huangxian Ju
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Gene recognition has extensively been applied in bioanalysis and bioimaging, whether in vitro or in vivo, as well as biomedicine such as clinical diagnosis and disease therapy. The rational functionalization of nanomaterials with target-specific DNA moieties to recognize different receptors both on cell surface and in cells has led to a large number of versatile theranostic nanosystems. Here I report several theranostic nanosystems developed in my group based on the specific gene recognition. Firstly, several signal switches were designed for sensitive bioimaging and in situ detection of cancer-related biomolecules. By functionalizing nanoparticles with cell-targeting moity and conjugated gene probe, a target-cell-specific delivery strategy for imaging and detection of intracellular miRNA was developed. By innovating DNA probes, a responsive “nano string light” and hydrogel microbeads were proposed for highly efficient mRNA and multi-miRNAs imaging in living cells. A photo zipper locked DNA nanomachine was also assembled for precise miRNA imaging in living cells. Besides RNA, two switchable fluorescent probes were developed for in situ “off-on” imaging of intracellular telomerase by its catalysis toward synthesis of telomeric repeats, and a hierarchical coding strategy was proposed for live cell imaging of protein-specific glycoform . Secondly, some siRNA delivery systems were designed for gene therapy of cancer. A DNA dual lock-and-key strategy was designed for cell-subtype-specific siRNA delivery, two upconversion nanoprobes were developed for near-infrared modulated efficient siRNA delivery and therapy, and in situ siRNA assembly was achieved in living cells for gene therapy. Thirdly, to enhance therapeutic efficiency, a DNA-azobenzene nanopump was designed for controllable drug release, a near-infrared photo-switched microRNA amplifier was proposed for precise photodynamic therapy of early-stage cancers, and a DNA nanomachine via computation across cancer cell membrane was recently developed for precise therapy of solid tumor.

Keyword: Gene recognition; Theranostics; Cancer; Theranostic nanosystems; Bioimaging

最终交流类型: Invited

On-demand synthesis of antiseptics at the site of infection for treatment of otitis media

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Otitis media (OM) is the main reason for pediatric antibiotic prescriptions. The current treatment mandates a rigorous regimen of multidose antibiotics over 5–10 days. The systemic antibiotic exposure and often prematurely terminated treatment due to the challenge of drug administration to young patients are believed to breed antibiotic resistance. To address these challenges, we designed a local treatment that converted a metabolic product (H2O2) of an OM pathogen (Streptococcus pneumoniae) into a potent antiseptic (HOBr), a reaction catalyzed by locally administered vanadium pentoxide nanowires (V2O5 NWs)1. The therapeutic, HOBr, was only synthesized in the presence of the pathogen, enabling on-demand generation of therapeutics for OM treatment. Hypohalous acids are broad-spectrum and have a long history in general disinfection applications without breeding substantial drug resistance. A single dose of the nanowire formulation eradicated OM in a standard chinchilla model in 7 days with no observable tissue toxicity or negative impact on hearing sensitivity.

Nontypeable Haemophilus influenzae (NTHi) is another major OM pathogen, which forms a biofilm that resists conventional antimicrobials and immune clearance. In another work, we designed a cascade nanozyme that generates an antiseptic, HOBr, from a ubiquitous non-ROS, i.e., O2, which successfully eradicates NTHi2. The cascade nanozyme simultaneously exhibits glucose oxidase (GOx)-like activity from gold nanoparticles (AuNPs) and haloperoxidase (HPO)-mimicking activity from V2O5 NWs connected using dopamine (DPA). The cascade nanozyme demonstrated strong antimicrobial efficacy against NTHi and its biofilm, while showing improved biocompatibility compared to the nanozyme of V2O5 NWs alone. The cascade nanozyme thus points to a material-oriented infectious disease treatment strategy, where small-molecule antimicrobials are generated in real time at the site of infection for the benefit of autonomous dosing.

Keyword: Otitis media, vanadium pentoxide nanowires,antibiotic resistance, nanozyme

最终交流类型: Oral

Achieving Effective Crosslinking Hydrogels via Bottle-Brush Polymers

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Due to the similarities with the extracellular matrix and highly tunable mechanical properties, polymer hydrogels have become an important class of material that holds great potential in biological and biomedical applications. However, regardless of the rapid progresses have been made in offering various crosslinks, such as thermal, light, or pH initiated chemical reactions and ironic interactions, or metal coordination assembled physical transient networks, topological defects and interchain entanglements observed in conventional hydrogels are inevitable and limit the development of mechanically robust hydrogels. In this study, we introduced a novel structure of polymer hydrogel, which aims to reduce the structure defects and intermolecular entanglements via bottle-brush polymers (BBPs), to address this challenge. It is found that, the densely packed side chains on BBP can significantly minimize the structure defects and provide more rigid scaffold for polymer networks. Compared with conventional polymer hydrogels, BBPs gels show much lower gelation point. In addition, with proper synthetic design, the effective crosslinking is able to offer evidently prolonged drug release period than conventional hydrogel, while maintain relatively robust polymer network upon swelling, which opens the possibilities for biomedical purposes.

Keyword: Hydrogel, Bottlebrush Polymer, Drug Release, Fast-setting, Non-swelling

最终交流类型: Invited

Cold-Responsive Nanotechnology-Enabled In Situ Engineering of an Immunologically Active Tumor Microenvironment for Immunotherapy of Primary and Metastatic Breast Cancer

Xiaoming (Shawn) He
University of Maryland, United States

Please see the attachment

Keyword: immunotherapy, tumor microenvironment, cryosurgery, nanoparticle, RNAi, chemotherapy, immune check point

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最终交流类型: Oral

Microfluidic platforms for droplet generation

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Droplet microfluidics offers exquisite control over the flows of multiple fluids in microscale, enabling fabrication of single and multiple emulsion droplets with precisely tunable structures and compositions in a high throughput manner[1,2]. These microdroplets provides an advanced platform for fabrication of monodisperse spherical, non-spherical, hollow, core-shell, and multi-compartment microparticles, which are widely used in various fields, such as delivery and controlled release of drugs, encapsulation and protection of active materials, micro-reactions and micro-separations[3]. Various microfluidic devices with different channel geometries including cross-flow, co-flow, and flow focusing have been explored to generate and manipulate droplets. Among these, glass capillary microfluidic device with a three-dimensional (3D) co-flow geometry was widely used due to its advantages of simple fabrication process, high chemical resistance and ideal coaxial hydrodynamic flow-focusing which enables preparation of droplets with wide range of material compositions and structures[4].

Current fabrication of glass capillary microfluidic devices involves capillaries and needles sealed onto the surface of microscope slides, which lack precise adjustment for nested capillaries alignment, long-term lifetime. Here we present a versatile, reconfigurable, reusable and easy to assemble glass capillary microfluidic device. This new device is based on the alignment of two capillaries immersed in a hexagonal prism-shaped glass chamber with mounting holes.This device uses standard fittings leading to sealed connections and its design allows for easy recovery and cleaning if clogging occurs. Remarkably, the device has a special structure design that enables to position capillaries with flexible and precise coaxial alignment. Different emulsion droplets (W/O, W/O, W/O/W and O/W/O droplets) , as well as microgels, microparticles, and microcapsules using these droplets as templates, can be fabricated via the device.

Keyword: droplets, microfluidics, microparticle, microgel, microcapsule

最终交流类型: Invited

Ultra-pH-sensitive (UPS) nanotechnology for precise drug delivery

Yiguang Wang
北京大学药学院

Stimuli-responsive nanomedicines that leverage pathophysiological signals to achieve a spatiotemporal control of therapeutic and diagnostic agents have been extensively investigated. Recently, we developed a novel ultra-pH-sensitive (UPS) nanotechnology based on the cooperative self-assembly of ionizable block copolymers. We further expanded this nanotechnology to a combinatorial library of UPS nanomedicines that composed of three modules: (i) a stimuli-responsive module for the sensing and remodeling of the complex tumor microenvironment; (ii) on-demand release module for precise delivery of therapeutics in vivo; (iii) multi-drug module for the synergistic efficacy of combined therapy. The UPS drug delivery nanotechnology has been exploited for binary reporting of endosome maturation, amplification of tumor microenvironment signals, precise drug delivery, quantification of intracellular nanoparticle exposure, immunotherapy, and nano-biology, etc. This cooperative nanotechnology provides a potential pharmaceutical platform to advance the fundamental research and clinical translation of nanomedicines.

Keyword: Stimuli-responsive nanomaterials, Tumor microenvironment, Intracellular trafficking, Nanomedicine, Tumor therapy

最终交流类型: Invited

Charge-transferrable Nano-Assembled Probes for Second Near-infrared Tumor Imaging and Biosensing

bengang xing
Nanyang Technological University

Currently, optical molecular imaging has been quickly recognized as an effective platform to comprehensively evaluate the essential biomolecules including DNA, RNA, proteins and metabolites in diseases management, and more importantly, it can improve every aspect of precise diagnosis and treatment in clinical practice.[1] Among the various imaging modalities, the emerging technique of photoacoustic imaging (PAT), especially in the near infra-red (NIR) window, enables high resolution, deep-penetration and clinically reliable sensing, which thus attract considerable interests in industry and clinics, however, by right, only few contrast agents are available that can specifically respond to intricate biological environments, and which are biodegradable and biocompatible. Recently, we introduce a new class of pH-sensitive organic photoacoustic contrast agents that operate in the second NIR window (NIR-II, 960–1,700 nm), which are derived from the self-assembled charge-transferrable nano-complexes (CTN) and their dication structure (TMB++)[2-4]. Such unique NIR-II-responsive nano-complexes can not only specifically respond to micro-environment in the physiological range and thus allow noninvasive and sensitive visualization of the tumor status in living mice with higher signal-to-noise ratio.[5] But also, such CTN nanocomplexes can function as NIR-II absorption-based photo-thermal-responsive colorimetric biosensor for anti-interference onsite dietary Myr enzyme determination and realization of rapid visualized outputs with the aid of smartphone calculation. Furthermore, the CTN nanocomplexes are biodegradable under physiological conditions, which can greatly alleviate the biosafety concern of nanoparticle accumulation in vivo. These nano-assemblies show the great potential as a promising environmental responsive and biodegradable molecular probe for specific tumor PAT imaging and high throughput food products screening in the NIR-II region.

Keyword: Charge-transferrable Nano-Assembly, Second Near-infrared Tumor Imaging. Biosensing, photoacoustic imaging

最终交流类型：Oral

Regulation of immune microenvironment enhances antitumor efficacy of tumor vaccines

Na Zhang
山东大学

Cancer immunotherapy has opened up a new way of cancer treatment, and tumor vaccine is one of the most important strategies of cancer immunotherapy, which has attracted wide attention. However tumor formed suppressive TME and TDLN severely hindered the efficacy of tumor vaccine. For example, TME inhibits the function of T cells, suppressive TDLN inhibits DC maturation and T cell activation. Therefore, TME remodeling and TDLN remodeling are expected to improve the effectiveness of tumor vaccines. Based on this, the research group built a series of tumor vaccine delivery systems. For example, Treg inhibition combined in situ tumor vaccine, T-cell promotion combined autologous vaccine, TDLN remodeling combined tumor vaccine. By adjusting the tumor microenvironment, the effect of tumor vaccine is enhanced, which has a clinical application prospect.

Keyword: Cancer；Immunotherapy；Tumor vaccine；Tumor microenvironment

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最终交流类型：Oral

Nanoadjuvants: From Nanocarriers to Immunomodulators

Jie Tang
华中科技大学

Although transcatheter arterial chemo-embolization (TACE) plays a key role on clinical treatment of hepatocellular carcinoma (HCC), it was greatly limited by the poor synergistic effect between chemotherapeutics and physical embolization to tumor-feeding arteries. In the present work, a temperature sensitive polymer poly(N-isopropylacrylamide-b-methacrylic acid) (PNA), which was modified with gold nanoparticles (AuNP@PNA), was successfully used to encapsulate doxorubicin (DOX) by electrostatic binding with their carboxyl groups. The resultant gold nanomedicines (AuNP@PNA/DOX) exhibited temperature responsive sol-gel phase transition, favorable shear thinning effect and X-ray angiography. By in vivo evaluation of vascular embolization on VX2-tumor-bearing rabbits, AuNP@PNA/DOX exhibited far better antitumor efficacy than Lipiodol/DOX, on either tumor growth inhibition, proliferation, apoptosis, necrosis or anti-metastasis. Owing to sufficient embolization to

tumor vascular networks, AuNP@PNA/DOX down-regulated the expression levels of HIF-1α, VEGF and MMP-9, and prompted more efficient activation on CD3+/CD8+ T cells and the related cytokines, suggesting the synergistic effect between AuNP@PNA and DOX on the improvement of post-operative tumor immunosuppressive microenvironment. With their favorable pharmcokinetics and biocompatibility, AuNP@PNA/DOX is promising to be developed as a multi-functional artery-imaging/embolic agent with immune-chemo-embolization for enhancing TACE efficacy on HCC.

Keyword: temperature sensitive nanogels, gold nanoparticles, transcatheter arterial chemo-embolization (TACE), antitumor immune response

最终交流类型: Invited

DNA molecular engineering of theranostic drugs

Zeyu Xiao
Shanghai Jiao Tong University School of Medicine

The bottleneck in the development of theranostic drugs is that the conformational relationship is difficult to be precisely regulated at the molecular level. The speaker has proposed the academic idea of "DNA molecular engineering of therapeutic drugs" through multidisciplinary cross-fertilization. The results include: 1) precise DNA helical spatial modification of the imaging molecule at the restricted scale, which can significantly enhance the optical signal and generate thermal therapy properties at 1 nm, refreshing the highest sensitivity for intraoperative diagnosis of micro lesions; 2) precise DNA base modification of drug-effective molecules with precise distance arrangement, which regulates the activation conformation of drugs on target proteins at the level of single base difference and greatly enhances the selectivity of treatment; and 3) precise DNA backbone modification of delivery carriers with precise response modification, which monitors the dynamic distribution of therapeutic dose at regular intervals and eliminates it on demand, revealing the whole-body dynamic process of DNA backbone carriers in human body. The results have revealed the systemic dynamic in vivo process of DNA backbone carriers in human body.

Keyword: DNA nanotechnology, aptamers, theranostics, bioimaging, drug delivery

最终交流类型: Oral

Dual Nanozyme-Driven PtSn Bimetallic Nanoclusters for Metal-Enhanced Tumor Photothermal and Catalytic Therapy

Yanlin Zhu
哈尔滨工程大学

Specific generation of reactive oxygen species (ROS) within tumors in situ catalyzed by nanozymes is a promising strategy for cancer therapeutics. However, it remains a significant challenge to fabricate highly efficient nanozymes acting in the tumor microenvironment. Herein, we develop a bimetallic nanozyme ($Pt_{50}Sn_{50}$) with the photothermal enhancement of dual enzymatic activities for tumor catalytic therapy. The structures and activities of PtSn bimetallic nanoclusters (BNCs) with different Sn content are explored and evaluated systematically. Experimental comparisons show that the $Pt_{50}Sn_{50}$ BNCs exhibit the highest activities among all those investigated, including enzymatic activity and photothermal property, due to the generation of SnO_{2-x} with oxygen vacancy (O_{vac}) sites on the surface of $Pt_{50}Sn_{50}$ BNCs. Specifically, the $Pt_{50}Sn_{50}$ BNCs exhibit photothermal enhanced peroxidase-like and catalase-like activities, as well as a significantly enhanced anticancer efficacy both in multicellular tumor spheroids and in vivo experiments. Due to the high X-ray attenuation coefficient and excellent light absorption property, the $Pt_{50}Sn_{50}$ BNCs also show dual-mode imaging capacity of computed tomography and photoacoustic imaging, which could achieve in vivo real-time monitoring of the therapeutic process. Therefore, this work will advance the development of noble-metal nanozymes with optimal composition for efficient tumor catalytic therapy.

Keyword: PtSn, bimetallic nanoclusters, multicellular tumor spheroid, catalytic therapy, photothermal therapy

最终交流类型: Keynote

Strategies to Improve Cancer Nanomedicine Clinical Translation

Twan Lammers
RWTH Aachen University Clinic

Nanomedicine formulations, such as liposomes, polymers and micelles, are extensively employed for anticancer drug delivery. By delivering drug molecules more efficiently to

pathological sites and by attenuating their accumulation in potentially endangered healthy tissues, nanomedicines assist in improving the balance between chemotherapy efficacy and toxicity. Nanomedicines are furthermore increasingly used to enable to in vivo application of nucleic acid therapeutics, such as siRNA and DNA. The tumor accumulation of nanomedicines is traditionally ascribed the Enhanced Permeability and Retention (EPR) effect, which is highly variable, both in animal models and in patients, and both inter- and intraindividually. To overcome issues associated with tumor targeting heterogeneity, and to help improve the clinical translation of cancer nanomedicines, we are working on systems and strategies to monitor and modulate tumor-directed drug delivery. In the present lecture, several of these strategies will be highlighted, including imaging-guided interventions to prime tumor blood vessels and the microenvironment, and the use of imaging and biopsy biomarkers for patient stratification, to thereby promote individualized and improved cancer nanomedicine treatment.

Keyword: Nanomedicine Clinical Translation

最终交流类型:

Radiofrequency-responsive nanocomplexes for enhancing synergistic therapy of tumor ablation

洪灿
华中科技大学

Radiofrequency ablation (RFA) therapy is the first-line treatment for early liver cancer, which widely used in clinical treatment with valuable effect (including excellent tissue penetration ability and efficient thermal deposition ability). RFA generates the friction heat in target sites by ionic agitation with the help of high-frequency alternating current delivered through a needle-electrode into tumor nodules. Amounts of RF-responsive nanoparticles has been applied fo developed as multifunctional drug delivery nanoplatform to regulate the release of payloads, realizing a synergistic antitumor effect between RFA and other therapy. In this tallk, we will give a presentation of RF-responsive nanocomplexes based smart and temperature-sensitive nanoparticles for cancer treatment.

Keyword: Radiofrequency ablation, Drug delivery nanoplatform

最终交流类型:

systematic co-delivery of dual agonists to enhance cancer immunotherapy

Xiangxia Li
University of Science and Technology of China

In the tumor immunosuppressive microenvironment (TIME), antigen presenting cells (APCs) usually exhibit a tumor suppressor phenotype. Toll-like receptors (TLRs) agonists could reprogram M2-type macrophages to M1-type and stimulate dendritic cells (DCs) maturation. The combination of TLR7/8 and TLR9 agonists seems to have synergistic therapeutic efficacy. Here, we designed a lipid-coated mesoporous silica nanoparticle (MSNs@Lipo) for the co-delivery of TLR7/8 agonist resiquimod (R848) and TLR9 agonist CpG oligodeoxynucleotides (ODNs) (CpG@MSNs-R@L-M). R848 was firstly conjugated onto the nanoparticle via silane chemistry, which is acidic responsive drug release. Then, CpG was loaded onto the nanoparticle through the positive charge mainly from TLR7/8 agonist R848. Our in vitro experiments further indicated that both drugs have acid-responsive release properties and could be taken up by DCs and located on the endosomes of APCs. More importantly, CpG@MSNs-R@L-M could significantly improve the antitumor efficacy in B16F10 melanoma model. The mechanistic study demonstrated that CpG@MSNs-R@L-M could remarkably modulate the TIME by promoting the maturation of DCs and repolarizing macrophages from M2 to M1 phenotype and facilitating the infiltration of tumor cytotoxic T cells. It was concluded that in comparison to single agonist, the codelivery of dual agonists, CpG and R848, can improve anti-tumor immune responses for cancer immunotherapy.

Keyword: toll-like receptors (TLRs) agonists, mesoporous silica nanoparticles (MSNs), drug delivery, tumor immunosuppressive microenvironment (TIME), cancer immunotherapy

最终交流类型:

Hemostatic Hybrid Hydrogel for Non-variceal Upper Gastrointestinal Bleeding Based on Blue Laser Endoscopy

罗杰
陆军军医大学第二附属医院

Endoscopic hemostasis is the preferred treatment for acute non-variceal upper gastrointestinal bleeding (ANVUGIB), while current treatment methods have limitations, necessitating the exploration of new strategies. Blue laser endoscopy (BLE) offers superior

visualization and targeted treatment options[1]. In this study, a novel hemostatic hybrid hydrogel (3H) based on BLE was developed. It consists of a hemostatic peptide and gelatin methacryloyl and can be conveniently delivered and solidified using the light source provided by BLE. 3H revealed ultrafast hemostasis and strong tissue adhesion in both rat and porcine models, exhibiting the potential for fast and lasting hemostasis through various mechanisms. This finding establishes the theoretical basis for applying 3H in the treatment of ANVUGIB using BLE.

Keyword: Hydrogel; Hemostatic; Acute Non-variceal Upper Gastrointestinal Bleeding, Blue laser endoscopy

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最终交流类型：Oral

Cationic Nanosheets Target Cell-free DNA to Attenuate Uncontrolled Inflammatory Diseases

涂召旭
中山大学附属第六医院

Increased levels of circulating cell-free DNA (cfDNA) are associated with poor clinical outcomes in patients with uncontrolled inflammatory diseases, such as acute kidney injury (AKI) and sepsis[1,2]. Scavenging cfDNA by nanomaterials is regarded as a promising remedy for cfDNA-associated diseases[1,2]. In my study, polyglycerol-amine (PGA)-covered nanosheets with suitable size were synthesized to bind negatively charged cfDNA in vitro, in vivo and ex vivo models. The nanosheets exhibited higher cfDNA binding capacity than corresponding polymers and nanospheres owing to the flexibility and crimpability of their 2D backbone. Moreover, with low cytotoxicity and mild protein adsorption, the nanosheets effectively reduced serum cfDNA levels and predominantly accumulated in the inflammatory sites to inhibit the formation of neutrophil extracellular traps (NETs) and the following inflammatory response. Further, they decreased the serum cfDNA levels in samples from AKI and sepsis patients. Thus, these cationic nanosheets could serve as a potent cfDNA scavenger for treating AKI, sepsis and other cfDNA-associated diseases. In addition, my work demonstrates the pivotal feature of a 2D sheet-like structure in the development of the cfDNA scavenger, which could provide a new insight into the future design of nanoplatforms for modulating inflammation.

Reference:

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Keyword: Cationic nanosheets, Cell-free DNA, Toll-like receptor, Uncontrolled inflammation, Sepsis, Acute kidney injury

最终交流类型：Invited

Smart Polymeric siRNA Delivery Systems for Tumor Therapy

Bingyang Shi
河南大学

siRNA is a very attractive therapeutic strategy for tumor therapy due to its high specificity, high efficiency as well as fast and easy to develop. However, lack of a safe and effective delivery carrier is the biggest challenge for siRNA clinical application. Polymer, as one of the most investigated siRNA delivery system has attracted broad attentions because of it is easy for large production, flexible for modification, and its biocompatibility. Nevertheless, the poor blood stability of polymer/siRNA complexed nanomedicine and positive charges induced toxicity severely limited its translation potential. To address these challenges, we have been focusing on the aim of improving delivery efficiency and carrier's safety by tackling the polymeric carrier assembling strategy, and achieved the following achievements: i) we developed novel polymeric siRNA delivery systems by extracellular triple-interactions synergistic assembly and intracellular interactions-responsive-depletion strategies, led to enhanced siRNA blood stability and minimized cation-caused carrier's cytotoxicity; ii) we raised the new method to prepare siRNA nanomedicine via hydrophilic-hydrophobic self-assembly approach. This approach is capable of realizing effective siRNA delivery in the absence of transfection agents, therefore avoided the cationic polymeric carriers-induced side-effects. All above-mentioned original polymeric siRNA nanomedicines showed excellent therapeutic outcomes in tumor models including glioblastoma and exhibited negligible side-effect.

Keyword: siRNA delivery; polymer; tumor therapy

最终交流类型：Invited

Enzyme-instructed peptide self-assembly for organelle-targetted nanomedicines

Zhimou Yang
南开大学

Enzyme-instrcuted self-assembly (EISA) is a powerful strategy for in situ generation of peptide-based nanomedicines for cancer therapy. Using the over-expressed enzyme of alkali phosphatase (ALP) in tumors/cancer cells, in combine with organelle targetted functional groups, we have successed in producing nanomedicines around or on the membrane of cancer cells, and in several organelles (e.g. mitochondria, nucleus) of cancer cells. Our strategy provides useful tools for precise therapy of cancer.

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Keyword: enzyme, peptide, self-assembly, precise therapy

最终交流类型：

Near-Infrared Light-Driven Bioimaging and Photodynamic Therapy

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Peking University, China

Nanoscale metal-organic frameworks (MOF) photosensitizers have attracted significant attention in photodynamic therapy (PDT). However, their limited tissue penetration depth restricts their application. Lanthanide (Ln)-doped upconversion (UC) nanoparticles, $NaLnF_4$, show potentials in converting near-infrared (NIR) light to visible one and can be used to activate the photosensitizers. Previous studies reported composites of NaLnF4 and MOF as a core/shell or Janus structure. Nevertheless, the imaging ability from $NaLnF_4$ is weakened due to decreased UC emission from the composites. Herein, we developed Er^{3+}-doped $NaLnF_4$@MOF nanocomposites that integrate NIR-driven PDT and NIR-II imaging under single 980 nm excitation. Enables efficient energy transfer from NaLnF4 to MOF, the composite can be activated under NIR irradiation to generate cytotoxic singlet oxygen and a good tumor inhibition ability was obtained. Additionally, the downshifting luminescence from $NaLnF_4$ was further used for NIR-II imaging simultaneously. This work demonstrates an all-in-one multifunctional nanoplatforms to integrate NIR light-driven PDT and NIR-II imaging for tumors.

NIR-IIb optical imaging, with minimized tissue scattering and negligible background fluorescence, enables high-resolution dynamic angiography. Er^{3+}-doped lanthanide nanoparticles (LNPs) emitting at 1530 nm in the NIR-IIb region were investigated for dynamic angiocardiography imaging with high spatiotemporal resolution. Following intracardiac injection of optimized LNPs in mouse, dynamic perfusion of major neck vessels and coronary arteries were vividly imaged with 150 ms temporal resolution and 162 μm spatial resolution. More strikingly, myocardial infarction and percutaneous coronary intervention in mice were successfully simulated and monitored in real-time with NIR-IIb imaging. These findings not only shed light on the modulation of NIR emissions from lanthanides but also represent a significant step forward in the clinical diagnostic applications of luminescent materials.

Keyword: NaLnF4 nanocrystals; Upconversion emission; Photosensitizer; Photodynamic therapy; NIRII Bioimaging

最终交流类型: Invited

Nanoelectrochemistry for Intracellular Measurement

黄卫华
武汉大学化学与分子科学学院

Numerous fundamental biological processes occur in subcellular locations and inside intracellular organelles, and electrochemistry using nanoelectrodes with high sensitivity and spatial resolution have been widely recognized as a powerful technique for real-time monitoring of such processes. To this end, we propose a new strategy to prepare a single nanowire electrode for real-time intracellular measurement. Through the preparation of conductive nanowire materials with core-shell structure, the controllable functionalization of nanowires is further carried out by means of such as physical adsorption, electrostatic assembly, covalent bonding, and the dynamic monitoring of intracellular ROS/RNS, NADH, GSH and glutamate was realized. Based on the results of real-time and dynamic monitoring of intracellular life activities, we studied the ROS/RNS homeostasis in phagolysosomes of living macrophages and their stress response to environmental pollutants, the content and release fraction of glutamate in neuronal vesicles as well as its dynamic changes in neurodegenerative diseases. These significantly increased our knowledge of relevant physiological and pathological processes at the single/subcellular level.

Keyword: Core-shell nanowires, Nanoelectrodes, Intracellular measurements, ROS/RNS, Glutamate

最终交流类型：

Lab on a single microbead: a new strategy for ultrasensitive detection of biomarkers at single-molecule level

李正平

University of Science and Technology Beijing, China

Many biomacromolecules of interest, especially for nucleic acids or proteins, exist with a few molecules in a cell or in circulating free DNA/RNA. Therefore, Ultrasensitive detection of biomarkers at single-cell level is of great significance for fundamental studies of life science and disease diagnosis. We have developed an unique single-microbead platform for ultrasensitive detection of various biomarkers, including protein kinase [1], antigens [2, 3], microRNAs[4], and exosomes[5]. The molecular probes specific to various biomarkers were firstly immobilized on the surface of single microbead to specifically recognize and capture the target molecules or their reaction products. Through intelligently designed signal amplification system, the specifically target-produced analytical signals were localized on the single-microbead surface. Then, the ultrahigh sensitivity to detect single molecule biomarkers

can be obtained by imaging the single-bead. More recently, we have also tried to realize one-by-one single-molecule counting for digital quantification of SARS-Cov-2 RNA. This method uses one fluorescent micromotor functionalized with peptide nucleic acids (PNAs) to specially capture one target RNA molecule. The RNA-micromotors can be propelled by the electric field to target district and accurately counted.[6] Combined with CRISPR-Cas systems, we have proposed the CRISPR-Cas-Driven Single Micromotor (Cas-DSM), which can directly detect the nucleic acid targets at a single-molecule level with high specificity.[7]

Keyword: single microbead, biomarker, single molecule detection, fluorescence analysis

最终交流类型: Keynote

Tackling the Challenges in Molecular Optical Imaging Probes for Diagnosis

Kanyi Pu
Nanyang Technological University, Singapore

Molecular optical imaging plays a crucial role in biology and medicine. However, the strong tissue autofluorescence and shallow tissue penetration of optical imaging not only compromise its sensitivity and specificity but also limit its clinical translation. In this talk, I will introduce our approaches (afterglow imaging and artificial urinary biomarkers) to tackle the challenges to advance the clinical translation of molecular optical probes. First, I will introduce molecular afterglow probes with long-lasting luminescence after removal of light excitation for ultrasensitive in vivo imaging. Molecular afterglow probes have the signal to background ratio more than two orders of magnitude higher than NIR fluorescence, allowing for sensitive detection of tiny peritoneal metastatic tumors and monitoring therapeutic outcome. Second, I will discuss how to design renal-clearable optical probes as artificial urinary biomarkers for early diagnosis of acute kidney injury (AKI) and allograft rejection. Molecular renal probes (MRPs) are developed to specifically activate their NIR/chemiluminescence signals towards the biomarkers of AKI or immune cells, followed by rapid renal clearance for urine tests. MRPs thus can act as artificial urinary biomarkers to bypass the in vivo imaging challenges, permitting optical urinalysis that outperforms typical clinical/preclinical assays. These studies provide the basis for an entirely new class of molecular optical probes with ultrahigh sensitivity and high translational potential for disease diagnosis and prognosis.

Keyword: Molecular probes, optical probes, diagnosis

最终交流类型: Invited

S-nitrosylation Produces NO Drugs: Challenges and Opportunities

Lee Jia
Minjiang University

Three gas signaling molecules synthesized in mammalian cells are carbon monoxide (CO), Nitric oxide (NO), and hydrogen sulfide (H2S). In the past 30 years plus, the physiological and pathological processes of NO in the human body have been extensively studied, and NO is granted the 1998 Nobel Medicine Prize. However, the biomedical translational research of NO is not easy, and often relies on S-nitrosylation technology that links NO to biological available sulfhydryl group of different molecules. S-nitrosocaptopril (CapNO) is one of the examples. CapNO possesses dual pharmacological functions of both angiotensin converting enzyme inhibitor (ACEI) and NO. Although the red aqueous solution of CapNO was easily made in 1989, its crystal or solid forms are not easy to obtain until 1998 when we obtained the first generation of CapNO crystals after 100 failures due to the unstable RS-NO bond. However, the large scale synthesis of stable CapNO was another great challenge. We solved the problem by using H2O and –SNO intermolecular stabilization chemistry that allows us to make hundreds of grams of CapNO in a single batch. We recently solved the drugability problem of CapNO by using pharmaceutical nano-encapsulation technology that makes CapNO stable at 50 degree and/or under light. Overall, the presentation focuses on the critical challenges and approaches by which we used for developing CapNO nebulizer for pulmonary delivery of CapNO for acute respiratory distress syndrome (ARDS) and pulmonary artery hypotension (PAH).

Keyword: NO, S-nitrosylation, S-nitrosocaptopril, Pharmaceutical Nano-encapsulation

最终交流类型: Oral

Functional Nucleic Acid-based Nanoprobes for Bioimaging

刘猛
大连理工大学

Functional nucleic acid (FNA) has emerged as an excellent recognition element to recognize and bind target molecules. The FNA-based sensors have been extensively explored

for the detection and imaging of a broad class of cellular analytes, ranging from small molecules to metal ions, and proteins. Such biosensors have important implications for disease diagnostics and fundamental pathophysiological studies by providing bio-information at molecular levels. In recent years, our group has developed several FNA-based nanoprobes for biosensing and bioimaging.

Keyword: Functional nucleic acid, DNAzyme; Aptamer; bioimaging

最终交流类型:

A Comparison Of Remdesivir Versus Au22Glutathione18 In COVID-19 Golden Hamsters: A Better Therapeutic Outcome Of Gold Compound

XUEYUN GAO
Beijing University of Technology

We firstly disclose single compound yields better therapeutic outcome than Remdesivir in COVID-19 hamster treatments as it is armed with direct inhibition viral replication and intrinsic suppression inflammatory cytokines expression. Crystal data reveals that Au (I), released from Au22Glutathione18 (GA), covalently binds thiolate of Cys145 of SARS-CoV-2 Mpro. GA directly decreases SARS-CoV-2 viral replication (EC50: ~0.24 μM) and intrinsically down-regulates NFκB pathway therefore significantly inhibiting expression of inflammatory cytokines in cells. The lung viral load and inflammatory cytokines in GA-treated COVID-19 transgenic mice are found to be significantly lower than that of control mice. When COVID-19 golden hamsters are treated by GA, the lung inflammatory cytokines levels are significantly lower than that of Remdesivir while their lung viral load are decreased to same level. The pathological results show that GA treatment significantly reduce lung inflammatory injuries when compared to that of Remdesivir-treated COVID-19 golden hamsters

Keyword: COVID-19 treatments, Remdesivir, Au22Glutathione18 (GA), lung inflammatory injuries

最终交流类型：Keynote

A critical role for glassy states biomolecular condensates in nanoscale regulation of biology

Kenneth Adrian Dawson
University College Dublin

Nanoscale objects are processed by living organisms using highly evolved and sophisticated endogenous cellular networks, specifically designed to manage objects of this size. While these processes potentially allow nanostructures unique access to and control over key biological machineries, they are also highly protected by cell or host defence mechanisms at all levels. A thorough understanding of bionanoscale recognition events, including the molecules involved in the cell recognition machinery, the nature of information transferred during recognition processes and the coupled downstream cellular processing, would allow us to achieve a qualitatively novel form of biological control and advanced therapeutics. Here we discuss evolving fundamental microscopic and mechanistic understanding of biological nanoscale recognition. We consider the interface between a nanostructure and a target cell membrane, outlining the categories of nanostructure properties that are recognized, and the associated nanoscale signal transduction and cellular programming mechanisms that constitute biological recognition.

Keyword: biological nanoscale recognition, nanostructure, nanoscale signal transduction, cellular programming mechanisms

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最终交流类型：

A Discovery Framework for Nanoparticle Shape-Based Adjuvants

Yan Yan
University College Dublin

With the ever growing universe of nanoscale shapes, names such as “nanoflowers” and “nanostars” no longer precisely describe or characterise the distinct nature of the particles. Conversely, it is of increasing interest to investigate shape-dependent effects in biology. Here, we introduce a conceptual framework to synthesis, capture, describe the nanoscale shapes. Furthermore, we introduce a novel approach for discovering biologically important nanoscale shapes without priori knowledge. biologically relevant inductive nanoscale shape discovery and evaluation that is ideally suited to, and will ultimately become, a vehicle for machine

learning discovery. In this framework, microfluidic flow synthesis is employed to achieve reproducibility and tunability. Computational imaging analysis is used for quantitative shape analysis. In vitro high-throughput biological responses are fed into an iterative feedback to guide the search for nanoscale shape regions. Early applications in vivo suggest the feasibility of such framework to identify significant forms of shape-induced biological and adjuvant-like immunological control.

Keyword: Nanoparticle, Shape-Based Adjuvants, microfluidic flow synthesis

最终交流类型:

Tackling Challenges in Electrochemical Sensing for In Vivo Analysis.

毛兰群
Institute of Chemistry, CAS, China

Electrochemical sensing methods aiming at providing the quantitative and spatiotemporally resolved picture accurately describing the chemical events during a physiological or pathological process have been facing big challenges in directly monitoring biomolecules in vivo. One of the long-standing obstacles is the selectivity issue due to the presence of numerous species displaying similar electroactivities on the probing electrode surface and thus overlapped potential windows for detection. To tackle this challenge, we have formulated an idea on engineering the electrode interface chemistry according to the positions of target molecules on the formal potential axis. For target molecules showing thermodynamic dominance in terms of lower formal potential for oxidation or higher formal potential for reduction, we modified the electrodes by carbon materials with high while promiscuous electrocatalytic activities, such as carbon nanostructures. As the overpotentials of all present molecules are reduced by different degrees, the detection potential of the analyte can be successfully distinguished from those of interferents. For target molecules showing no formal potential dominance, new nanomaterials possessing structural, electronic and chemical uniqueness, such as graphdiyne and single-atom catalyst, are employed to retard or inactivate interfering processes at the sensing interface by tailoring heterogeneous electron-transfer pathways and metal-adsorbate interactions. Following this idea, a series of implantable electrochemical sensors have been constructed for highly selective, real-time monitoring of important neurochemicals like ascorbate, dopamine, glucose, lactate, oxygen, nitric oxide at cellular or in vivo level.

Keyword: In Vivo Analysis

最终交流类型:

Nanozymes based on magnetic nanoparticles in cancer immunotherapy

王術人
北京大学

Cancer immunotherapy has emerged in the field of biomedicine thanks to the good therapeutic prospects. Nanozyme as a new type of nanotechnology has attracted the attraction of more and more researchers to expand its application in cancer immunotherapy. Therefore, we have developed a series of nanozymes with immunomodulatory functions, aiming to address the issue of conventional cancer immunotherapy.

At first, we have designed a kind of immunomodulatory visualized nanozyme Cu@Fe2C@mSiO2-R848-ICG-AS1411 with temperature- and pH-sensitive dual stimulus-response. Under these two exogenous dual stimulations, loaded immune agonist R848 is continuously and reasonably released, further activate dendritic cells, improve the function of CD8+T cells, and reduce the population of myeloid-derived suppressor cells, ultimately achieving the MRI/NIR-II dual mode imaging-guided PTT/CDT/immunotherapy. Moreover, we systematically explore the molecular mechanisms of antitumor effect of these nanozymes, which provides important therapeutic strategy and theoretical basis for the clinical treatment of cancer[1]. To further expand the application of nanozymes in cancer immunotherapy, we also fabricate a new kind of catalytic immune activator base on Au-Fe/Fe3O4. These activators can achieve enhanced chemodynamic therapy/immunotherapy under the guidance of CT/NIR-II dual-mode imaging through maturing dendritic cells, polarizing tumor-associated macrophages, and regulating the cytokines secreted by tumor cells, reprogramming the triple-negative breast cancer from the "cold" tumor to a "hot" tumor[2].

In conclusion, we have developed various nanozymes with immunomodulatory functions, aiming to optimize conventional cancer immunotherapy and promote the application prospects of biological nanozymes based on magnetic nanoparticles in this field.

Reference

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Keyword: Magnetic nanoparticles, Theronastic, Drug delivery system, Nanozymes, Immunotherapy

最终交流类型:

Chemotherapy induced neoantigen nanovaccines enhance αPD-1 immunotherapy

陈贵远
中国科学技术大学

Chemotherapeutics have the potential to increase the efficacy of cancer immunotherapies by stimulating the production of damage-associated molecular patterns (DAMPs) and eliciting mutations that result in the production of neoantigens, thereby increasing the immunogenicity of cancerous lesions. However, the dose-limiting toxicity and limited immunogenicity of chemotherapeutics are not sufficient to induce a robust antitumor response. We hypothesized that cancer cells in vitro treated with ultrahigh doses of various chemotherapeutics artificially increased the abundance, variety and specificity of DAMPs and neoantigens, thereby improving chemoimmunotherapy. The in vitro chemotherapy-induced (IVCI) nanovaccines manufactured from cell lysates comprised multiple neoantigens and DAMPs, thereby exhibiting comprehensive antigenicity and adjuvanticity. Our IVCI nanovaccines exhibited enhanced immune responses in CT26 tumor-bearing mice with a significant increase in CD4+/CD8+ T cells in tumors in combination with αPD-1. The concept of IVCI nanovaccines provides an idea for the manufacturing and artificial enhancement of immunogenicity vaccines to improve chemoimmunotherapy.

Keyword: nanovaccine; immunogenicity; immunotherapy; chemotherapy; immune checkpoint inhibitors

最终交流类型:

Paratensile signaling regulates correlated cell migration and synapse formation

叶方富
中国科学院物理研究所

The migration and other functions of cells are affected by various factors in the microenvironment. In addition to the widely studied biochemical molecular signaling pathways, recent studies have shown that physical factors in the microenvironment also play a crucial role. Type I collagen is a major component of extracellular matrix (ECM) in vivo. Due to the nonlinear viscoelastic mechanical properties of type I collagen, the attenuation of the mechanical signal can be largely slowed down.

Therefore, we constructed a quasi-3D system using collagen with tunable stiffness to mimic the microenvironment as in vivo. We found that the contraction force of cells during migration can be transmitted remotely through the collagen fibers. Cell mechanical communications are realized through dynamic remodeling of collagen fiber bundles among cells. Then, there is a strong correlated migration between interconnected cell pairs. We integrated the femtosecond laser ablation technology into the 3D real-time tracking system, and proved that tension force does exists in the dynamically reconstructed collagen fiber bundles between cells. Based on the directed migration regulation of collagen fibers, the study found that multi-cellular populations can self-organize and aggregate along the remodeled fibers.

we further constructed a quasi-3D system to mimic an in vivo-like microenvironment for neurons by using mouse cortex primary neurons and neuronal cell line PC12, and strikingly found out that neuronal cells can remotely sense each other and precisely extend axons for synaptic formation via extracellular matrix-transmitted mechanical signals. It is also proved that this mechano-response of neuronal cells is related to the activation of mechanosensitive ion channels and the increase of calcium signaling within specific neurite confronting to the remote mechanical stimuli. This mechanotaxis mechanism brings up a new and important concept for regulating axon pathfinding and synapse formation, which has much higher spatial precision for guiding neurons than chemotaxis does. We believe this finding can provide new insights for understanding the early development of nervous system and potentially assist clinical applications aiming to neural regeneration and other neuronal system related diseases.

Keyword: Collagen fiber bundles, Correlated cell migration, Fibrous proteins, Long-range force propagation, Synapse formation

最终交流类型:

S-nitrosylation produces NO drugs: challenges and opportunities.

贾力
闽江大学

Three gas signaling molecules synthesized in mammalian cells are carbon monoxide (CO), Nitric oxide (NO), and hydrogen sulfide (H2S). In the past 30 years plus, the physiological and pathological processes of NO in the human body have been extensively studied, and NO is granted the 1998 Nobel Medicine Prize. However, the biomedical translational research of NO is not easy, and often relies on S-nitrosylation technology that links NO to biological available sulfhydryl group of different molecules. S-nitrosocaptopril (CapNO) is one of the examples. CapNO possesses dual pharmacological functions of both angiotensin converting enzyme inhibitor (ACEI) and NO. Although the red aqueous solution of CapNO was easily made in 1989, its crystal or solid forms are not easy to obtain until 1998 when we obtained the first generation of CapNO crystals after 100 failures due to the unstable RS-NO bond. However, the large scale synthesis of stable CapNO was another great challenge. We solved the problem by using H2O and –SNO intermolecular stabilization chemistry that allows us to make hundreds of grams of CapNO in a single batch. We recently solved the drugability problem of CapNO by using pharmaceutical nano-encapsulation technology that makes CapNO stable at 50 degree and/or under light. Overall, the presentation focuses on the critical challenges and approaches by which we used for developing CapNO nebulizer for pulmonary delivery of CapNO for acute respiratory distress syndrome (ARDS) and pulmonary artery hypotension (PAH).

Keyword: NO, S-nitrosylation, S-nitrosocaptopril, Pharmaceutical Nano-encapsulation

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最终交流类型:

Metformin Reprogramming the Tumor Immune Microenvironment and Boosting Chemoimmunotherapy

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Tumor stroma plays important role in the occurrence, development, and metastasis of colorectal cancer (CRC). The dense collagenous stroma forms a physical barrier for antitumor drugs and sustains a highly tumor immunosuppressive microenvironment. To

address this issue, a spatiotemporal combination of antitumor stroma and nanoscale antitumor strategies for reprogramming the tumor immune microenvironment was proposed. In this combination, metformin (MET) was intraperitoneally injected to disrupt the dense tumor stroma for promoting the drug delivery and remodeling the tumor immune microenvironment, and subsequent intravenous injected MIL-100/mitoxantrone/hyaluronic acid nanoparticles (defined as MMH NPs) for generating a robust immune response via immunogenic cell death (ICD). More importantly, the combination treatment also synergistically with the anti-OX40 agonist antibody (αOX40), which enhanced the treatment of orthotopic CRC (Scheme 1). In summary, the combination strategy of MET/MMH NPs/αOX40 provides a novel and effective clinical option for CRC therapy.

Keyword: Tumor stroma, Colorectal cancer, Immunotherapy, Metformin, Tumor microenvironment

最终交流类型:

Nano-inhibitors Self-assembled In Situ for Improving Colorectal Cancer Immune- Chemotherapy By Disrupting Membrane and Blocking PD-1/PD-L1

望应
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Despite recent advances in tumor immunotherapy, the efficacy of this approach remains to be improved. Looking forward to high rates of objective clinical response, cancer immunotherapy combined with chemotherapy has gained increasing attention. Herein, we constructed a pH responsive peptide-polymer system IICs, which was able to enhance the antitumor efficacy by blocking PD-1/PD-L1. Firstly, IICs nanoparticles could target and accumulate in tumor, followed by in situ transforming into nanofibers induced by weak acidity of tumor site, resulting in prolonged retention time and local drug concentration which is beneficial for improving tumor treatment efficacy. What’s more, the fibers wrapped on the surface of tumor cells can significantly blocking the combination of PD-1/PD-L1 by increasing the contact area and contact site between the IICs fibers and PD-L1, which effectively enhanced the immunotherapeutic effect of colorectal cancer. Meanwhile, the chemotherapeutics loaded in IICs NFs gradually released in tumor upon the occurrence of fibrillogenesis which could directly kill tumor cells, further improving the curative effect of colorectal cancer.

Keyword: Colorectal cancer, immune checkpoint, PD-1/PD-L1, immunotherapy, chemotherapy, combination therapy, peptide, self-assembly

最终交流类型: Invited

The research of smart drug delivery systems based on oncolytic microorganism.

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Oncolytic microorganism therapy has shown the potential to overcome the disadvantage of conventional immunotherapy. We developed a combination of chemotherapy and biotherapy intravenous drug delivery system based on the tumor targeting characteristics of bacteria. An oral probiotics delivery system that can be valued at colon cancer sites was designed by coating technology. Then, we constructed intelligent responsive bacterial delivery systems using the techniques of synthetic biology, such as micro-to-nano oncolytic microbial system. In addition, bacterial outer membrane vesicles (OMVs) can remold the tumor immunosuppressive microenvironment due to the unique nanosize and immunogenicity. Oncolytic adenovirus (Ad) infection promotes intracellular autophagy in tumors. This could kill cancer cells and contribute to Ads-mediated anticancer immunity. However, the low intratumoral content of intravenous-delivered Ads is far from to activate tumor over-autophagy. Herein, we report bacterial outer membrane vesicles (OMVs)-encapsulating Ads as microbial nanocomposites that are biomineral engineered for autophagy-cascade-augmented immunotherapy. Biomineral shells cover the surface antigens of OMVs to circumvent the clearance during in vivo circulation and enhance intratumoral enrichment. After entering tumor cells, there is excessive H2O2 accumulation through the catalytic effect of overexpressed pyranose oxidase (P2O) from microbial nanocomposite. It increases oxidative stress levels and triggered tumor autophagy. The autophagy-induced autophagosomes further promote Ads replication in Ads-infected tumor cells, leading to Ads-overactivated autophagy. Moreover, OMVs are powerful immunostimulants for remolding the immunosuppressive tumor microenvironment, facilitating autophagic antitumor immune response in preclinical cancer models in female mice. Therefore, the present autophagy-cascade-boosted immunotherapeutic method can expand OVs-based immunotherapy. Our researches are devoted to the construction of intelligent delivery systems based on oncolytic bacteria, providing theoretical basis and strategies for the study of the immunotherapy.

Keyword: oncolytic microorganism.

最终交流类型: Oral

Polypept(o)ides-based PEG-free Nanomedicine: Focus on RNA.

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Polyethylene glycol (PEG) is the most widely used stealth polymer in nanomedicine and bioconjugation to prolong blood circulation time and improve drug efficacy. However, safety concerns associated with PEG (e.g., anti-PEG immunity, accelerated blood clearance phenomenon and storage diseases) have gained considerable attention. Therefore, safe and efficient PEG-free nano-delivery systems are required to facilitate RNA implementation. We have developed a versatile PEG-free nano-platform based on polypept(o)ides (e.g., polysarcosine), providing comparable stealth-like properties, pronounced RNA/DNA shielding, low immunogenicity compared to PEG counterparts or even lead to a total absence of immediate immune responses (e.g., cytokine release). In the previous work, we incorporated these novel (lipo)polymers into different formulations including liposomes, lipid nanoparticles and polymeric micelles, and achieved efficient RNA delivery both locally and systemically. Further efforts on stimuli-responsive nano-delivery systems will be directed to novel treatment options of auto-immune diseases, such as atherosclerosis and neurodegeneration.

Keyword: Focus on RNA

最终交流类型: Oral

Fluorinated dendrimer for 19F MRI-based theranostic.

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luorinated dendrimer for 19F MRI-based theranostic

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Magnetic Resonance Imaging (MRI) is a widely used imaging modality in clinic for disease diagnosis, thanks to the high spatial resolution and deep-tissue penetration. In particular, fluorine-19 Magnetic Resonance Imaging (19F-MRI) is an emerging modality for MRI, thanks to no background 19F-MRI signal in biological systems. However, designing an ideal 19F-MRI agent with high fluorine content, good water solubility and optimal MRI properties for bioimaging is challenging. We have recently developed self-assembling dendrimer nanosystems composed of amphiphilic dendrimers [1-4], which hold the promising feature to carry a large number of fluorine atoms yet in a modular and controllable way. Here, we report our design and synthesis of fluorinated amphiphilic dendrimers, which have high fluorine content by virtue of the multivalent characteristics of dendrimer. Importantly, these fluorinated dendrimers are highly soluble in water yet having suitable 19F-MRI properties. They were able to self-assemble into small and stable nanomicelles and accumulate within tumor lesions via enhanced permeability and retention (EPR) effect for effective tumor imaging. Remarkably, the formed nanomicelles also enabled encapsulation of near infrared fluorescent probe and anticancer drug, offering both 19F-MRI-based multimodal imaging and chemotherapy-based cancer treatment at the same time. These dendrimer nanosystems constitute therefore promising 19F-MRI agents and theranostics for cancer management. This study also opens new perspectives in exploiting advancement of self-assembling dendrimer nanotechnology to address challenging 19F-MRI for biomedical applications.

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Keyword: 19F MRI-based theranostic

Topical Sessions =》 14. Safety, Environment and Health of Nanomaterials

最终交流类型: Oral

Defining the surface oxygen threshold that switches the interaction mode of graphene oxide with bacteria

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As antimicrobials, graphene materials (GMs) may have advantages over traditional antibiotics due to their physical mechanisms of action which ensure less chance of development of microbial resistance. However, the fundamental question as to whether the antibacterial mechanism of GMs originates from parallel interaction or perpendicular interaction, or from a combination of these, remains poorly understood. Here, we show both experimentally and theoretically that GMs with high surface oxygen content (SOC) predominantly attach in parallel to the bacterial cell surface when in the suspension phase. The interaction mode shifts to perpendicular interaction when the SOC reaches a threshold of ~ 0.3 (the atomic percent of O in the total atoms). Such distinct interaction modes are highly related to the rigidity of GMs. Graphene oxide (GO) with high SOC is very flexible and thus can wrap bacteria while reduced GO (rGO) with lower SOC has higher rigidity and tends to contact bacteria with their edges. Neither mode necessarily kills bacteria. Rather, bactericidal activity depends on the interaction of GMs with surrounding biomolecules. These findings suggest that variation of SOC of GMs is a key factor driving the interaction mode with bacteria, thus helping to understand the different possible physical mechanisms leading to their antibacterial activity.

Keyword: graphene oxide, surface oxygen content, oxidative potential, membrane damage, antibacterial activity, interaction mode

最终交流类型: Invited

Ferroptosis contributes to particulate matter-induced pulmonary fibrosis

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Particulate matter (PM) is an environmental air pollutant that threatens human health. Once inhaled into the human airway, it triggers tracheal mucosa damage, ventilatory disorders, respiratory acute and chronic inflammation, and even fibrosis through inflammation. PM-induced pulmonary fibrosis is a progressive life-threatening disease that seriously endangers people's health. The wide application of nanoproducts leads to an increase in environmental exposure to nano-size PMs. Recent studies have established a correlation between inhalation exposure to PMs and pulmonary fibrosis. Moreover, macrophage damage is known to play a pivotal role in PM-induced pulmonary fibrosis. However, the cellular-level mechanisms involved in these processes are not entirely clear. Ferroptosis, a non-apoptosis programmed cell death, is involved in various pathological conditions and diseases. Recently, ferroptosis was reported in some nanomaterials (NMs)-treated macrophages and NM-exposed animal models. However, whether ferroptosis is widely involved in inhaled nano-size PM-induced pulmonary injury and fibrosis is still unknown. The mechanisms underlying nano-size PM-induced ferroptosis also warrant further exploration.

In the current study, we found the accumulation of lipid peroxidation in alveolar macrophages (AMs) of pulmonary fibrosis patients. Thus, we established a nanomaterial library to assess the widespread induction of ferroptosis by NMs in macrophages (RAW 264.7), and NM-induced ferroptosis was evidenced by elevated cellular iron level, radical oxygen generation, and lipid peroxidation. Interestingly, ferroptotic toxic effects were found in multiple kinds of NMs. And these effects were also influenced by various parameters of NMs. These findings were also validated in mice after oropharyngeal aspiration of particles. Importantly, NM-induced ferroptosis in macrophages significantly contributed to the activation of lung fibroblasts in vitro and lung fibrosis in vivo, and these effects were suppressed by the co-treatment with ferroptosis inhibitors, ferrostatin-1 and liproxstatin-1. Overall, our study highlights that ferroptotic effects are widely found in NM-induced cytotoxicity, which is further involved in the pathogenesis of nano-size PM-induced lung fibrosis. These findings could also be carefully considered in the safety design of nanoproducts.

Keyword: particulate matter; pulmonary fibrosis; ferroptosis; lipid peroxidation

最终交流类型: Invited

Integration of mass spectrometric and spectroscopic approaches to investigate the in vivo fate of noble metal nanoparticles

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Nobel metal nanoparticles, such as silver (Ag) and gold (Au) nanoparticles (NPs), have a wide range of applications in disinfection, drug delivery, diagnosis, etc. Recently, we found that the physicochemical properties of Ag NPs and Au NPs including the shape, size and surface coating could significantly affect their "nano-bio interaction" [1-3]. However, there is still a lack of research on how Ag and Au NPs distribute at the subcellular level and sub-organ level and in what form they exist in the body.

Noble metal nanoparticles, such as silver (Ag) and gold (Au) nanoparticles (NPs), have a wide range of applications in commercial and medical products, owing to their unique physicochemical properties. Recently, we found that the intrinsic properties of Ag NPs and Au NPs including the shape, size and surface coating could significantly affect their "nano-bio interaction", thereby leading to unexpected biological effects [1-3]. However, there are only few studies exploring how Ag NPs and Au NPs distribute at the subcellular level and sub-organ level and in what form they exist in the body. Hence, there is a great need for the development of versatile tools to examine the in vivo fate of noble metal NPs, elucidating their potential health risks.

In order to achieve in situ imaging of Ag NPs and Au NPs in organs and tissues, we integrated laser ablation plasma mass spectrometry (LA-ICP-MS) with hyperspectral dark-field microscopy (HSI-DFM) to investigate the translocation, transformation and distribution of Ag NPs and Au NPs in the body and cells, by which Ag NPs and Au NPs can be qualitatively and quantitatively determined on the basis of their elemental and spectral characteristics. Our results show that after entering the body and cells, Ag NPs and Au NPs underwent complicated transformation processes, including dissolution and aggregation, which further determine their behaviors and effects [2,4]. For example, Au NP aggregates formed intracellularly have a longer retention time and are more difficult to be exocytosed than well-dispersed Au NPs by cells, which is helpful for the mesenchymal stem cell-mediated delivery of Au NPs to tumors [5]. On the contrary, ionic Ag leached from AgNPs in the gastrointestinal tract is more easily absorbed by the intestines than particulate Ag after oral ingestion. Our findings provide important insights for understanding the fate of noble metal nanoparticles in vivo.

Keyword: LA-ICP-MS; hyperspectral imaging; noble metal nanoparticles; transformation; distribution

最终交流类型: Invited

Design and fabrication of smart nanoradiosensitizer for radiotherapy enhancement

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Radiotherapy (RT) nowadays is one of the most important clinical cancer therapeutic strategies. According to the reports, approximately 70% of patients are treated with RT. The therapeutic rationale of RT is to directly cause DNA damage, or indirectly react with water molecules to produce highly toxic reactive oxygen species (ROS, such as O2•−, H•, and HO•) to destroy DNA or other cellular components. As a classical cancer therapy method, RT has its special superiority such as no tissue depth restriction. However, some intrinsic shortcomings such as damage to normal tissue or hypoxic tumor resistance to radiation still accompany RT which greatly limits its practical application. Therefore, in order to solve these problems, nanomaterials-mediated radiosensitization is now receiving increasing attention. Our group recently developed a new nanomaterials-based radiosensitizing strategy: radiocatalysis. On the one hand, aiming at the tumor microenvironment, we designed a few novel nanoradiosensitizers to improve radiotherapy by improving hypoxia, reducing GSH content, catalyzing H2O2 conversion, and inhibiting DNA repair. This provides a new solution for overcoming tumor cell irradiation tolerance, improving radiotherapy selectivity and controllability, and achieving accurate radiotherapy. It can also ensure the highly efficient radiotherapeutic effect in tumor upon the relatively low dose of radiation, so as to reduce the side effect that is commonly associated with clinical radiotherapy. On the other hand, the use of irradiation catalysis could also selectively generate free radicals, and promote tumor cell immunogenic death and antigen presentation, so as to activate the immune response of solid tumors, while clearing tumors in situ. This strategy could inhibit the growth of distal metastatic tumors, break through the shortcomings of local radiotherapy, and provide a new idea for the development of immunoradiotherapy. Despite the achievement we’ve obtained so far, systematic investigation of the toxicology and biosafety

of nanosensitizers is still needed. We hope to promote more nanosensitizers into clinical translation.

Keyword: radiotherapy, nanomedicine, immunoradiotherapy, radiocatalysis

最终交流类型: Invited

Converting Nanotoxicity Data to Critical Information Using Artificial Intelligence Approaches

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The rapid development of nanotoxicology research has led to an exponential increase in data being accumulated, and urgent need of developing computational methods for extracting and processing critical nanostructure-activity relationships from large datasets. During the past several years, artificial intelligence approaches, especially deep learning has emerged as a powerful method to mine useful information from complex big data, which has been widely used for face recognition, autonomous driving, and medical diagnosis. Inspired by these successes, researchers have successfully applied these technologies in the areas of toxicology. Compared with small molecules, the complexity and diversity of nanostructures lead to many challenges (e.g., lack of available database and suitable nanodescriptors) in the application of artificial intelligence to nanotoxicology. Therefore, in our recent studies, we have focused on the construction of effective databases, development of suitable nanodescriptors, and application of end-to-end deep learning methods3 that will enable big data and artificial intelligence to make a deeper contribution to nanosafety.

Modern nanotechnology research has generated numerous experimental data for various nanomaterials. However, the few nanomaterial databases available are not suitable for modeling studies due to the way they are curated. Here, we report the construction of a large nanomaterial database containing annotated nanostructures suited for modeling research. The database, which is publicly available through http://www.pubvinas.com/, contains 705 unique nanomaterials covering 11 material types. Each nanomaterial has up to six physicochemical properties and/or bioactivities, resulting in more than ten endpoints in the database. All the nanostructures are annotated and transformed into protein data bank files, which are downloadable by researchers worldwide. Furthermore, the nanostructure annotation procedure generates 2142 nanodescriptors for all nanomaterials for machine learning purposes, which are also available through the portal. This database provides a

public resource for data-driven nanoinformatics modeling research aimed at rational nanomaterial design and other areas of modern computational nanotechnology.

Rational nanomaterial design is urgently demanded for new nanomaterial development with desired properties. However, computational nanomaterial modeling and virtual nanomaterial screening are not applicable for this purpose due to the complexity of nanomaterial structures. To address the challenge, a new computational workflow is established in this study to virtually profile nanoparticles by (1) constructing a structurally diverse virtual gold nanoparticle (GNP) library and (2) developing novel universal nanodescriptors. The emphasis of this study is the second task by developing geometrical nanodescriptors that are suitable for the quantitative modeling of GNPs and virtual screening purposes. The feasibility, rigor and applicability of this novel computational method are validated by testing seven GNP datasets consisting of 191 unique GNPs of various nano-bioactivities and physicochemical properties. The high predictability of the developed GNP models suggests that this workflow can be used as a universal tool for nanomaterial profiling and rational nanomaterial design.

Artificial intelligence approaches, such as machine learning and deep learning, may predict nano−bio interactions. However, such a prediction is now hindered by the paucity of suitable nanodescriptors with applicable nanostructure annotation methods. Inspired by face recognition technology, we have developed a novel nanostructure annotation method to automatically convert nanostructures to images for convolutional neural network modeling. In this operation, nanostructure features were directly learned from nanoparticle images without complicated nanodescriptor calculations. The constructed convolutional neural network models were successfully used to predict physicochemical properties (i.e., logP and zeta potential) and biological activities (i.e., cellular uptake and protein adsorption) of 147 unique nanoparticles, including 123 gold nanoparticles, 12 platinum nanoparticles, and 12 palladium nanoparticles. Our nanostructure diversity and wide distribution of experimental values are beneficial for building predictive deep learning models. The deep learning models provide highly accurate predictions with all determination coefficients (R2) higher than 0.68 for both cross validation and external prediction. In addition, the constructed model is explainable because we can visualize how it learns from the class activation map. This approach enables a much more efficient end-to-end deep learning modality suitable for design of next generation nanomaterials.

Keyword: nanotoxicity data, artificial intelligence, machine learning, nanodescriptors generation, nano-QSAR

最终交流类型: Invited

Developing New Nano-adjuvants for Vaccines

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Background: Vaccination is recognized as one of the most effective and low-cost ways to control the spread of infectious diseases worldwide.[1] However, protective immune responses triggered by vaccines alone are still insufficient.[2] We devote to developing new nano-adjuvants to improve the efficacy of vaccines.

Methods: We have constructed a series of nano-adjuvants such as morphologically virus-like fullerenol nanoparticles, polyvinylpyrrolidone−poly (ethylene glycol) modified silver nanorods and peptidic nanofibers (in situ formation) and comprehensively evaluated their enhancements in the quantity and quality of immune responses induced by DNA and protein vaccines *in vivo*.

Results: (1) Morphologically virus-like fullerenol nanoparticles as adjuvant can not only improve special immune response, but also protect DNA antigen from enzymatic degradation *in vivo*. Morphologically virus-like fullerenol nanoparticles promoted dendritic cells (DCs) maturation and activated the function of DCs via TLRs signaling pathway, thus inducing more production of multiple pivotal cytokines (IL-2, IFN-γ and IFN-α) [3]; (2) The noncarrier adjuvant, silver nanorods coated by polyvinylpyrrolidone (PVP) and polyethylene glycol (PEG), integrates surface modification-based immunostimulation and shape-dependent improvement of biosafety. This adjuvant can significantly improve HIV protein vaccine-triggered antibody and T cell immune response (remarkably increasing the titer of IgG and crucial cytokines such as IL-2, IL-4 and IFN-γ), and show a satisfactory biosafety [4]; (3) *In situ* formed peptidic nanofibers facilitated HIV vaccine-induced polyfunctional T cell response, broad IgG subclasses response and V1/V2 loop-specific antibody response, all of which can hardly be triggered by HIV vaccine alone. Such peptidic nanofibers may allow a better inhibition against HIV than reported adjuvants [5].

Conclusion: We have designed a series of nano-adjuvants and effectively induced the enhancement of vaccine-induced humoral and cellular immunity, thus providing some promising principles and guidelines for designing a safe and high-efficacy nanoadjuvant for improving the efficacy of vaccines.

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Keyword: Vaccines, nanoadjuvants, biosafety, efficacy

最终交流类型: Invited

Basic research on the health risks of oral intake of titanium dioxide nanoparticles

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Titanium dioxide containing nano-fractions is widely used in the field of food and medicine due to their excellent whitening and brightening capability. Recently, European Commission has banned titanium dioxide as a food additive, raising public concern about its health risk, especially the nanoparticles contained therein. It is crucial to evaluate the health risks of oral intake of titanium dioxide nanoparticles (TiO2 NPs). Our research group estimated the dietary exposure level of TiO2 NPs among Chinese population by measuring the content of TiO2 NPs in food sold in China, and found that children are the highest exposure population due to their love of sweets. Through animal experiments of oral exposure, it was found that young rats are more susceptible than adult rats, mainly manifested as liver and heart damage, which worsens with the increase of exposure dose and exposure time. The combination of TiO2 NPs and glucose showed an interaction, but TiO2 NPs had no significant effect on glucose absorption. TiO2 NPs can alter the intestinal epithelial structure and thereby affect intestinal function, manifested in changes in amino acid absorption and metabolism levels, and increase intestinal barrier function when LPS coexists. TiO2 NPs play an important role in the course of acute colitis by affecting the gut microbiota and activating the ROS-TXNIP-NLRP3 inflammatory pathway. It can also be observed that TiO2 NPs is absorbed into the blood through the intestine, and nanoparticles are found in the liver, but the absorption and transportation amount is relatively low. TiO2 NPs can also induce DNA double strand breaks in rat bone marrow cells and HPRT gene mutations in V79 cells. To sum up, oral intake of TiO2 NPs carries certain health risks. Foods supplemented with TiO2

NPs should be carefully consumed by people with high protein requirements, such as children, the elderly, and patients with high metabolic disease or intestinal inflammation.

Keyword: titanium dioxide, nanoparticles, oral toxicity, intestinal injury, nanosafety

最终交流类型：Keynote

From joint nanotoxicology assessment to nano-bioremediation technology

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Nanomaterials (NMs) are utilized in various sectors of everyday life and releases into ground/surface waters, soils, and sediments are likely significant. Concerns over the combined risks of NMs and co-existing pollutants have led to investigations into co-contamination scenarios. Synergistic, additive, antagonistic, and independent effects are all possible toxic interactions resulting from NMs and co-contaminant exposure. Interestingly, NMs may antagonize the toxicity of co-existing contaminants by adsorption/reductive-oxidation reactions, or decrease toxicity through altered biological processes such as antioxidation, detoxification, or biodegradation, along with the removal of contaminants. These types of interactions clearly suggest the potential use of NMs to facilitate the bioremediation of contaminated sites. Based on this consideration, we put forward a strategy extracting valuable information from joint nanotoxicity studies as an indicator for the development of nano-enabled bioremediation (nano-bioremediation) technologies.

We have worked on developing nano-phytoremediation, nano-microbial remediation, and nano-zooremediation technologies. We established a new soil remediation strategy using nanoscale zero-valent iron (nZVI) coupled with safe rice-production in a paddy soil contaminated with pentachlorophenol (PCP). The specific role of nZVI-derived root iron plaque formation in the safe production of rice was described, and the synergistic effect of nZVI-treatment and rice cultivation was identified as nZVI-facilitated rhizosphere microbial degradation of PCP. nZVI was also found to interact with alfalfa and synergistically remediate polychlorinated biphenyl-contaminated agricultural soil. An indigenous dehalogenation bacteria was isolated from the agricultural soil, and a synergistic effect of soil organic matter and nZVI was observed on the biodegradation of organochlorines. We have also drawn inspiration from nano-bio interaction and established a hybrid remediation framework using nZVI and nematodes for organochlorine-contaminated soil. We found that the exposure to nZVI stimulated the synthesis of reductive biomolecules which significantly mitigated the toxicity of PCP and strongly accelerated nZVI-induced PCP dechlorination by facilitating the reductive dissolution of nZVI oxide shell and electron transfer from Fe0 core to PCP. I will briefly present these nano-bioremediation technologies and introduce how to develop nano-bioremediation technologies from joint nanotoxicology assessment, with a focus on the interactions among NMs, biota, and pollutants.

Keyword: Nanotechnology, joint nanotoxicity, bioremediation, bioresponse, soil pollution.

最终交流类型: Invited

Potential implications and applications of nanotechnology in bacterial evolutionary biology

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Extensive researches have been conducted on nanomaterials for their potential applications as antimicrobials. However, there is a paucity of information regarding the utilization of nanomaterials as "resistance breakers" to impede the evolution of antibiotic resistance. This introduces a unique perspective in the field of antibacterial therapy.

First, we present recent studies exploring the potential applications of nanotechnology in disrupting the evolution of resistance by leveraging the distinctive action patterns of nanomaterials. The term "bacterial memory" is employed to describe the phenomenon wherein bacterial cells respond to their present conditions based on past experiences. This history-dependent behavior plays a vital role in facilitating rapid adaptation, enabling bacteria to survive in fluctuating environments, and ultimately leading to the development of genetic resistance. i) Our results showed that carbon nanomaterials have the ability to influence bacterial memory by disrupting the process of respiration, which is crucial for providing energy required for detoxification or repair processes during a lag phase. For instance, when graphene oxide (GO) interacted with the transmembrane protein cytochrome c, it facilitated the transfer of electrons from the respiratory chain to extracellular oxygen. This transfer ultimately resulted in the generation of extracellular reactive oxygen species[1]. This interruption effect has also been reported for other nanomaterials with high electron transfer activity, e.g., carbon nanotubes and fullerene[2]. ii) Additionally, nanoparticles have been found to play a role in regulating motility, which is crucial for nutrient sensing, evading persistent states, and the formation of biofilms. In a previous study conducted by our team, it was demonstrated that graphene-based nanomaterials can interact with chemosensors present on bacterial surfaces. This interaction transiently influenced cell motion and, at the same time, stimulated long-range swimming by inducing the production of the quorum sensing molecule AI-2[3]. iii) Furthermore, our research delved into the impact of nanomaterials on the evolution of antibiotic resistance through cyclic treatment. Our findings revealed that bacteria exhibited a gradual development of adaptive tolerance to ciprofloxacin (CIP) when subjected to cyclic treatment involving both CIP and silver ion co-treatment. However, when CIP exposure was alternated with silver nanoparticle (AgNP) exposure, no discernible resistance or tolerance was observed. In contrast, continuous selection through exclusive CIP treatment resulted in the rapid induction of CIP resistance[4].

Secondly, we conducted an assessment of the development of bacterial tolerance/resistance to various nanomaterials, which raises concerns about potential nanoresistance[5-8]. For example, in a study where Escherichia coli (E. coli) was repetitively exposed to 5 mg/L graphene oxide for 200 subcultures spanning 400 days, the evolved E. coli cells exhibited significant differences compared to their ancestor cells[6]. Contact with GO surfaces induced transformative effects on E. coli by activating the Cpx envelope stress response (ESR), resulting in over a twofold increase in extracellular protease release and biofilm formation. The ESR also influenced the structure and function of the bacterial envelope by promoting membrane fluidity, permeation, and lipopolysaccharide content to meet growth requirements and combat envelope stress. Interestingly, the regulatory networks and genetic mechanisms responsible for this adaptation partially overlapped with those involved in the development of drug resistance and pathogenicity, albeit with reduced efficiency.

Thirdly, evolution is a continuous process that seeks to minimize stress and develop distinct characteristics that improve fitness across different time frames. Can we trace the evolutionary trajectory and identify the factors that potentially influence the course of evolution? To address this question, we have conducted a comprehensive analysis of the physiological transition in bacteria before, during, and after developing resistance to AgNPs. The results indicated that E. coli MG1655 initially developed resistance by employing flagellin-mediated AgNP precipitation and enhancing antioxidant activity. This led to a five-fold increase in the minimum inhibitory concentration (MIC) value when cultured repeatedly in a medium containing AgNPs at a concentration of 10 × MIC. Subsequently, we observed the overexpression of cus efflux pump genes and the formation of biofilms as mechanisms to maintain AgNP tolerance in the absence of AgNP precipitation. Our study revealed a noteworthy increase (approximately 1,000-fold) in the fraction of persister variants only at later stage. Consequently, the evolved strains exhibited tolerance not only to AgNPs but also to multiple drugs. Our research offers valuable insights into the complex and dynamic nature of bacterial adaptive strategies when exposed to AgNPs.

These findings suggest a potential opportunity to intervene in the evolution of resistance and present a promising perspective for utilizing nanotechnology in directed evolution. However, there exists a knowledge gap concerning the correlation between the structural properties of nanomaterials and their evolvability. This understanding is essential for informed nanostructure design and the development of strategies that can effectively address or combat the emergence of resistances.

Keyword: antibiotic resistance, evolution, nanomaterials

最终交流类型: Invited

High Spatial Resolution Imaging Spectrometry Unraveling the In Vivo Organ-Specific Capture, Transfer, Degradation and Metabolic Responses of Nanoparticles

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Nanomedicine, the combination of nanotechnology with pharmaceutical and biomedical sciences, holds great promise for revolutionary advancements in the efficacy of drugs, drug delivery systems, diagnostics, and therapeutics in combating devastating human diseases. However, a significant concern and challenge lie in understanding the implications of nanomaterial interactions within the mammalian biological milieu. Gaining insights into the organ-specific capture, transfer, degradation, and biological effects during these processes is crucial for the design of highly efficient and safe nanomaterials. In our recent study, we employed several high spatial resolution imaging spectrometry techniques, including laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), laser ablation single-particle ICP-MS (LA-sp-ICP-MS), and desorption electrospray ionization mass spectrometry (DESI-MS), to investigate the in vivo transfer behaviors, deposition, degradation and metabolic responses of graphene oxide nanosheets (GO NSs), gold nanoparticles (GNPs), and silver nanoparticles (AgNPs) following intravenous administration. Our findings demonstrate that while the majority of injected nanoparticles accumulate in the reticuloendothelial system

(RES), particularly in the lung, spleen, and liver, the sub-organ transfer, distribution, and accumulation are strongly influenced by their physicochemical properties, such as size, surface chemistry, dissolution and deformability. For instance, we observed that GO-PVP NSs, which exhibited higher deformability compared to GO-PEG NSs, showed enhanced targeting and retention in the lower respiratory tract, resulting in lung/liver and lung/spleen ratios that were approximately 230-fold and 30-fold higher, respectively, compared to GO-PEG treated mice. Moreover, the surface chemistry of GNPs influenced their in vivo dispersion and aggregation. PEG-coated GNPs maintained dispersion properties, facilitating their passage through the liver sinusoidal endothelium and Disse space, likely leading to clearance from the liver via the hepatobiliary route. On the other hand, chitosan (CS) and polyethylenimine (PEI) capped GNPs exhibited agglomeration/aggregation in vivo and were captured by hepatic Kupffer cells and endothelial cells, resulting in long-term storage in the liver. Utilizing LA-sp-ICP-MS imaging, we were able to visualize the degradation of silver nanoparticles (AgNPs) into AgI species, which were widely distributed in the spleen and liver. Furthermore, metabolic imaging provided early molecular events associated with nanoparticle administration, contributing to a deeper understanding of nano-bio interactions.

Keyword: nanomaterials, physicochemical properties, bio-nano interplay, high spatial resolution imaging spectrometry

最终交流类型: Keynote

The effect of As4S4 nanoparticles to induce multiple-lineage differentiation and post-differentiation apoptosis in leukemia and myelodysplastic syndromes

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Induction treatment is an ideal therapeutic strategy for leukemia with relative low toxicity in comparison with chemotherapies, which induces leukemia cells into different lineages and enhances the cells apoptosis. However, there is little induction therapeutics up to date. Meanwhile, therapeutic choice for refractory anemia arising from ineffective erythropoiesis in myelodysplastic syndromes (MDS) has long remained an unmet demand, and a part of MDS patients would develop to refractory acute myeloid leukemia.

Arsenic sulfide (As_4S_4) is a mineral drug that can be administrated orally and has been applied in several Chinese medicine formulations for blood cancers. However, As_4S_4 are poor water soluble in its original crystal form, which makes it very low bioavailability, meanwhile, difficult to mine mechanisms due to little cellular uptake. In this talk, we will introduce the fabrication of water dissolvable arsenic sulfide nanoformulation (ee-As_4S_4) that is able to induce erythroid and megakaryocytic differentiation in chronic myeloid leukemia (CML) cells [1], induce multiple-lineage differentiation and post-differentiation apoptosis in AML cells and a refractory AML animal model [2], and promote terminal erythropoiesis in the bone marrow mononuclear cells (BMMNCs) of MDS patients with different subtypes (manuscript submitted). We will show that ee-As_4S_4 can be largely internalized by the cells and plays strong reduction role inside the cells to down regulate the intracellular reactive oxygen species (ROS), which leads to the inhibition of histone deacetylase (HDAC) activity in the CML cells [3] and triggers the phosphorylation of eukaryotic translation initiation factor 2α (eIF2α) in the bone marrow cells of MDS patients [manuscript submitted]. Interestingly, the phosphorylation of eIF2α consequently led to the increase of globins in mRNA and protein levels, as well as induced the formation of stress granules (SGs) that caused the segregation and inactivation of eIF4E and inhibited the synthesis of general protein in the BMMNCs. Besides, ee-As_4S_4 mitigated the oxidative stress in BMMNCs by eliminating intracellular reactive oxygen species. All mechanisms together contributed to the effective differentiation of erythroblasts of early and terminal stages.

In conclusion, ee-As_4S_4 holds significant potentials for the treatment of leukemia and refractory anemia that arises from ineffective erythropoiesis.

Keyword: Arsenic sulfide nanoparticles, leukemia, myelodysplastic syndromes, ROS, differentiation

最终交流类型: Invited

Development of safe and efficacious silicasome nanocarrier for drug delivery to gastrointestinal tumors

刘湘圣

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Gastrointestinal (GI) tract cancers (such as gastric cancer, pancreatic cancer, colorectal cancer) are a major category of refractory malignant tumors in clinical practice. The traditional chemotherapy is still an important treatment for GI cancers but generally inefficient and highly toxic. Therefore, a new drug delivery system is urgently needed to improve the efficacy and safety of drugs used for GI cancer treatment. In recent years, we have developed a lipids coated mesoporous silica nanocarrier, i.e., silicasome, which is used for efficient delivery of drugs to tumors in vivo[1-5]. Studies have shown that systematic administration of silicasome can effectively improve the blood circulation time of drugs in the body, and enhance drug accumulation in tumor tissues through transcytosis, showing excellent anti-tumor efficacy in orthotopic pancreatic cancer and colorectal cancer models. Recently, in view of the urgent need for improvement in intraperitoneal thermal infusion chemotherapy, an important treatment for gastric cancer with peritoneal metastasis, the possibility of treating peritoneal metastasis by intraperitoneal administration of silicasome nanodrugs was investigated. It was found that intraperitoneal administration could achieve the same or even better tumor targeting effect than intravenous administration in a variety of gastric cancer mouse models. At the same time, the safety evaluation showed that intraperitoneal administration of silicasome can effectively reduce the side effects of drugs. The study is actively investigating the therapeutic effect of this silicasome nanodrug on peritoneal metastasis of gastric cancer under the intraperitoneal administration mode, which is expected to provide a new effective treatment strategy for this refractory digestive tract tumors. Moreover, we have established the good laboratory practice (GLP) of silicasome nanocarrier in a scale-up procedure, and comprehensively evaluated the safety of the silicasome in cooperating with Nanotechnology Characterization Lab (NCL) at NCI, including the in vitro immunology safety assessments such as hemolysis, complement activation, platelets aggregation, plasma coagulation time Leukocyte procoagulant activity, cytokines in whole blood etc., which showed the silicasome has good biocompatibility for clinical development.

Keyword: nanomedicine, silicasome, gastrointestinal cancers, mode of administration, biocompatibility

最终交流类型: Invited

2D MoS2 Nanosheets Induce Ferroptosis by Promoting NCOA4-Dependent Ferritinophagy and Inhibiting Ferroportin

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Two-dimensional transition metal sulfides (2D TMDCs), such as MoS2 and WS2, can be used as lubricants, catalytic materials, and carriers for drug delivery due to their unique

physicochemical properties. The widespread use of 2D TMDCs increases the risk of human exposure and threatens human health. It has been reported that the exposure of MoS2 nanosheets can cause cytotoxicity, which causes health risks and affects its medical applications. However, knowledge of the underlying molecular mechanisms remains limited. Ferroptosis is an iron-dependent mode of programmed cell death and is closely associated with many human diseases. However, whether 2D MoS2 nanosheets cause ferroptosis and the biological mechanism is unclear. To address the above questions, we selected the lung epithelial cell line BEAS-2B and monocyte-macrophage RAW264.7 (involved in immune defense regulation) as in vitro models. Meanwhile, in order to simulate the exposure of MoS2 nanosheets more realistically, we constructed a mice inhalation exposure model. Our study confirmed that MoS2 nanosheets induce ferroptosis in vivo and in vitro, which is caused by the nanosheet themselves rather than by the dissolved ions. MoS2 nanosheets induce ferroptosis in BEAS-2B and RAW264.7 cells due to nuclear receptor coactivator 4 (NCOA4)-dependent excusive ferritinophagy and the inhibition of ferroportin-1 (FPN). After the cells were exposed to MoS2 nanosheets, most of the MoS2 nanosheets entered the cells via macropinocytosis and were localized to the lysosome, contributing to an increase in the lysosomal membrane permeability (LMP). At the same time, NCOA4-dependent ferritinophagy was activated, and ferritin was degraded in the lysosome, which generated Fe2+. Fe2+ leaked into the cytoplasm, leading to ferroptosis. Inhibition of autophagy using the autophagy inhibitor 3-MA and knockdown of NCOA4 by small interfering RNA were both able to reverse MoS2 nanosheet induced ferroptosis, further confirming that NCOA4-dependent ferritinophagy plays a critical role in MoS2 nanosheet induced ferroptosis. Furthermore, the inhibition of the iron export protein FPN aggravated the overload of Fe2+ in the cell. We found that the expression of FPN was reduced after MoS2 nanosheet exposure, and exogenous overexpression of FPN using an overexpression vector significantly attenuated MoS2 nanosheet induced ferroptosis. It demonstrates that the disruption of FPN may further promote intracellular iron ion overload and ultimately exacerbate cellular ferroptosis. It was also observed that ferroptosis increased in lung tissue in mouse models exposed to MoS2 nanosheets, and the effect of MoS2 nanosheets on mice lung tissue replicated the in-vitro results. In conclusion, this work highlights a novel mechanism by which MoS2 nanosheets induce ferroptosis by promoting NCOA4-dependent ferritinophagy and inhibiting FPN, which could be of importance to elucidate the toxicity and identify the medical applications of 2D nanoparticles.

Keyword: MoS2 nanosheets, ferroptosis, ferritin, ferritinophagy, NCOA4

最终交流类型: Oral

Unsaturation in Lipid Nanoparticles Potentially Enhanced Inhibitory Effects of Gold Nanocluster on Breast Cancer Cells and Lung Carcinoma Cells

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Gold nanoclusters (AuNCs) have proven to be useful in various biomedical applications, such as imaging, diagnosis, drug delivery, and cancer treatment, due to their unique properties like luminescence, catalysis, and ability to generate singlet oxygen and photothermal conversion. However, the instability of AuNCs impedes their fundamental and biomedical application. To address this issue, several studies have employed different capping ligands to stabilize AuNCs, but the ligand-protected AuNCs exhibit a low quantum yield of less than 1% or low catalytic activities, making their in vivo applications limited. To improve AuNCs physicochemical properties, hybrid structures have been developed using various biocompatible organic materials. Among these structures, liposomes have gained much attention because their lipid bilayers can significantly increase colloidal stability and enhance intracellular delivery efficiency.1 Therefore, in this study, we synthesized a series of AuNCs-loaded pH-sensitive lipid nanoparticles (AuNCs@LNPs) by varying the ionizable lipid component's length, unsaturation, and tail branches. We characterized the physicochemical properties of AuNCs@LNPs, such as morphology, size distribution, fluorescence, encapsulation efficiency, and pKa. Five types of AuNC@iLNPs with different pKa values ranging from 5.30 to 5.90 exhibited similar encapsulation efficiency of AuNCs (~66.7%). The administration of lipid nanoparticles without AuNCs showed no significant cytotoxicity, while AuNCs@LNPs showed inhibitory effects on MCF-7 and A549 cells. Especially, AuNCs@C10LNPs with unsaturated tail showed the most significant inhibitory effects on MCF-7 and A549 cells, and present time and dose-dependent inhibition effects, with the lowest cellular viability of 30% and 13% respectively for MCF-7 and A549 cells at 24 h after treatment. Further, dynamic light scattering (DLS) and small angle X-ray scattering (SAXS) analysis indicated that the AuNCs@C10LNPs swell in the artificial endosomal

environment and promote the release of AuNCs. The significant inhibitory effect induced by AuNCs@C10iLNPs may be closely correlated with their intracellular effective release and higher peroxidase-like catalytic activity activities in bio-microenvironments.

Keyword: Lipid nanoparticles, Unsaturation, Gold nanocluster, Inhibitory effects, Cancer cells

最终交流类型: Invited

Environmental particulate matter triggering chronic diseases based on NLRP3 inflammasome activation

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NLRP3 inflammasome is an intracellular protein complex assembled under various stimuli that controls the activation of caspase-1 and regulates the secretion of interleukin-1β (IL-1β) and interleukin-18 (IL-18). Activation of NLRP3 inflammasome has been found to be associated with many chronic diseases. At present, a variety of nanomaterials have been found to activate NLRP3 inflammasome through lysosomal rupture, reactive oxygen species production and potassium ion efflux, which are closely related to their unique physicochemical properties. Fine particulate matter (PM2.5) contains complex physicochemical properties, of which 80-90% are nanoscale particles, which may bypass the blood-brain barrier through the respiratory system and enter the brain directly through the olfactory nerve. We used the APP/PS1 mouse model to evaluate the level of Aβ aggregation and cognitive ability after intranasal perfusion of PM2.5. The results showed that PM2.5 could activate the NLRP3 inflammasome of BV2 cells, release ASC spots, accelerate Aβ aggregation, which led to apoptosis of neuronal cells, induced obvious neuronal function decline and spatial memory impairment in AD mice, and aggravated the occurrence of Alzheimer's disease. In addition, rare earth fertilizers have been widely used in more than 100 crops such as wheat, rice, tea, etc., and these soluble rare earth elements easily enter the human body through the food chain and are converted into insoluble phosphate and bicarbonate particles under normal physiological conditions. Our study found that these rare earth particles can activate NLRP3 inflammasome through the pathways of K+ leakage and lysosomal rupture, and long-term ingestion of soluble rare earth elements by mice can lead to significant renal and liver fibrosis diseases.

Keyword: Environmental particulate matter; NLRP3 inflammasome activation; chronic diseases

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最终交流类型:

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Inhaled nanomaterial (NM) can cause acute and chronic inflammation, with the latter considered a crucial step for the pathogenesis of pulmonary fibrosis. Accordingly, the adverse outcome pathway (AOP) framework for NM inhalation generated fibrosis relies on the

involvement of the inflammatory component. Here we applied single-cell transcriptomics to identify NM-specific cellular perturbations and underlying key cell types. We exposed mice to carbon black (CNP), tangled double-walled (DWCNT) and rigid, multi-walled carbon nanotubes (MWCNT).

At the chosen dose, all NMs induced comparable acute inflammation, which increased further until d6 only for CNTs. Elevated levels at d28 were only observed for MWCNT, allowing a differentiation of the key events (KE) acute and chronic inflammation. To understand which cells elicit the initiation of inflammation, we compared 12h bronchoalveolar lavage (BAL) cytokine levels with scRNA-seq profiles. CNP uniquely triggered GM-CSF and CXCL1 release, with Csf2 and Cxcl1 mRNAs induced mainly in alveolar epithelial cells. DWCNT caused a release of the monocyte attractants CCL2, -3 and -4, involving interstitial macrophages and monocytes. MWCNT however caused the most extensive BAL cytokine response and specifically induced the Th2-cytokines CCL11 and IL10, seen as a crucial KE in fibrosis. Cell-communication-analysis demonstrated MWCNT-specific networks between epithelial cells, fibroblasts, and macrophages.

MWCNT exposure causes the induction of an alveolar differentiation intermediate (ADI), a type 2 alveolar epithelial cell (AT2) state, previously shown to contribute to alveolar regeneration [1]. RNA-velocity analysis revealed the differentiation of AT2 cells to ADI, NicheNet-analysis reveals a pro-inflammatory injury crosstalk within the epithelium. Cell death analysis localizes lung injury to AT2 cells and indicates ferroptosis as a specific cell death pathway.

Our study demonstrates that depending on NM quality different cell types are already early involved in the induction of inflammation and respective KEs and suggests more complex cell-cell communications might be considered on AOP predictive cell-based testing strategies.

Keyword: Single cell transcriptomics, nanomaterial, adverse outcome pathway (AOP), epithelial cells, ferroptosis

最终交流类型: Invited

Mucus penetration of surface engineered nanoparticles in various pH microenvironments

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During the transport of the drug carriers in the airway, the mucus lines the surface of the airway and hinders the effective delivery of active ingredients. The penetration behavior of nanoparticles in mucous depends on physicochemical properties of the nanoparticles and the mucus microenvironment, due to particle-mucin interactions and the presence of the mucin mesh space filtration effect. To date, it is still unclear how the surface properties of nanoparticles influence their mucus penetration behaviors in various physiological and pathophysiological conditions. In this study, we have prepared a comprehensive library of amine-, carboxyl- and PEG-modified silica nanoparticles (SNPs) with well controlled surface ligand densities. Using multiple particle tracking (MPT), we have studied the mechanism responsible for the mucus penetration behaviors of these SNPs. It was found that PEG- and amine-modified SNPs exhibited pH-independent immobilization under iso-density conditions, while carboxyl-modified SNPs exhibited enhanced movement only in weakly alkaline mucus. Further mechanistic biophysical characterizations demonstrated that amine- and carboxyl-modified SNPs were trapped in mucus due to electrostatic interactions and hydrogen bonding with mucin. In contrast, high-density PEGylated surface formed a brush conformation that shields particle-mucin interactions. We have further investigated the surface property-dependent mucus penetration behavior using a murine airway distribution model. This study provides insights for designing efficient transmucosal nanocarriers for prevention and treatment of pulmonary diseases.

Keyword: Mucus penetration, Mucus pH microenvironment, Surface engineering, Multiple particle tracking, Silica nanoparticle

最终交流类型: Oral

Mixed Effects and Co-Transfer of CeO2 NPs and Arsenic in the Pakchoi-Snail Food Chain.

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南京大学

The application of nanomaterials in agriculture offers new solutions for soil As pollution control, meanwhile, concerns also arise about their safety along the food chain to humans. In this study, we comprehensively evaluated the effect of foliar application of CeO_2 nanoparticles (NPs) on As uptake by pakchoi and their co-occurrence along the pakchoi-snail food chain. It was found that CeO_2 NPs reduced the transfer factor of As from pakchoi roots to shoots by 37.9%, and decreased As in snail foot (the edible portion) by 39%, thereby reducing the exposure risk of As to humans by about half. The CeO2 NPs might alleviate As toxicity in pakchoi shoots by regulating the antioxidant system and stimulating photosynthesis and phosphatidylinositol signaling system. On the other hand, although the foliar application of CeO2 NPs resulted in a high accumulation of Ce on pakchoi leaves and a certain transfer to snails, the exposure risk of Ce was low due to its low bioavailability. The plant-snail-human food chain acts as a "risk filter" for CeO2. Our results contribute to a comprehensive assessment of the trophic transfer of NPs along the terrestrial food chain when used as heavy metal passivators and their subsequent effects on higher-level consumers.

Keyword: nanoparticle; pollution control; food chain; trophic transmission; risk assessment

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最终交流类型: Invited

“Fishing” Nano-Bio Interactions at the Key Biological Barriers

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同济大学

Understanding nano-bio interactions is pivotal to the safe implementation of nanotechnology for both biological and environmental applications. Zebrafish as a model organism provides unique opportunities to dissect nano-bio interactions occurring at different biological barriers. This talk will focus on four key biological barriers, namely cell membrane, blood-brain barrier (BBB), skin and gill epithelia, and gastrointestinal tract (GIT), and highlight the recent advancement achieved by using zebrafish to conduct both visualized observations and mechanistic investigations on a diversity of nano-bio interactions for understanding of the hazard potential of engineered nanomaterials.

Keyword: Nano-bio interactions, zebrafish, nanoEHS

最终交流类型: Oral

New Thermodynamic Mechanism of Membrane fouling and Preparation of Antifouling Membrane

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Despite the huge contribution of membrane-based brine and wastewater purification systems in today’s life, biofouling still affects the sustainability of membrane engineering.

Aimed at reducing membrane module wastage, the need to study biofouling monitoring as one of the contributory factors stemmed from the short time between initial attachment and irreversible biofoulant adhesion. Hence, a membrane for monitoring is introduced to determine the right cleaning time by using fluorescent sensing as a non-destructive and scalable approach. The classical solid-state emissive fluorophore, tetraphenylethylene (TPE), was introduced as a sustainable, safe and sensitive fluorescent indicator in order to show the potential of the method, and polyethersulfone (PES) and nonsolvent-induced phase separation method, the most popular material and method, are used to fabricate membrane in industry and academia. Since the employed filler has an aggregation-induced emission (AIE) characteristic, it can track the biofouling throughout the operation. The fabricated membranes have certain characterizations (i.e., morphology assessment, flux, antibiogram, flow cytometry, surface free energy, and protein adsorption), which indicate that a hybrid membrane with 5 wt % of TPE has identical biofouling activity compared to neat PES membrane and its optimal luminescence properties make it an appropriate candidate for non-destructive and online biofouling monitoring.

Keyword: Luminescent membrane； Membrane cleaning； Aggregation-induced emission；Tetraphenylethylene

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最终交流类型: Keynote

Understanding Nanoparticle-Cell Interactions by Multi-dimensional Single Particle Tracking in Live Cells

方宁
厦门大学

Understanding the characteristic motions of functionalized nanoparticles is crucial to understand their interactions with cells. A multi-dimensional single particle tracking technique has been developed to fully disclose the 3D translational and rotational motions of anisotropic imaging probes, as well as relevant biomolecular information, in live cells. Using plasmonic gold nanorods as probe in our recent studies, we have visualized the live endocytic and intracellular transport events of nanoparticle cargos with unprecedented details in live cells. These experiments have led to new insights on the working mechanisms of molecular motors (dynamin in clathrin mediated endocytosis and kinesin/dynein in microtubule-based intracellular transport).

Keyword: Nano-bio Analysis,Nanobioimgaing and Diagnostics

最终交流类型：Invited

Multimodal Precise Cancer Theranosis by Selenium Nanomedicine

陈填烽
Jinan University

Overview: This talks will center on the key scientific issues in tumor radiotherapy and the ways to solve the three bottlenecks of radiotherapy toxicity, radiotherapy resistance and immunosuppression to conduct research on innovative selenium nanomedicine (SeNPs). Based on the biochemical characteristics of tumors, the applicant designed targeted SeNPs to achieve precise drug delivery and reduce toxic side effects. Precise controlled-release SeNPs with tumor microenvironment-responsive properties have also been constructed to overcome inhibitory bottlenecks, improve radiosensitivity, and to reverse radioresistance. The applicant also explored radio-/immune- synergistic therapy strategy through activation of natural/adoptive immune systems through regulating selenoprotein activities by SeNPs, and revealed the molecular mechanisms for reverse of radiotherapy-induced immunosuppression.

Keyword: Selenium Nanomedicine,Theranosis, Radiation immunotherapy

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最终交流类型：Invited

The hematological effects of silica nanoparticles: Particle size-related effect

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Silica nanoparticles (SiNPs), as the second largest engineered nanomaterial, has been widely applied in diverse areas, which concomitantly leads to their inevitable contact with, and subsequent exposure to human bodies. The entering of SiNPs into circulatory system causes the interaction with blood components. How the artificial nanoparticles would affect these functional components and induce unfavorable consequence to the hematological homeostasis is of utmost importance in concern of their hazardous impact on human health.

Testing the effect of SiNPs on the plasma kallikrein-kinin system (KKS) using ex vivo mouse plasma assay showed that this nanomaterial could induce exposure concentration-dependent plasma prekallikrein (PPK) cleavage, showing its perturbation on plasma zymogen cascade. The initial zymogen of Hageman factor XII (FXII) in the KKS could adsorb on the negatively-charged surface of SiNPs, processed the conformational alteration, subsequent autoactivation and self-cleavage, triggering the cascade activation of the KKS. Exposure to

SiNPs also increased the maturation and differentiation of the megakaryocytes, which was characterized by the occurrence of irregular cell morphology, cell size enlargement, DNA content and DNA ploidy increase, spore-lie protrusion formation, thus inducing the platelet formation. All the alterations of bioindicators were inversely correlated with the particle size of SiNPs, showing the higher effects of smaller particles on megakaryocyte development. The encounter of erythrocytes with high levels of SiNPs could cause acute erythrocytotoxicity and hemolysis. Low levels of SiNPs induced the phosphatidylserine exposure through the regulation of overproduction of reactive oxidative species and phosphorylation of p38 and ERK1/2, which would consequently trigger thrombin-dependent platelet activation in plasma, perturbing hematological homeostasis. Moreover, the particle size was also inversely correlated with SiNP-induced effects on blood red cells.

Altogether, exposure to SiNPs poses deleterious hematological risk via disturbing multitargets in circulatory system, and the particle size is one of the crucial influencing factors mediating their bioactivities.

Keyword: Silica nanoparticles, hematological effect, particle size, plasma zymogen, megakaryocyte development

最终交流类型: Invited

Toxic effects of microplastics and their influences on the bioavailability of emerging pollutants

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深圳大学

Microplastics (MPs) have been increasingly widespread in environment and can sorb various hydrophobic organic contaminants, leading to a possible threat to non-target organisms. In the present study, the impact of polystyrene MPs with different diameters on non-target organisms was investigated, and their influences on the bioavailability of emerging pollutants were also studied. In natural waters, MPs (0.03 μm, 1 mg L-1) presented a significant inhibition on algal growth, but the growth rate of Euglena sp. was recovered after 2 d exposure. Their toxicity decreased in the presence of MPs with larger diameters. What’s more, the toxicity mechanisms of MPs varied with algal species. Furthermore, the sorption of diclofenac (DCF) by MPs increased with the increase in particle size, and the sorption was a chemisorption based on the sorption isotherms and Fourier transform infrared spectroscopy (FTIR) results. Due to the sorption, PS MPs alleviated the toxicity of DCF in P. tricornutum

and the DCF toxicity continually decreased as their diameter increased. Meantime, the Euglena sp. revealed a higher removal for DCF, especially in the presence of MPs, but the higher accumulation and bioaccumulation factors (BCFs) indicated a possible ecological risk in natural waters. What's more, BPS had no effect on plant growth, but could accumulate in roots of plant and less trans -location to leaves based on the low TF values. MPs also posed no effect on plant growth, but negatively affected the translocation of BPS in plants. MPs with large size (5 μm) also increased the distribution of BPS in organelles. These findings showed that the toxicity and behavior of MPs in environment should be paid more attention, which may be helpful for their risk assessments.

Keyword: Microplastics, Toxicity, Sorption, Emerging pollutants, Non-target organisms

最终交流类型: Invited

Environmental molecules affect microbial effect of ceria nanoparticles: Two distinct mechanisms

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The rapid development of nanotechnology and the widespread use of engineered nanoparticles (NPs) have raised concerns about the environmental health risks caused by NPs' improper use, disposal, or leakage. Ceria NPs are widely used for their unique properties, thus highly prioritized among engineered NPs for risk screening. Given the critical role of microbes in ecosystem function and productivity, the toxicity of ceria NPs toward microbes has sparked great concern. The speaker has utilized synchrotron radiation techniques to investigate the biotransformation of ceria NPs on nano-bio interfaces, the biochemical mechanism underlying the biotransformation, and the toxicological consequences of the ion release following the biotransformation. Our studies demonstrate that the formation of eco-corona, which occurs when environmental molecules (proteins, electrolytes, natural organic or inorganic matter, etc.) adsorb onto the particle surfaces, alters the physicochemical properties of ceria NPs and, subsequently, their microbial toxicity. In addition, environmental molecules can also change the outcomes of nano-bio interactions by changing the microbial susceptibility to ceria NPs. These findings are of great significance for a more comprehensive understanding of the environmental impacts of NPs.

Keyword: Ceria, microbes, biotransformation, ionic toxicity, susceptibility

最终交流类型: Invited

Understanding engineered nanomaterials-induced inflammation to improve inflammation resolution and inflammation-related disease treatment

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Engineered nanomaterials (ENMs) are widely used in commercial and medical products, such as cosmetics, vaccines, and drug carriers. The widespread production and use increase the risk of ENMs-induced inflammation, which would develop into chronic inflammation and lead to various diseases including tissue fibrosis as well as damage to organs, raising significant public health concerns. The understanding of ENMs-induced inflammation and subsequent control of inflammation and inflammation-related damage have been vital issues. Here, we first detailed the molecular processes underpinning ENMs-induced inflammation actions. Further, using resolvins and their precursors for inflammation resolution, we demonstrate a nano-enabled approach for accomplishing robust anti-fibrotic effects in ENMs-induced pulmonary fibrosis (PF) models in vivo. Targeting the lipid peroxidation-triggered NLRP3 inflammasome and NF-κB pathway in macrophages and the ROS-mediated TGF-β/Smad and S1P signaling in epithelial cells result in these potent protective effects at the ng/mL dosimetry. We further develop an inhalable biocompatible nanoparticle that encapsulates fish oil, a chosen resolvin precursor, with phosphatidylcholine and polyethyleneglycol to enhance drug permeability and facilitate crossing the mucosal barrier, forming “fish-oilsome” (FOS). Oropharyngeal aspiration and inhalation of FOS improved anti-inflammatory status, histological characteristics, and pulmonary function in fibrotic lungs, which was mechanistically supported by transcriptomic and proteomic analyses. Further, scale-up engineered FOS samples with the desired physicochemical properties, anti-PF efficacy, and in vivo biocompatibility were validated in different batch sizes (up to 0.2 L/batch). This study provides a practical and translatable approach to improving ENMs-induced inflammation resolution and inflammation-related disease treatment.

Keyword: Engineered nanomaterials, pulmonary fibrosis, specialized pro-resolving mediators, inflammation resolution, nanomedicine

最终交流类型: Invited

Graphene oxide disruption of homeostasis and regeneration processes in freshwater planarian Dugesia japonica

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The aquatic system is a major sink for engineered nanomaterials released into the environment. Here, we assessed the toxicity of graphene oxide (GO) using the freshwater planarian Dugesia japonica, an invertebrate model that has been widely used for studying the effects of toxins on tissue regeneration and neuronal development. GO not only impaired the growth of normal (homeostatic) worms, but also inhibited the regeneration processes of regenerating (amputated) worms, with LC10 values of 9.86 mg/L and 9.32 mg/L for the 48-h acute toxicity test, respectively. High concentration (200 mg/L) of GO killed all the worms after 3 (regenerating) or 4 (homeostasis) days of exposure. Whole-mount in situ hybridization (WISH) and immunofluorescence analyses suggest GO impaired stem cell proliferation and differentiation, and subsequently caused cell apoptosis and oxidative DNA damage during planarian regeneration. Mechanistic analysis suggests that GO disturbed the antioxidative system (enzymatic and non-enzymatic) and energy metabolism in the planarian at both molecular and genetic levels, thus causing reactive oxygen species (ROS) over accumulation and oxidative damage, including oxidative DNA damage, loss of mitochondrial membrane integrity, lack of energy supply for cell differentiation and proliferation leading to retardance of neuron regeneration. The intrinsic oxidative potential of GO contributes to the GO-induced toxicity in planarians. These data suggest that GO in aquatic systems can cause oxidative stress and neurotoxicity in planarians. Overall, regenerated tissues are more sensitive to GO toxicity than homeostatic ones, suggesting that careful handling and appropriate decisions are needed in the application of GO to achieve healing and tissue regeneration.

Keyword: Graphene oxide, planarian, regeneration, toxicity

最终交流类型: Invited

Analysis for nano-bio interface and its application in nanomedicine

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To understand the nature of biological effects, it is necessary to capture biological process and physicochemical behaviors of nanomaterials. It is still largely unknown about interaction details in situ and the structure at nano-bio interface. To understand the mechanism of biological effects caused by nanomaterials, we have developed methods to capture nanomaterials and quantify their interaction with biological systems at different levels. Synchrotron radiation (SR) techniques are powerful not only to provide the information for elemental component, chemical structure, and form, but also for chemical imaging. Based on SR analysis, we used quantitative methods to characterize binding structure of proteins/phospholipids on nanomaterials, which well explained the roles of nano-bio interaction in inducing biological effects [1,2]. Second, SR-based methods were used to in situ detect chemical reaction of nanomaterials in the biological systems such as lysosomes and tumor microenvironment, which showed chemical behaviors of nanomaterials caused biological effects [3]. Third, we combined high resolution chemical imaging with chemical form analysis in situ for single particle, single cell, and tissue/organs which revealed how nanomaterials are trafficked, accumulated, and metabolized in vivo [4-6]. Finally, we used these methods to study how surface properties induce nanotoxicity [1], how they affect the circulation and clearance of nanocarriers in vivo, and how powerful nanomedicines work in inhibiting microbial infection efficiently [6].

Keyword: Biomedical effects of nanomaterials, nanotoxicity, synchrotron radiation, nano-bio interface

最终交流类型: Oral

Novel polyoxometalate composites for cesium capture and retention: facilitation by the affinity of tungsten

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Yanshan University

Polyoxometalates (POM) exhibit excellent adsorption capacity for radioactive nuclides, but their impotent ability to sequester adsorbates poses a risk of Cs migration in radioactive waste decontamination and disposal. By the Cs adsorption capacity of POMs and the beneficial regulatory effects of ionic liquids (IL), POM composites are promising for the efficient capture and retention of Cs. Herein, we fabricated two POM composed of the phosphotungstate anion (PW) and tetrabutylammonium cation (TBA), i.e., the {WO_6}-saturated TBA-PW_{12} and mono-lacunary TBA-PW_{11}, for the capture and retention of aqueous

Cs. The composites were then characterized, and the performance and mechanism of Cs uptake were investigated. TBA-PW_{12} exhibited ~300 nm aggregate of particles around 20 ~ 60 nm. TBA-PW_{12} retained the Keggin structural features of $PW_{12}O_{40}^{3-}$, which was proven essential for the binding of Cs^+. With a desorption efficiency of only 2.7% in an NH4Cl eluent and a maximum adsorption capacity of 400.9 mg/g at 333 K, Cs capture and retention by TBA-PW_{12} was superior to the ammonium phosphomolybdate POM composite TBA-AMP. The Cs adsorption onto TBA-PWs achieved equilibrium within 180 minutes. Cs uptake by TBA-PWs was monolayer chemisorption of Cs+ accompanied by H^+ release, and the removal efficiencies stabilized around initial pH 5 – 10. Due to intense affinity between W and Cs^+, TBA-PW_{12} efficiently sequestered Cs^+ through $\{WO_6\}$ octahedra so that the $\{WO_6\}$-saturated TBA-PW_{12} presented better Cs uptake performance than the mono-lacunary TBA-PW_{11}. These results provided insight into the potential application of the saturated POM composite and offered an efficient adsorbent for Cs capture and retention from wastewater.

Keyword: polyoxometalate; phosphotungstate; ionic liquid; cesium; removal

最终交流类型: Invited

Design, Fabrication, Efficacy and Safety Evaluation of Nitric Oxide Releasing Nanodrugs for Cancer Therapy

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Nitric oxide (NO) plays a pivotal and multifaceted role in various physiological processes. Consequently, NO-based therapy has garnered increasing attention as a promising approach in the treatment of diverse diseases. Nonetheless, the clinical application of NO therapy has been hampered by significant challenges associated with existing nitric oxide donors. These challenges include poor stability, uncontrolled release behavior, and unclear target specificity. To overcome these limitations, nanotechnology has emerged as a powerful tool with immense potential. In our recent study, we successfully developed a series of functional nanoparticles capable of controlled NO release. These nanoparticles were subsequently applied in the field of biomedicine, encompassing the following applications: 1) A near-infrared-controlled NO delivery system based on upconversion nanoparticles for tumor NO therapy and the reversion of chemo-drug resistance; 2) NO-releasing nanoparticles utilizing photothermal conversion agents for mild photothermal therapy and antibacterial applications; 3) X-ray-triggered NO releasing nanoparticles based on scintillators for enhancing tumor radiotherapy sensitization; and 4) ratiometric co-delivery of NO and chemotherapeutic agent using biomimetic liposomes for the treatment of pancreatic cancer. We conducted thorough evaluations of the therapeutic efficacy of single NO therapy as well as NO-based combination therapies in various tumor models, and further explored the synergistic mechanism between NO and other therapeutic strategies. Furthermore, we performed preliminary safety assessments of these NO-releasing nanodrug candidates. Moving forward, our research aims to advance the clinical translation of these NO-based nanodrugs by focusing on target identification, druggability, and safety considerations concerning NO and its therapeutic combinations. We anticipate that our findings will offer valuable insights into the application of NO nanodrugs or nanomedicine in tumor therapy and other biomedical fields.

Keyword: Nitric oxide, Nanodrug, Tumor therapy, NO-based synergism, Efficacy and safety evaluation

最终交流类型: Oral

Se@Albumin Nanoparticles Attenuates DSS-Induced Colitis via Modulation of Intestinal Barrier Function, Microbiome and Adenosine Metabolism

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Ulcerative colitis (UC) is a chronic inflammatory bowel disease closely related to the imbalance of gut microbiota and intestinal homeostasis.[1] However, the progress in exploring its pathogenesis and finding effective prevention and treatments is still not ideal. A new form of Se@Albumin complex nanoparticles (Se@HS) with significant antioxidant properties and anti-inflammatory activity was developed, [2] but its mechanism of action on UC has not been clarified. In this work, the intervention effect of Se@HS on UC, and its potential mechanism were investigated. Our results showed that Se@HS can obviously alleviate the symptoms of UC in mouse model: improving the weight loss of mice, alleviating the degree of diarrhea and hematochezia in mice, and reducing the inflammatory damage of colon tissue. Compared to DSS-induced colitis group, The expression of TNF- α, and claudin-2 decreased, while the expression of IL-10 and claudin-1 increased in Se@HS treated group ($P<0.05$); The 16S rRNA sequencing of gut microbiome showed that the diversity of intestinal microbiota in the model group mice decreased, and supplementation of Se@HS

could significantly enhance the diversity of intestinal microbiota ($P<0.05$); In the DSS-induced colitis group, the abundance of Verrucomicrobia at the phylum level was reduced, and the abundance of Dubosiella newyorkensis, Akkermansia muciniphila (AKK), Lactobacillus and Vibrio butyricus at the genus level were reduced. After Se@HS intervention, the relative abundance of the above bacterial communities were increased, with the increase in AKK bacteria being more significant in the high-dose group ($P<0.01$). Colonic tissue metabolomics suggest that significant changes of arginine and proline metabolism, purine metabolism were occurred after Se@HS intervention. Our study found that AKK bacteria were significantly positively correlated with purine metabolites.

In summary, Se@HS can significantly alleviate DSS-induced UC in mice, and intestinal microbiota and metabolic remodeling may plays an important role in Se@HS ameliorating acute colitis in mice.

Keyword: Se@Albumin nanoparticles, Colitis, Akkermansia muciniphila, Metabolomics, Inosine

最终交流类型：Invited

Mechanistic toxicity assessment of differently sized and charged polystyrene nanoparticles based on human placental cells

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复旦大学

Nanoplastics, as emerging contaminants, may be degraded from microplastics and released into aquatic systems globally, which pose threats to human health via ingestion with food or water. Although plastic fragments have been isolated from placental tissues in pregnant women, little is known about the direct toxicity of nanoplastics on human placental cells that plays a critical role in maintaining healthy growth of fetus. This study explored the mechanistic toxicity of polystyrene nanoplastics (PS-NPs) with different sizes (25, 50, 100 and 500 nm) and surface charges ($-NH_2$, $-COOH$ and unlabeled) on human placental cells. Results showed that PS-NPs had size- and surface charge-specific toxicity pattern. The smaller the PS-NP size was, the greater the toxicity induced on human placental cells. In terms of surface charges, NH_2-labeled PS-NPs caused greater effects on cytotoxicity, inhibition of protein kinase A (PKA) activity, oxidative stress, and cell cycle arrest compared to COOH-labeled and unmodified PS-NPs. PS-NPs also induced size- and surface charge-

dependent expression profiles of genes involved in various and interrelated toxicity pathways. In particular, PS-NPs increased intracellular reactive oxygen species in human placental cells, which can induce DNA damage and lead to cell cycle arrest in G1or G2 phase, inflammation and apoptosis. Our findings provide empirical evidences that the negative effects of nanoplastics on human placental cells, and highlight the necessity to conduct risk assessment of nanoplastics on female reproduction and fetal development.

Keyword: Polystyrene nanoplastics, human placental cells, pathway-based toxicity assessment, reproductive toxicity, reactive oxygen species

最终交流类型: Invited

Predictive models for hazard assessment of nanomaterials

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Risk assessment of engineered nanomaterials is essential to protect human health and the environment. These materials display high heterogeneity regarding their physicochemical properties, quantum-mechanical properties, and, as such, their toxicological impact. Traditional risk assessment relies mostly on in vivo testing. Rather than extensive testing based on phenotypic responses in animals, there has been a growing shift toward exploiting mechanistically based approaches to underpin data-driven decision-making frameworks. In order to avoid testing of each new nanomaterial from scratch, we aim to develop in silico models for predicting the physicochemical properties as well as biological effect of nanomaterial.

Keyword: Keywords: nanotoxicity, inflammation, computational toxicology, machine learning

最终交流类型: Keynote

Injury target, toxic effect and molecular mechanism of atmospheric fine particulate matters

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China is experiencing the period with most complex air pollution in the world. Fine particulate matter (PM2.5) is not only a key indicator of air quality, but also an important

contributor to air pollution induced health effects. For this reason, we established integrated technology of component screening, function detection, omics screening and pathway analysis to identify new targets, define the effect endpoint and health outcome, and reveal the molecular mechanism for diseases phenotype. Firstly, we determined the metal contents of PM2.5 samples collected from a typical coal-burning city and then investigated the metabolic distributions of six metals (including Zn, Pb, Mn, As, Cu, and Cd) following PM2.5 inhalation in mice in different developmental windows, and found that fine particles mainly deposited in the lung, but PM2.5-bound metals could reach and gather in secondary off-target tissues (the lung, liver, heart and brain) with a developmental window-dependent property. Based on this, (1) PM2.5 aspiration caused histone modification associated lung dysfunction and inflammation, and the action restored after exposure ending and 2-week recovery.[1] (2) PM2.5 exposure reversibly elevated heart rate and blood pressure, induced cardiac systolic dysfunction of older mice, and reversibly induced fibrosis in juvenile and older mice. The mechanism by which PM2.5 exposure resulted in cardiac lesions might involve oxidative stress, NADPH oxidase, TGFβ1, and Smad-dependent pathways.[2] (3) PM2.5 aspiration caused neuroinflammation and deteriorated synaptic function integrity and spatial learning and memory, and the effects were associated with the induction of BACE1. The action was mediated by NF-κB p65-regulated downregulation of miR-574-5p, which targeted BACE1.[3] (4) Gestational exposure to PM2.5 led to histopathological changes and vascularization injuries of the placenta, and caused developmental toxicity and functional damages in offspring.[4] These findings provide new evidence for exposure evaluation and protective treatment for local population.

Keyword: fine particulate matters, injury target, toxic effect, molecular mechanism

最终交流类型: Invited

Glucose-responsive insulin delivery

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People with type 1 diabetes or type 2 with deficient endogenous insulin secretion require exogenous insulin administration to maintain the blood glucose (BG) in the normal range. However, this treatment procedure requires the individuals to monitor BG multiple times daily (or continuously) and administer adequate insulin doses accordingly. The discomfort and inconvenience of BG monitoring and insulin injection could reduce people's

compliance with insulin treatment. In addition, the BG still frequently fluctuates out of the normal range even with the administration of both rapid-acting insulin and long-acting insulin, which may lead to many hyperglycemia-associated chronic complications, such as limb amputation and blindness, and kidney failure. At the same time, hypoglycemia can increase the risk of seizures, unconsciousness, brain damage, or even death.

In healthy individuals, endogenous insulin is precisely secreted by β-cells to match BG fluctuations. Therefore, synthetic insulin delivery systems mimicking the β-cell function to release insulin in response to blood glucose levels have great potential for improving blood glucose control. Building on glucose-responsive mechanisms including glucose oxidase (GOx), phenylboronic acid (PBA), and glucose-binding molecules, we have synthesized various types of stimuli-responsive polymeric materials and developed a series of corresponding glucose-responsive insulin carriers like microneedle array patch, hydrogels, insulin complexes, and insulin analogs. After evaluating these systems in mice and minipigs, the glucose-responsive insulin release performance has been confirmed. Furthermore, the relevance between in vitro and in vivo glucose-responsive insulin release performance has also been evaluated.

However, the clinical translation of the current glucose-responsive insulin delivery system remains challenging. One of the major obstacles that hinder the translation arises from the possible safety concerns associated with the glucose-responsive delivery system. Here, along with introducing the prepration and performance of the glucose-responsive insulin delivery systems, we will also disscuss about the possible safety issues related to glucose-responsive mechanisms and carriers.

Keyword: glucose-responsive carrier, insulin delivery, smart insulin, glucose-responsive mechanism

最终交流类型: Invited

Antagonistic effects of graphene oxide-based nanomaterials on the toxic response to environmental pollutants

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Graphene oxide (GO) chemically exfoliated from oxidized graphite has promising applications in various fields owing to its unique structure and its mechanical, optical, and

electronic properties. Owing to its high specific surface area and abundance of oxygen-containing groups, GO has been extensively explored as one of the most promising nanomaterials for application in environmental remediation and water purification. However, related toxicity studies focusing on GO and environmental pollutants are largely unknown. Here, we found the prominently antagonistic capacity of GO against the toxicity induced by organic and inorganic environmental contaminants both *in vitro* and *in vivo*. Pretreatment with GO dramatically decreased PCB52 induced cytotoxicity and gene mutation in mammalian cells, which was mainly mediated by triggering a genuine autophagic process. With *Caenorhabditis elegans (C. elegans)* as an in vivo model, along with adsorption, the beneficial effects of GO in reducing As(III)-induced toxicity in vivo were through protective autophagy coupled with downregulation of arsenic target protein expression. Comparing with ZnO NPs or GO alone, ZnO/GO nanocomposites manifested more excellent Cd detoxification efficiency both *in vitro* and *in vivo* through sharply decreasing the bioaccumulation of Cd via modulating the uptake-excretion process of Cd. Additionally, ZnO/GO nano-composites possessed elevated biocompatibility than ZnO NPs. Our data provided new insights into the potential application of GO-based nanomaterials in prevention and detoxification of environmental pollutants.

Keyword: GO-based nanomaterials, Antagonistic effects, Toxic response, Environmental pollutants

最终交流类型：Invited

Interactions between biomaterials and membrane interfaces - from biomedical to bioagricultural applications

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Nano-biointerface aims to study the basic rules of interaction between nanomaterials and biological interface at the nanoscale, which is a frontier and hot direction in the development of nanobiotechnology. An important issue at the nano-biological interface is investigating the potential interactions between nanomaterials and the components of living systems. Solving the above problems is of guiding significance to fully understand nanomaterials' biological effects and biosafety and to complete the design of biointerfaces for specific biomedical and agricultural applications. However, the structure of living systems is dynamic, ordered, and

highly complex, making it difficult to study the effects of nano-biological interfaces in life processes. How to construct a nano-biological interface interaction model is the core problem. Focusing on this problem, we took the nano-membrane interface (including lipid, cell, and cell membranes with a cell wall) as a breakthrough. We clarified various new nano-lipid membrane interface interaction mechanisms for biomedical and bio-agricultural purposes. We established a controllable assembly and precise regulation method of nanomaterials on lipid membranes and designed nano-drug carriers at the nano-cell membrane interface. Studies on plant nanotechnology have enriched the connotation of nano-bio interface at the cell wall-containing cell membrane interface.

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Keyword: Nano-biological effect, Nano-biointerface, Delivery carrier material design, Plant nanotechnology

最终交流类型：Keynote

Airborne fine particles drive H1N1 viruses deep into the lower respiratory tract and distant organs

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Mounting data suggest that environmental pollution due to airborne fine particles (AFPs) increases the occurrence and severity of respiratory virus infection in humans. However, it is unclear whether and how interactions with AFPs alter viral infection and distribution. We report synergetic effects between various AFPs and the H1N1 virus, regulated by physicochemical properties of the AFPs. Unlike infection caused by virus alone, AFPs facilitated the internalization of virus through a receptor-independent pathway. Moreover, AFPs promoted the budding and dispersal of progeny virions, likely mediated by lipid rafts in the host plasma membrane. Infected animal models demonstrated that AFPs favored

penetration of the H1N1 virus into the distal lung, and its translocation into extrapulmonary organs including the liver, spleen, and kidney, thus causing severe local and systemic disorders. Our findings revealed a key role of AFPs in driving viral infection throughout the respiratory tract and beyond. These insights entail stronger air quality management and air pollution reduction policies.

Keyword: airborne fine particles， viral infection ， extrapulmonary organs

最终交流类型: Invited

Multi-Dimensional Characterization of Ambient Nanoparticles in the Human Body

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Characterization at nanoscale plays a crucial role in in-depth understanding the nature and processes of environmental nanoparticles (NPs). Unfortunately, current techniques suffer from many limitations, like lack of accurate molecular information, inability to real-time monitor intermediates, or vulnerability to sample matrix interference. To probe NPs in the human body, we developed some MS-based techniques to analyze and characterize NPs. Specifically, we developed a chemical multi-fingerprinting platform (integrating elemental fingerprinting, high-resolution structural fingerprinting, and natural isotopic fingerprinting) for particle characterization and source tracing. We found that exogenous NPs are widely present in the human blood samples with extreme diversity in chemical species, concentration, and morphology. Furthermore, we have also developed detection platforms for airborne magnetic NPs and soot particles in complex media based on different MS techniques. These methods will greatly rich the toolbox of nanotoxicological research and nanomaterial risk assessment.

Keyword: Nanoparticle, Mass spectrometry, Exposure, Nanotoxicology, Characterization

最终交流类型: Keynote

Catalytic Toxicology Study on Nanomaterial

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The high surface area of single-atom layers in nanoparticles endows them with significant catalytic activity. Some engineered nanomaterials are reported to even mimic the

activity of natural enzymes. When these nanoparticles are exposed to organisms, they may catalytically speed up a specific biochemical reaction, disrupt the metabolic balance of organisms and cause severe toxic effects. Understanding the toxic mechanism of enzyme-like nanomaterial is a key issue in environmental toxicology research. To address this challenge, this report focuses on the interaction between the nanoparticle-biological interface and develops advanced analytical methods, such as liquid chromatography-mass spectrometry, fluorescent and radiological imaging. Interestingly, surface atomic vacancy was found to dictate the enzyme-like activity of nanomaterials. These enzyme-like nanomaterials could catalyze the peroxidation of polyunsaturated lipids, dephosphorylation of phospholipids, oxidation of NAD(P)H, dehydrogenation of metabolites and esterolysis of lactones, resulting in ferroptosis, NLRP3 inflammasome activation, immune activation, reductive stress and disruption of bacterial communications, respectively. Furthermore, based on the exploration of the structure-activity relationship in nanotoxicity, new strategies for safe design of nanomaterials are proposed, including vacancy healing and protein corona regulation. These findings provide new methods for analyzing nano-bio interactions, expand the knowledge of nanotoxicology, and the developed safety design methods contribute to the sustainable development of nanotechnology and industry.

Keyword: Nanotoxicity, biocatalysis, nanozyme, ferroptosis, reductive stress

最终交流类型: Keynote

Direct entry of micro(nano)plastics into human blood circulatory system by intravenous infusion

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Southern University of Science and Technology

Micro(nano)plastics (MNPs) are widely distributed in the global environment and biota, posing risks on human health. However, their impacts on human health at large are still poorly known, partly due to the lack of knowledge on the exposure of MNPs to human body that greatly impedes thorough assessment of their potential risks on human health[1]. Current studies mainly focus on particle inhalation and ingestion, which are considered as the dominant pathways for MNPs to enter human body[2]. It remains unclear whether there is a direct and serious exposure route of MNPs into the human blood circulatory system, such as intravenous infusion. Although most intravenous infusion products (IVIPs) are made of plastics, the numbers of MNPs released from plastic IVIPs during the intravenous infusion

remain unknown, partly due to the lack of efficient analytical methods. Here, we develop comprehensive analytical methods by combined use of Pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS), scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy (SEM-EDS) and Raman spectroscopy to identify and quantify polyvinyl chloride MNPs down to 20 nm. Using the established methods, this study found about 0.52 μg equal to $10^5 \sim 10^{11}$ particles of PVC-MNPs were released from PVC-IVIPs and should be directly introduced into the human blood circulatory system during each intravenous infusion of 250 mL injection. we also demonstrated that the released amounts of MNPs from IVIPs were dependent on the plastic materials, and the injection volume and composition. Our study reveals a previously ignored but important pathway of human exposure to MNPs, and calls for further research on the potential risks of these MNPs on human health.

Keyword: micro(nano)plastics, identification, intravenous infusion, human exposure

最终交流类型: Keynote

Mechanistic Insights into the Biodegradation of Carbon Dots by Two Typical Oxidoreductases.

Liang Mao
Nanjing University

As a new carbon nanomaterial, carbon dots (CDs) with unique physicochemical and luminescent properties have wide-ranging applications.1 The rapid increase in production and use of CDs will inevitably lead to their release into the environment, and the potential environmental impacts of CDs have also raised significant concerns. CDs have been found to induce toxic effects on various organisms, including mammalian cells, algae, and bacteria. Therefore, it is needed to assess the possible environmental impacts and health risks of CDs to ensure their safe use.

Understanding the biodegradability of nanomaterials is of particular importance for both minimizing their adverse impacts on living organisms and eliminating their contamination from the environment.2 Like many nanomaterials, once administered in vivo or released into the natural environment, CDs will confront the different types of oxidoreductases enzymes. To date, many studies have reported the degradation of nanomaterials catalyzed by naturally occurring enzymes.3 Nevertheless, the research on the biodegradation of CDs by enzymes is still in the initial stage. The enzymatic transformation of CDs at the molecular level, in particular, is largely unknown.

Laccase and peroxidase, are two typical oxidoreductases in the natural environment, which are critically involved in natural transformation processes like humification, lignocellulosic degradation, and recalcitrant contaminants elimination.4 Therefore, it is important to investigate their potential catalytic roles in the transformation of CNMs including CDs. The enzymatic transformation may alter the physicochemical properties of CDs, thereby affecting their biological effects.5 Nevertheless, quantification of CDs in vivo remains a challenge because plant tissues have high background carbon levels that obstruct the high-precision quantification of CDs in biological samples.

Herein, we presented a comprehensive investigation into the transformation of CDs by two typical oxidoreductases, i.e., laccase and horseradish peroxidase (HRP). The degradation rates of CDs were determined to be first-order in both substrate and enzyme. Computational docking studies showed that CDs preferentially bonded to the pocket of the enzyme on the basal plane rather than the edge through hydrogen bonds and hydrophobic interactions. Electrospray ionization-Fourier transform-ion cyclotron resonance mass spectrometry (ESI-FT-ICR MS) and other characterizations revealed that the phenolic/amino lignins and tannins portions in CDs are susceptible to biotransformation, resulting in graphitic structure damage and smaller-sized fragments. By using the 13C stable isotope labeling technique, we quantified the uptake and translocation of 13C-CDs by mung bean plants. 13C-CDs (10 mg L-1) accumulated in the root, stem, and leaf were estimated to be 291, 239, and 152 μg g-1 at day 5. We also evidenced that laccase treatment alters the particle size and surface chemistry of CDs, which could facilitate the uptake of CDs by plants and reduce their nanotoxicity to plants.

We further examined the co-transformation of CDs and phenolic compounds (Phenols) via HRP-catalyzed reactions. In the binary system, both the removal rates of CDs and phenolic compounds (paracetamol, trimethylphenol, and trichlorophenol) were enhanced. The presence of CDs is able to protect HRP from inactivation as demonstrated through enzyme activity test. In addition, the enzymatic reaction kinetics further indicated that the CDs-Phenols complex has a higher binding affinity with HRP than the sole CDs. Moreover, both X-ray photoelectron spectrometer and ESI-FT-ICR MS characterizations demonstrated that the phenolic radicals would attack CDs and generate cross-coupling products. overall, this study provided experimental evidence and fundamental mechanistic insights into the biodegradation of CDs by two typical oxidoreductases. The results of this study highlighted the non-negligible influence of enzymatic transformation on the environmental impacts and the biological effects of CDs.

Keyword: Carbon dots, enzyme-mediated biodegradation, 13C stable isotope labeling techniques, co-transformations, biological effects

最终交流类型：Keynote

Dynamic Nano-Assemblies for Biological Sensing, Imaging and Regulation

Dynamic Nano-Assemblies for Biological Sensing, Imaging and Regulation

Keyword: Dynamic Nano-Assemblies for Biological Sensing, Imaging and Regulation

最终交流类型: Oral

Nanozyme: An emerging raw material for food preservation

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Food-borne microorganisms often cause food contamination and food spoilage throughout the food supply chain. Traditional food preservatives either have limited capability to preserve food, or may greatly increase the risk of microbial resistance, thereby losing effective control over food safety and quality. Inspired by the antiseptic activities of natural enzymes, "nanozymes" with enzyme-like characteristics may effectively fight against harmful microorganisms through sustained biomimetic catalytic reactions, and thus are expected to be a class of candidate food preservatives with long-lasting and safer bacteriostatic efficacy. This presentation will illuminate the foreseeing potentials of smart-responsive nanozymes designed for the application of food preservation.

Keyword：Food safety; food-borne microorganisms; nanofood; nanozyme; nanocatalysis

最终交流类型: Invited

Nanozymes for translational medicine: a preliminary study

魏辉
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Nanozymes are functional nanomaterials with enzyme-like activities. Nanozymes combine the unique features of artificial enzymes and nanomaterials. Therefore, they have superior properties compared with natural enzymes and conventional artificial enzymes. First, they have multiple functionalities beyond catalysis, such as optical, electric, and magnetic properities. Second, the rich surface chemistry and high surface area enable facile conjugation of biorecognition molecules, which is critical for developing bioanalysis probes. Moreover, the catalytic activity of nanozymes can be tuned by various strategies such as

composition, structures, morphologies, surface modifications, allowing for rational design of high performance nanozymes. Here, we will introduce our recent efforts on nanozyme design and their applications for translational medicine. First, an orally administered CeO2@montmorillonite nanozyme targeting inflammation for inflammatory bowel disease therapy is introduced. Second, a probiotic nanozyme hydrogel regulateing vaginal microenvironment for Candida vaginitis therapy is discussed.

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A probiotic nanozyme hydrogel regulates vaginal microenvironment for Candida vaginitis therapy

Science Advances, 2023, 9, in press.

Keyword： nanozymes, translational medicine

最终交流类型: Invited

Unveiling the Reaction Mechanisms in Nanozyme-Catalyzed Oxidation of o-Phenylenediamine

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Nanozymes, as an emerging class of nanoengineered artificial enzymes, have offered significant advantages over natural enzymes in terms of stability, activity, cost, and scale-up production.[1] Due to these key advantages, nanozymes have garnered increasing interest over the past decade and found their way in various applications including biosensors, immunoassays, nanomedicines, and environmental remediation.[2,3] Oxidation of o-phenylenediamine (OPD) by nanozymes has been listed as a standard protocol for determining nanozyme activities[4]. Given the complexity of OPD oxidation reactions, elucidation of the mechanism of nanozyme-catalyzed oxidation of OPD is of vital importance for its standardization as a protocol for determining the catalytic activity of nanozymes. To date, however, no mechanistic study has ever been done to study the mechanism of oxidation of OPD in the case of nanozymes.

In this talk, I'll introduce our mechanistic studies of nanozyme-catalyzed oxidation of OPD and the discovery of a distinguishably different mechanism from that of natural enzymes[5]. A combination of Fourier transform infrared spectroscopy, nuclear magnetic resonance, electrospray ionization mass spectrometry, and electron microscopic studies provides compelling evidence that polymerization of OPD occurs on the surface of several different nanozymes. The unexpected polymerization causes a dense coating layer of poly(o-phenylenediamine) (POPD) on nanozymes, blocks the active sites of nanozymes, and renders the intrinsic properties of nanozymes. This phenomenon can be generalized on the surface of several different nanozymes, including Au, Fe3O4, Pd, Pt, CeO2, and Prussian blue nanozymes. Therefore, this fundamental discovery raised serious concerns using OPD-based colorimetric method for determining nanozyme activities. Without examining the surface change of nanozymes after catalytic reactions, the use of OPD-based colorimetric method for determining nanozyme activities is strongly discouraged. Furthermore, POPD is discovered as a new oxidase mimic, and this new mechanism also provides a general and robust method to coat many nanomaterials with POPD polymers of enzyme-mimicking properties.

Keyword： nanozyme, o-phenylenediamine, polymerization, peroxidase, colorimetry

最终交流类型: Keynote

Ceria-based nanoparticles for therapeutic antioxidants and radioprotectants

Taeghwan Hyeon
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We demonstrated that ceria nanoparticles and related ceria–based nanoparticles can work as therapeutic antioxidants to treat various intractable diseases, including ischemic stroke, Alzheimer's disease, sepsis, and Parkinson's disease.[1] Furthermore, we showed that CeO_2/Mn_3O_4 nanoparticles are highly catalytic antioxidants that can protect tissue-resident stem cells from irradiation-induced ROS damage and can protect the regenerative capabilities of intestinal stem cells in an organoid model after a lethal dose of irradiation.[2] We also demonstrated that the use of CeO_2/Mn_3O_4 nanoparticles can protect the parasympathetic ganglion and tissue-resident stem cells in an *ex vivo* culture model of embryonic salivary gland. We developed manganese ferrite and ceria nanoparticle-anchored mesoporous silica nanoparticles (MFC-MSNs) that can synergistically scavenge ROS and produce O_2 for reducing M1 macrophage levels and inducing M2 macrophages for rheumatoid arthritis (RA) treatment.[3] Very recently, we demonstrated that ceria nanoparticle and mesenchymal stem cell works not only individually but also cooperatively toward a comprehensive RA treatment.[4] Ceria nanoparticles deposited with copper ions, the cofactors for the indigenous antioxidant enzyme, superoxide dismutase 1 (SOD1), are synthesized for effective and synergistic antioxidant therapy to treat ischemic vascular diseases.[5] Through H_2O_2-mediated edge generation, we modulate local coordination environment and electronic structure of single-atomic iron (FeN_4) sites, which significantly boost multi-enzymatic properties for bio-catalytic therapeutics.[6]

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6. "Geometric Tuning of Single-Atom FeN_4 Sites via Edge-Generation Enhances Multi-Enzymatic Properties," *Adv. Mater.* **2023**, *35*, 2207666.

Keyword： ceria nanoparticles, therapeutic antioxidants, radioprotectants, reactive oxygen species (ROS), enzymatic properties

最终交流类型: Invited

Prussian blue nanozyme regulates microenvironment to prevent and treat diseases

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The homeostasis of microenvironment is an important condition for maintaining normal cell proliferation, differentiation, metabolism and functional activities. Abnormal changes in microenvironment components can cause cell lesions. Reactive oxygen species, inflammation, oxidative stress and other microenvironment are closely related to the occurrence and development of diseases. Therefore, how to maintain the homeostasis of cell microenvironment is the key to disease prevention, and how to remodel the cell microenvironment of disease is the key to disease treatment. Guided by clinical issues, centering on the scientific issue of "how bioactive nanomaterials regulate microenvironment to prevent/treat diseases", Prussian blue approved by the US Food and Drug Administration was selected as a representative bioactive material, and we focus on the research main line of "Prussian blue biological activities and cell microenvironment regulation". Using polyvinylpyrrolidone as reducing agent and stabilizer, a variety of mesoporous Prussian blue were constructed, which solved the shortcomings of clinical Prussian blue. A prevention strategy of Prussian blue mediated "maintaining normal microenvironment homeostasis" and a treatment strategy of Prussian blue mediated "remodeling disease microenvironment" was proposed.

(1) Ischemia reperfusion injury can occur during organ transplantation, surgical procedures, and blood circulation disorders such as thrombosis. In tissue ischemia-reperfusion cascades, a large amount of ROS are generated, attacking cell membrane lipids, proteins, DNA, and RNA, causing a series of damage. The production of excessive ROS can stimulate the expression of cytokines and adhesion molecules, thereby mediating inflammation and immune response, ultimately leading to further inflammatory damage. Timely and continuous removal of excess ROS and maintenance of normal microenvironment homeostasis are the key to the prevention of ischemia-reperfusion injury, which is still a challenge. In our studies, the effectiveness, feasibility, safety, and mechanism

of the proposed prevention strategy were elucidated in animal models of ischemia-reperfusion skin flap injury, ischemia-reperfusion brain injury, and ischemia-reperfusion liver injury, providing new strategies and references for the prevention of ischemia-reperfusion injury and drug development.

(2) Degenerative diseases have become a major health and social issue faced by various countries, with degenerative diseases such as Parkinson's disease, Alzheimer's disease, osteoarthritis, and osteoporosis being one of the most unmet clinical areas. ROS, inflammation, oxidative stress, and other factors are closely related to the occurrence and development of degenerative diseases. How to continuously regulate the microenvironment such as ROS, inflammation and oxidative stress at the site of degenerative diseases, and how to remodel the disease microenvironment is the key to the treatment of chronic diseases such as degenerative diseases, which is still a challenge. The effectiveness, feasibility, safety, and mechanism of the proposed treatment strategy have been elucidated in animal models of neurodegenerative diseases (Alzheimer's disease and Parkinson's disease) and bone related degenerative diseases (osteoporosis and osteoarthritis), providing new ideas for the treatment and drug development of chronic diseases such as degenerative diseases.

Keyword： Prussian blue nanozyme; Cell microenvironment; Bioactivity; Ischemia-reperfusion injury; Neurodegenerative diseases

最终交流类型: Invited

Nanozymes inspired by natural enzymes

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Nanozymes, nanomaterials with enzyme-like activities, with high structural stability, adjustable catalytic activity, functional diversity, recyclability and feasibility in large-scale preparation, have become a hot spot in the field of artificial enzymes in recent years, and are expected to become potential surrogates and competitors for natural enzymes in practical applications. With the development of in-depth research and a wide range of application requirements, creating nanozymes with catalytic performance comparable or even surpassing natural enzymes has been the key research topic in this field. Most of the nanozymes reported in the past were obtained based on random synthesis and screening, of which the catalytic efficiency is far inferior to that of natural enzymes. Natural enzymes that have evolved over

hundreds of millions of years have developed a lot of high-efficiency catalysis know-how hidden in their structural features. To create highly active nanozymes, we assumed that there is a general structure-activity relationship between nanozymes and natural enzymes, and proposed the nanozyme optimization strategy by grafting the catalytic principles of natural enzymes into the rational design of nanozymes. Based on this bioinspired strategy, a series of nanozymes that exhibit similar catalytic activities that are closer or even beyond those of natural enzymes have been successfully synthesized. By now, rationally designed high-activity bioinspired nanozymes have become a hot topic in the current research on nanozymes.

Here, we focus on recent representative research progress in systemic design and construction of bioinspired nanozymes, and are devoted to introducing the strategic concepts in bioinspired optimization of nanozymes. We show that de novo design of nanozymes by simulating the amino acid microenvironment, metal-free architecture, and coordination structure of metal active sites in natural enzymes are effective strategies to significantly improve the catalytic performance of nanozymes. A future perspective of the challenges and countermeasures of bioinspired nanozymes is proposed on the basis of these achievements. We hope that the biologically inspired perception will arouse widespread interests in fundamental research and practical applications, as well as provide inspiration for the rational design of nanozymes.

Keyword： Nanozymes, structure-function relationship, catalytic activity, catalytic therapy, disease diagnosis and treatment.

最终交流类型: Invited

Surface-bound reactive oxygen species generating nanozymes for selective antibacterial action

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Killing microbes by producing reactive oxygen species (ROS) in situ, nanozymes are promising as antimicrobials. ROS’ intrinsic inability to distinguish bacteria from mammalian cells, however, deprives nanozymes of the selectivity necessary for an ideal antimicrobial. To make nanozymes selectively active against bacteria over mammalian cells, we herein propose nanozymes that generate surface-bound ROS. Using a silver-palladium bimetallic alloy nanocage, AgPd0.38, that converts oxygen into surface-bound singlet oxygen-like ROS as a

first model for surface-bound ROS generating nanozymes, we show that AgPd0.38 is potent against a wide-spectrum of bacteria but lacks cytotoxicity to diverse mammalian cell-lines and that the observed selectivity is retained even in mouse models bearing bacterial infection, indicative of successful acquisition of the selectivity necessary for an ideal antimicrobial. Of note, AgPd0.38 exhibits similar potency against methicillin-resistant Staphylococcus aureus as against the otherwise antibiotic-sensitive Staphylococcus aureus strain and, after repeated dosage, fails to induce the emergence of resistance in Gram-positive and -negative bacteria — which contrasts significantly with silver nanoparticles, suggesting that the surface-bound nature of the ROS generated by AgPd0.38 does not impact this nanozyme's potential in fighting against antimicrobial resistance in bacteria. In addition to AgPd0.38, two other nanozymes that are distinct from AgPd0.38 both in chemical composition and in the ROS type they generate but similar as AgPd0.38 in the ability to generate surface-bound ROS are used as two extra models and are found to selectively kill bacteria over mammalian cells as does AgPd0.38, suggesting selective action against bacteria over mammalian cells as a property global for nanozymes that generate surface-bound ROS. Moreover, using AgPd0.38 as a model, we show that the observed selectivity is attributable to both the surface-bound nature of ROS these nanozymes generate and an unexpected antidote role of endocytosis that is common to mammalian cells but absent in bacteria. In addition, we use AgPd0.38 as a model for surface-bound ROS generating nanozymes and find that, though generating surface-bound ROS, AgPd0.38 when used as coating additives enables an inert substrate to inhibit biofilm formation and to suppress infection-related immune responses in mouse models. This work opens an avenue toward biocompatible nanozymes and may have implication in our fight against antimicrobial resistance.

Keyword： antimicrobial resistance, biofilm, nanoparticle, artificial enzyme, reactive oxygen species

最终交流类型: Invited

Research and application of nano-enzyme-based bionanomaterials in the field of orthopedic implant-associated infections

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As a common morbidity after orthopedic prosthesis replacement, periprosthetic infections continue to cause many intractable diseases. The evolution of bacterial resistance due to antibiotic use cannot be ignored. For this reason, there is a growing need to develop non-antibiotic antimicrobial strategies to eliminate periprosthetic biofilms without bacterial resistance evolution.(1)

To this end, we propose a novel non-antibiotic strategy based on the synergistic effect of thermally amplified chemodynamic therapy driven by a bionic catalyst and innate immune modulation for specific biofilm removal by intelligently designing biofilm microenvironment-responsive bilayer metal-organic framework bionic catalysts (MACG) composed of MIL-100 and CuBTC. Once reaching the acidic BME, the acidity-triggered degradation of CuBTC allows the sequential release of glucose oxidase (GOx) and an activable photothermal agent, 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) (ABTS). GOx converts glucose into H2O2 and gluconic acid, which can further acidify the BME to accelerate the CuBTC degradation and GOx/ABTS release. The in vitro and in vivo results show that horseradish peroxidase (HRP)-mimicking MIL-100 in the presence of self-supplied H2O2 can catalyze the oxidation of ABTS into oxABTS to yield a photothermal effect that breaks the biofilm structure via eDNA damage. Simultaneously, the Cu ion released from the degraded CuBTC can deplete glutathione and catalyze the splitting of H2O2 into •OH, which can effectively penetrate the heat-induced loose biofilms and kill sessile bacteria (up to 98.64%), such as E. coli and MRSA.(2)

In another work, we prepared microneedle patches enriched with ferric tetroxide and proposed to kill bacteria by Fe overload of Fe-like death-assisted mild thermotherapy based on Fe elemental competition between bacteria and normal immune cells in the infected microenvironment. At the same time, the phagocytic function of immune cells that received Fe element supplementation was restored, and the two synergistically cleared biofilm and inhibited infection recurrence.(3)

Subsequently, we reported on novel "interference-regulation strategy" based on bovine serum albumin–iridium oxide nanoparticles (BIONPs) as biofilm homeostasis interrupter and immunomodulator via singlet oxygen (1O2)-sensitized mild hyperthermia for combating BAIs. The catalase-like BIONPs convert abundant H2O2 inside the biofilm-microenvironment (BME) to sufficient oxygen gas (O2), which can efficiently enhance the generation of 1O2 under near-infrared irradiation. The 1O2-induced biofilm homeostasis disturbance (e.g., sigB, groEL, agr-A, icaD, eDNA) can disrupt the sophisticated defense system of biofilm, further enhancing the sensitivity of biofilms to mild hyperthermia.(4)

Further research and application of bionic nanoenzyme-based materials in the field of periprosthetic infections in orthopedic prostheses is yet to be carried out.

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Keyword：Periprosthetic infection, bionic nanoenzyme, biofilm

最终交流类型: Oral

Bioinspired hierarchical self-assembled nanozyme for efficient antibacterial treatment

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Along with the rapid development and ever-deepening understanding of nanoscience and nanotechnology, nanomaterials hold promise to mimic the highly evolved biological exquisite nanostructures and sophisticated functions. Here, inspired by the ubiquitous antibacterial nanostructures on the wing surfaces of some insects, we develop a $NiCo_2O_4$ nanozyme with self-adaptive hierarchical nanostructure that can capture bacteria of various morphotypes via the physico-mechanical interaction between the nanostructure and bacteria. Moreover, the developed biomimetic nanostructure further exhibits superior peroxidase-like catalytic activity, which can catalytically generate highly toxic reactive oxygen species that disrupt bacterial membranes and induce bacterial apoptosis. Therefore, the mechano-catalytic coupling property of this $NiCo_2O_4$ nanozyme allows for an extensive and efficient antibacterial application, with no concerns of antimicrobial resistance. This work suggests a promising strategy for the rational design of advanced antibacterial materials by mimicking biological antibiosis.

Keyword： Self-adaptive structure, Nanozyme, NiCo2O4, Antibacterial treatment, Mechano-chemical coupling behavior

最终交流类型: Keynote

Research progress of noble metal-based nanozymes

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国家纳米科学中心

Since the discovery of peroxidase-like activity of Fe3O4 nanoparticles (NPs), [1] many different nanomaterials, such as carbon nanomaterials, oxide nanomaterials, metal nanoparticles, two-dimensional nanostructures, etc., have been found to exhibit enzyme-like catalytic activities. Owing to inherent high chemical stability, nanozymes, nanomaterials with enzyme-like catalytic activities, have demonstrated broad application scenarios, such as energy, environment, and human health. [2] The rapid development in this field also aroused a new upsurge of nanozyme research. Among various nanozymes, metal -based nanomaterials have attracted special attention owing to their unique property of localized surface plasmon resonance (LSPR), collective oscillation of free electrons. The LSPR features can be easily regulated via particle size, shape, composition, structure, and surface chemistry, to name a few. Such rich tuning parameters make the maneuver of LSPR-related properties, such as local field enhancement, hot carrier injection, and local photothermal effect, easy and flexible. Local plasmons not only endow the light modulation of metal-based nanozymes and improve their enzyme-like catalytic activities, but also bring in new catalytic mechanisms /pathways and induce new types of enzyme activity. Furthermore, the multimode imaging modalities of noble metal nanostructures themselves, such as surface enhanced Raman scattering (SERS), multi-photon fluorescence (two- or three-photon fluorescence), photoacoustic and photothermal imaging, give them extra functionalities. In this talk, I will first give a brief introduction of new achievements in this field, such as exciting single atom catalysis, which makes nanozymes realize single site catalysis, close to their natural counterparts. Then, I will present the research progress of noble metal-based nanozymes, including our own effort, [3-6] from 1) characteristics of LSPR and its benefits for catalysis, 2) design and controlled wet-chemical synthesis, 3) activity regulation via crystalline facet, composition, and/or forming hybrid structure, 4) catalytic mechanism investigation both experimentally and theoretically, 5) multiply- substrates and multiply-enzymes features and substrate specificity improvement strategy, and 6) potential application fields. In the end, future perspectives are highlighted.

Keyword： Nanozymes, Localized Plasmon, Photocatalysis, Catalytic mechanism, Substrate specificity

最终交流类型: Invited

The fabrication of nano-biocatalysts with amplified therapeutic effects in pathological environments

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Life activities and organism metabolism are accomplished through biocatalysis, and many physiological and pathological processes are related to biocatalysis. Recently the introduction of catalysts into the body were reported to regulate the biochemical reactions. Especially, nano-biocatalysts which possess enzyme-like activity, were able to modulate the intracellular microenvironment and play a role in disease treatment. In addition, nano-biocatalysts can use the metabolic substances at the focal point to produce the desired therapeutic effect only at the disease site, and therefore are expected to reduce or eliminate the side effects on the whole body to achieve site-specific treatment. Thus, nanobiocatalysts exhibit great potential in the diagnosis and treatment of many major diseases, such as cancer, cardiovascular diseases, infectious diseases, neurodegenerative diseases, etc. However, the current therapeutic efficiency of nano-biocatalysts in living organisms is poor because of their low catalytic efficiency, poor specificity, and limited variety of substrate molecules they can catalyze, which severely limit the long-time and continuous treatment of nano-biocatalysts in disease areas. Therefore how to enhance the efficiency of nano-biocatalysts and promote therapeutic efficiency in the physiological environment is the key scientific issue facing the current development of molecular engineering of nano-biocatalysts.

This report focuses in our group's research on functional enhancement and application of nano-biocatalysts in pathological environments: 1) for the enhancement of interfacial redox reaction kinetics, we have developed a coupling enhancement strategy to promote the adsorption and activation of substrate molecules, and to enhance the surface reaction rate. 2) To enhance the energy absorption and response to external field irradiation, a new strategy of "dimensional tailoring" design is proposed to enhance the separation and migration of photogenerated carriers through dimensionality reduction engineering and chemical bond mediated engineering, which can solve the problem of external field energy response insensitivity and carrier migration of nano-biocatalysts. (3) To strengthen the tandem mechanism of composite functional photosensitizers, we propose a new "orthogonal/auxiliary tandem enhancement" strategy, which significantly improves the therapeutic efficiency under physiological environment and expands the application of photosensitizers in antibacterial, antitumor and neurodegenerative disease treatment.

Keyword： interfacial reaction kinetics, nanozyme, anti-cancer therapy

最终交流类型: Invited

Promotion of nanozymes with human self-generated electric field

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Development of high-performance nanozymes for producing excessive reactive oxygen species (ROS) in local tumor tissues to induce lethal oxidative damage is a highly specific and efficient pathway for cancer therapy. In addition to improving the intrinsic activities of nanozymes, external stimuli can promote the catalytic activity. Natural protein enzymes have strong and permanent electrostatic fields in their active sites, which are believed to be the major factor responsible for the binding of these enzymes with substrates and subsequent catalytic reactions, namely the electrostatic preorganization effect. Accordingly, external electric fields have been utulized to remodel the internal electrostatic field of enzymes to control the reactivities and selectivities of catalytic reactions.

In light of this, we have utilized human self-generated electric field through wearable nanogenerator to improve the catalytic activities of a variety of nanozymes. We find that the electric field can modulate the electron mobility and electron structure of nanozymes, and also the interaction of nanozymes with substrates. Compared to other external stimuli, electricity has a broad actuation field to cover the entire tumor volume, thereby avoiding the possibility of escape of a small number of tumor cells from damage and the risk of tumor relapse. These works also propose a new pathway for future smart therapy that can overcome the space-time limitation of the current therapies.

Keyword： Nanozymes, electric field, nanogenerator, ROS, cancer therapy

最终交流类型: Invited

Precise Construction of Enzyme-mimetic Materials for Antibacterial and Wound Healing Applications

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Diseases caused by pathogenic microorganisms (bacteria, viruses, etc.) are considered to be one of the world's greatest health challenges, and the high variability of microorganisms, such as bacterial resistance and high mutation of RNA viruses, pose serious problems for the maintenance of public health. Therefore, the research and development of broad-spectrum antibacterial and antiviral agents have become a common goal for researchers all over the world. In recent years, our team has designed and screened a large number of low-dimensional functional materials engineered by coordination polymers and nanotechnology. We have constructed a variety of intelligent and efficient broad-spectrum antibacterial and antiviral nanostructures or targeted inhibitors, and proved their large-scale preparation and anti-pathogen mechanisms (1-4). In addition, by combining novel coordination polymers, organic conjugate coordination molecules, metal-organic frameworks, conjugated organic frameworks, and other new low-dimensional functional materials, our team has constructed abundant biomimetic catalytic materials that can be used for diverse biomedical fields, including anti-tumor, arthritis, stem cell protection, anti-inflammatory, and tissue regeneration (4-5). These studies have expanded the material type, clinical application scope, and transformation values of the intelligent and bionic nanomaterials and polymeric biomaterials.

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Keyword: Nanoagents, drug-resistant bacteria, wound healing, biomedical polymers, biomimetic catalysis

最终交流类型: Invited

Molybdenum-Based Nanozymes and their Bioapplications

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Nanozymes can make up the deficiency of natural enzymes and become a new frontier in the fields of biocatalytic therapy and biosensors, and so on. It was found that the variable valence state of molybdenum-based nanozymes such as MoS2 and MoOx have unique physicochemical properties and advantages of large surface area, biodegradability, low toxic as well as high near-infrared photothermal conversion efficiency, which endowed them with great potential applications in the biomedical fields. In recent years, our teams have carried out research on three parts of molybdenum-based nanozymes, including (1) construction and regulation of catalytic activity, (2) applications of biocatalytics, including anti-tumor and anti-bacteria, and (3) biological effects and safety research, and achieved a series of research results. Related works have been published in international academic journals such as JACS, Angew.Chem. Int. Ed., ACS Nano, Nano Today, Biomaterials, and so on 1-6.

ACKNOWLEDGMENTS

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Keyword： Nanozymes, MoS2, MoOx, Regulation of catalytic activity

最终交流类型: Invited

Engineering Biocatalytic Framework Material through Enzyme Encapsulation

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Nanozyme is a rising class of materials featuring natural enzyme-like catalytic function.[1] Structurally imitating the active center of a natural enzyme is an efficient strategy to engineer nanozyme so far.[2] However, this method requires precise design route and complicated synthesis steps, which limits the diversity of nanozyme that can be accessed in multidisciplinary applications. Herein, we impart an alternative strategy to engineer biocatalytic nanomaterials by means of spatial integration of enzyme and porous framework crystal.[3] In this protocol, the robust and porous framework crystals are in situ grown onto a fragile enzyme through biomimetic mineralization or co-precipitation principles.[4,5] This straightforward synthesis procedure affords a hierarchical bio-nano-architecture (Figure 1), well integrating the catalytic activity and selectivity of natural enzyme and the materials property of framework crystal. In addition, when enzymes are encapsulated in a framework crystal, the compact framework can tightly confine the tertiary structure of enzymes, while allowing the entrance of catalytic substrates and the transport of the intermediates/products owing to its high porosity. This exquisite bio-nano-architecture protects enzymes from external stimuli while preserving their desirable activity, which have provided great opportunities in biosensing, biocatalysis, pollutant degradation, energy harvest, and healthcare, etc. This straightforward encapsulation strategy offers new insight into the nanozyme engineering with high activity and catalytic selectivity, and may accelerate the progress of nanozyme in different applications.

Keyword： nanozyme, enzyme encapsulation, porous framework crystal, hierarchical structure

最终交流类型: Oral

A series of functional hydrogenase-mimic nanozymes for efficient and robust H2 evolution in aqueous environment

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Hydrogen, as one of the clean and high energy-density carriers, is attracting much attention now. However, its sustainable and green production methods are still under continuous developments. [NiFe]-Hydrogenase, with turnover rate around 103 s-1, offered a great template for clean hydrogen production catalyst, but its implementation is currently limited by its low resistance to environmental changes (such as temperature, pH, etc.). Here, inspired by the active center structure of the hydrogenase, we designed and synthesized a variety of transition metal-based hydrogenase-like nanozymes and applied those nanozymes to different green hydrogen production methods. We were able to achieve a high hydrogen production (HER) rate of 915 L h-1 per grams of nanozyme using aluminum as electron donors and achieved a fully consumption of Al. Also, we assembled a perovskite oxide/[NiCo]-based nanozyme composite and realized a 60-fold increase in photocatalytic HER rate compared to perovskite oxide alone. In conclusion, we envision that the transition mental based hydrogenase-like nanozymes can potentially offer an upgrade for current hydrogen production.

Keyword： hydrogenase mimics, nanozyme, HER, photocatalyst

最终交流类型: Invited

Porous Organic Frameworks (POFs) Nanozyme Engineering for Biomarker Colorimetric Sensing

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Nanozymes, an emerging class of artificial enzymes, have gained sustained advances in the fields of biomarker sensing for disease diagnosis, treatment and prognosis.[1,2] Among various categories of nanozymes, porous organic frameworks (POFs) including metal organic frameworks (MOFs), covalent organic frameworks (COFs) and hydrogen-bonded organic frameworks (HOFs) have drawn enormous attention due to their unique features of ultrahigh surface area, high porosity, and intercommunicating channels. Most importantly, POFs have unambiguous yet predictable topologies, which are structurally favorable for mimicking the

active sites as well as microenvironments of natural enzymes.[3] Inspired by these, we engineered a series of POF nanozymes with diverse and high-efficiency enzyme mimicking activities, e.g., peroxidase-, oxidase-, superoxide dismutase-, catalase-, or phosphatase-like activities. Attributing to their explicit topological architecture, the catalytic mechanisms were well investigated. Further, colorimetric sensing platforms were developed and successfully applied for the rapid and in situ analyses of biomarkers such as glucose, H2O2, glutathione, ascorbic acid, phosphorylated peptides and proteins, alkaline phosphatase, etc.[4-8]

Keyword： nanozyme, porous organic framework, biomarker, sensing

最终交流类型: Oral

Nanozymes for Cardioprotection

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Distressing and lethal cardiotoxicity is one of the major severe side effects of using anthracycline drugs such as doxorubicin for cancer chemotherapy. The currently available strategy to counteract these side effects relies on the administration of cardioprotective agents such as Dexrazoxane, which unfortunately has unsatisfactory efficacy and produces secondary myelosuppression. In the present work, aiming to target the characteristic ferrous iron overload in the doxorubicin-contaminated cardiac microenvironment, a biocompatible nanomedicine prepared by the polyvinylpyrrolidone-directed assembly of magnesium hexacyanoferrate nanocatalysts is designed and constructed for highly efficient intracellular ferrous ion capture and antioxidation. The synthesized magnesium hexacyanoferrate nanocatalysts display prominent superoxide radical dismutation and catalytic H2O2 decomposition activities to eliminate cytotoxic radical species. Excellent in vitro and in vivo cardioprotection from these magnesium hexacyanoferrate nanocatalysts are demonstrated, and the underlying intracellular ferrous ion traffic regulation mechanism has been explored in detail. The marked cardioprotective effect and biocompatibility render these magnesium hexacyanoferrate nanocatalysts to be highly promising and clinically transformable cardioprotective agents that can be employed during cancer treatment.

Keyword： Nanozymes, antioxidation, cardioprotection, prussian blue analogue, chemoprotection

最终交流类型: Invited

Nanozymes Combined with Cell Therapy for Acute Liver Failure Treatment

陶玉
中山大学

Reactive oxygen species (ROS)-associated oxidative stress, inflammation storm, and massive hepatocyte necrosis are the typical manifestations of acute liver failure (ALF), therefore specific therapeutic interventions are essential for the devastating disease. We developed a platform consisting of versatile biomimetic copper oxide nanozymes (Cu NZs)-loaded PLGA nanofibers (Cu NZs@PLGA nanofibers) and decellularized extracellular matrix (dECM) hydrogels for delivery of human adipose-derived mesenchymal stem/stromal cells-derived hepatocyte-like cells (hADMSCs-derived HLCs) (HLCs/Cu NZs@fiber/dECM). Cu NZs@PLGA nanofibers could conspicuously scavenge excessive ROS at the early stage of ALF, and reduce the massive accumulation of proinflammatory cytokines, herein efficiently preventing the deterioration of hepatocytes necrosis. Moreover, Cu NZs@PLGA nanofibers also exhibited a cytoprotection effect on the transplanted HLCs. Meanwhile, HLCs with hepatic-specific biofunctions and anti-inflammatory activity acted as a promising alternative cell source for ALF therapy. The dECM hydrogels further provided the desirable 3D environment and favorably improved the hepatic functions of HLCs. In addition, the pro-angiogenesis activity of Cu NZs@PLGA nanofibers also facilitated the integration of the whole implant with the host liver. Hence, HLCs/Cu NZs@fiber/dECM performed excellent synergistic therapeutic efficacy on ALF mice. This strategy using Cu NZs@PLGA nanofiber-reinforced dECM hydrogels for HLCs in situ delivery is a promising approach for ALF therapy and shows great potential for clinical translation.

Keyword： nanozymes, stem cell, differentiation, acute liver failure, treatment

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最终交流类型: Keynote

Carbon nanodots and Traditional Chinese Medicine derived nanozyme in cellular stress and PARP signaling

Yingqiu Xie
Nazarbayev University

Carbon nanodots have been widely studied and applied in anti-cancer, imaging, and anti-microbes. We recently found carbon nanodots and Traditional Chinese Medicine derived nanozyme exhibit alkaline phosphatase or co-phosphatase activity. Here we report the modified carbon nanodots and Traditional Chinese Medicine derived nanozyme may mediate cellular stress and PARP-cleavage in cell death. PARP inhibitor olaparib with high dose carbon nanodots form a “synergetic lethality” through an intermolecular interaction. In addition, Traditional Chinese Medicine derived nanozyme also induces DNA damage response which may be applied for anti-cancer treatment by targeting PARP.

Keyword： Nanozyme, PARP, Carbon nanodots, Traditional Chinese Medicine

最终交流类型: Invited

Design and Application of Cold-Adapted Nanozymes

张连兵
西北工业大学

The development of cold-adapted enzymes with high efficiency and good stability is an advanced strategy to overcome the limitations of catalytic medicine in low and cryogenic temperatures. Inspired by natural enzymes, a novel cold-adapted nanozyme based on a manganese-based nanosized metal–organic framework (nMnBTC) is designed and synthesized. The nMnBTC as an oxidase mimetic not only exhibits excellent activity at 0 °C, but also presents almost no observable activity loss as the temperature is increased to 45 °C. This breaks the traditional recognition that enzymes show maximum activity only under specific psychrophilic or thermophilic condition. The superior performance of nMnBTC as a cold-adapted nanozyme can be attributed to its high-catalytic efficiency at low temperature, good substrate affinity, and flexible conformation. Based on the robust performance of nMnBTC, a low-temperature antiviral strategy is developed to inactivate influenza virus H1N1 even at −20 °C. A series of cold-adapted nanozymes are developed for various applications, such as black water treatment and plant fiber degradation. These results not only provide an important guide for the rational design of highly efficient artificial cold-adapted enzymes, but also pave a novel way for cryogenic applications.

Keyword： nanozyme, cold-adapted, MOF, cryogen, nanozyme design

最终交流类型: Keynote

Engineering Metal Nanoclusters for Biomedical Applications

Jianping Xie
National University of Singapore, Singapore

Ultrasmall metal nanoclusters (NCs) have attracted increasing attention from the scientific community due to their fascinating physicochemical properties. Today, functional metal NCs are finding growing acceptance in biomedical applications. To achieve a better performance in biomedical applications, metal NCs can be interfaced with biomolecules, such as proteins, peptides, and DNA, to form a new class of biomolecule-NC composites (or bio-NCs in short), which typically show synergistic or novel physicochemical and physiological properties. In this talk, I will discuss some of our recent studies at the interface of metal NCs and biomolecules, highlighting some unique physicochemical properties (e.g., luminescence) and the biological functions of bio-NCs. Before discussing the ultrasmall metal NCs, I will also briefly introduce the synthesis, characterization, functionalization, properties and applications of inorganic nanomaterials, demonstrating how chemical engineering principles can contribute to nanomaterials-driven sustainability.

Keyword： Nanomedicine; Nanozymes; Metal Nanoclusters

最终交流类型: Invited

Photo-responsive Nanozyme

刘惠玉
北京化工大学

Nanozymes, as natural enzyme mimics with high efficiency and stable performance, have extremely promising applications in biosensing, disease diagnosis, and treatment. However, it is still a challenge to modulate the performance of nanozymes to suit their biomedical application at this stage. To solve this problem, we proposed the strategy of "photo-responsive nanozyme" which enhanced the therapeutic efficiency of nanozyme with near-infrared light irradiation, and conducted an in-depth study on its activity regulation and extended applications. Meanwhile, we have designed and developed various photo-responsive nanotherapeutic platforms, such as MOF-derived metalloporphyrin-centered nanostructures, degradable porous palladium nanosheets, PtFe@Fe_3O_4, etc. Moreover, we also constructed a bionic single-atom nanozyme and realized the development of photo-responsive nanozyme with single-atom active centers of transition metals, revealed the enhanced mechanism of catalytic effect of photo-responsive nanozyme with enhanced electron transfer, proposed the stretching strain to achieve Palladium sheets for the modulation of photo-responsive catalytic activity strategy. Based on these works, we further designed more efficient and novel photo-responsive therapeutic platforms, such as degradable carbon-silica nanocomposites, FePc/HNCS, providing a wider range of means for the efficient photo-responsive treatment of tumor and other disease. This report will mainly introduce the design and application expansion of the photo-responsive nanozymes in our group, and provide new ideas for the development of new photo-responsive platforms.

Keyword： Photo-Responsive Nanozyme, Single-Atom Nanozyme

最终交流类型: Oral

Enantioselective detection of glucose with chiral noble metal nanozymes

陈佳琪
Chengdu University

Glucose monitoring is essential to evaluate the degree of glucose metabolism disorders. The enzymatic determination has been the most widely used method in glucose detection [1]. Noble metal nanomaterials (NMs), inheriting their excellent electronic, optical and enzyme-like properties, are classified as noble metal nanozymes (NMNZs) [2-4]. By employing NMNZs with glucose oxidase (GOx) and peroxidase (POD) mimicking activities, the NMNZs are often involved in two series of reactions, the oxidation of glucose and the chromogenic reaction of peroxide [1]. Although the NMNZs have been successfully used in the enzymatic determination of glucose, there are still some problems to be solved. For instance, the glucose enantiomer recognition ability of natural enzymes is difficult to achieve by artificial nanozymes. In the GOx-POD nanozyme system, the detection specificity depends on the enantioselective catalysis of GOx to glucose. The combination of chirality and GOx-like activity in NMNZs may not only get rid of the defects of natural enzymes, but also introduce enantio-selectivity, similar to their natural counterparts. The design and synthesis of GOx-like NMNZs with chiral structures may be beneficial for the enantioselective detection of glucose. With thiolated bimolecular cosurfactants, we demonstrated a chemical strategy for the synthesis of intrinsically helical plasmonic nanorods (HPNRs) with strong and tailorable plasmonic circular dichroism (PCD) responses [5]. The influence of structural parameters of HPNRs on PCD responses was analyzed systematically by theoretical simulations. Among the different structural parameters, the pitch depth was found to have the greatest impact on the PCD signals, in agreement with the experimental results. The obtained HPNRs were found to have GOx-POD-like tandem catalytic activities under the illumination of sunlight. Molecular imprinting was used to realize the specific recognition and improved catalytic efficiency of chiral NMNZs. Chiral NMNZs exhibit great potentials for the enantioselective detection of glucose.

Keyword： Plasmonic circular dichroism, Noble metal nanozymes, Glucose detection, Activity regulation, Enantioselective recognition

最终交流类型: Oral

Design of Nanozymes Capable of Degrading Organic Molecules in Antibacterial Application

高梦
Soochow University

Bacterial infections pose a significant risk to human health, resulting in the deaths of approximately 7.7 million individuals annually. This makes it the second most common cause of death worldwide. Traditional antibiotic drugs or conventional antimicrobial agents failed to conquer superbugs, leading to an urgent requirement of new strategy (Angew. Chem. 2023, 62, e202217345). Among bacterial infection induced death the most common lethal factors are the lipopolysaccharide (e.g. endotoxin, LPS) induced sepsis and the biofilm colony induced antimicrobial resistance (AMR). According to our previous investigations, nanomaterials with unique enzyme-like activities often performed superior catalytic activities toward important organic molecules (JACS 2020, 142, 19602; JACS 2023, 145, 3108). In this research, we designed two new nanomaterials with phosphatase- and lactonase-like activities, which were specifically degraded the most detrimental parts during bacterial infection, i.e. the LP,S and biofilm. We engineered a dephosphorylation reaction on endotoxins by a synthetic nanozyme (CeO_2) to attenuate its toxicity (Nano Today, 2023, 44, 101456). CeO_2 prepared in phosphate-free hydrothermal reaction selectively and efficiently catalyzed the breaking of P-O bonds in endotoxins. Catalytic depletion of phosphates from endotoxins attenuated their binding with Toll-like receptors, NF-κB activation and pro-inflammatory cytokine release. Airborne LPS was, for the first time, inactivated (98%) by this facile dephosphorylation reaction. Moreover, an efficient lactonase-like Zn-N_x-C nanomaterial was synthesized by tuning the coordination environment around zinc atoms to mimic the active domain of lactonase for catalytical interception of bacterial communications in biofilm formation (Angew. Chem. 2023, 62, e2023054). The Zn-N_x-C material could selectively catalyze 77.5% hydrolysis of N-acylated-L-homoserine lactone (AHL), a critical bacterial quorum sensing (QS) signal in biofilm construction. Consequently, AHL degradation downregulated the expression of QS-related genes in antibiotic resistant bacteria and significantly prevented biofilm formation.

Keyword： Nanozyme; Biofilm; Endotoxin; Lactonase; Phosphatase

最终交流类型: Invited

Self-assembled structures and properties of short peptides with catalytic functions

董昊
南京大学

Peptide molecules can form stable nanostructures or supramolecular systems through non-covalent interactions. This self-assembly process is influenced by peptide sequence, environmental conditions and other factors, which can control the structure and properties at different levels. Many catalytic peptides have been found in peptide self-assembly, which can catalyze various important biochemical reactions such as ester hydrolysis and redox reactions. Compared with traditional small molecule catalysts, enzyme mimics have higher selectivity and specificity, and stronger adaptability to environmental changes. Studies have shown that factors such as peptide sequence, spatial arrangement, and non-covalent interactions can affect their structure and performance. In previous work, we used multi-scale simulations combined with experiments to study the effect of sequence differences on the catalytic performance of amphiphilic peptides self-assembling into highly ordered fiber bundles1, as well as the construction of enzyme-mimicking nanoscale superstructures based on cyclic dipeptides2. We further investigated the structural and morphological changes and spectral characteristics of such peptide-based self-assembled catalysts under different solution conditions, and explored new types of catalytic reactions. These studies contribute to

developing new peptide self-assembled enzyme mimic systems, which have broad applications in materials science, biotechnology, and environmental protection, among other fields.

Keyword： catalytic peptide, self-assembly, molecular modeling

最终交流类型: Keynote

Atomically precise metal nanozymes

伍志鲲
中国科学院合肥物质科学研究院

Since the intrinsic peroxidase-like property of Fe3O4 NPs was reported in 2007, nanozymes has specifically referred to nanomaterials with intrinsic enzyme-like characteristics, and they, as a new type of promising artificial enzyme, have attracted considerable interest over the past decade owing to their obvious advantages over natural enzymes and conventional artificial enzymes, such as high and tunable catalytic

activities, low cost, easy large-scale production, and high stability. However, the undefined compositions and structures, as well as the multiple dispersity retard the composition (structure)-property correlation and the iterative optimization of their performances. The recently emerging metal nanoclusters, which can be viewed as ultrasmall metal nanoparticles with atomically precise compositions and structures, provide opportunities for developing nanozyme with atomic precision. Indeed, we revealed the enzyme-like property of Au42 nanoclusters in 2020, after that, the enzyme-like property of atomically precise metal nanoclusters was also reported by other groups, and even the cluster-zyme concept was proposed by Zhang group. Very recently, we extended the application of nanocluster-zyme in biosensing. Herein, we will report the progress of nanozymes with atomical precision and attract the consideration of colleagues for future development of nanocluster-zymes.

Keyword： Atomically precise nanozymes; metal nanoclusters;enzyme-like property; biosensing

最终交流类型: Oral

Exploring for Catalytic Performance Regulation of Multi-composition Metal Nanozymes

Qi Yang
Xuchang University

Colorimetric sensing based on nanozymes is a burgeoning and important strategy for bioassay. The difficulties and challenges lie in further improving the catalytic activity, selectivity and stability of nanozymes. Noble metal-based nanozymes have the advantages of easy preparation and outstanding stability in tough environments, which have been widely used to construct the biosensing platforms for diverse biomolecules [1,2]. The combining of abundant catalytic active sites from noble metals and polyvalent state from transition metals is an effective strategy to construct high performance metal nanozymes. The controllable electronic structure induced by multi-composition could effectively adjust the d-band center of metal nanoparticales, contributes to boosting the charge separation and transfer, influence the interface adsorption/desorption behavior between the metal surface and substrate, and finally improve the catalytic efficiency [3,4]. It seems that continuously increasing the member of component may achieve further enhanced effects, which inspires an interesting research direction to constructing novel nanozymes with high selectivity and catalytic activity, as well as revealing their potential enhancement mechanisms. Therefore, ternary, quaternary and even high entropy alloy nanozymes are urgently required to be explored for biosensing applications. The simple, green and economic preparation methods for multi-composition metal nanozymes need to be developed. Furthermore, The interaction mechanism between complex elements and reactants/intermediates need to be revealed. The surface charge density, d-band center and lattice mismatch response induced by the change of components need to be described. Herein, we tentatively explored the catalytic performance regulation of multi-composition metal nanozymes. The effects of metal kind and proportion on multiple enzyme-mimetic activities were discussed. We hope to enhance one or two certain target activity to functionalize the metal nanozymes for promising application through component adjusting, instead of promoting the non-target activity simultaneously. We think this is potential to motivate ideas and accumulate theory for the development of novel nanozymes.

Keyword: Metal nanozymes, Multi-composition, Targeted regulating, Colorimetric sensing

最终交流类型: Invited

Atomic insights into the catalytic activity and reaction specificity of CeO2-based nanozymes

PENG Yung-Kang
City University of Hong Kong

Nanozymes are promising alternatives to natural enzymes, but their use remains limited owing to poor specificity. For example, CeO2 activates H2O2 and displays peroxidase (POD)-like, catalase (CAT)-like, and haloperoxidase (HPO)-like activities. Since they unavoidably compete for H2O2 affecting its utilization in the target application, the precise manipulation of reaction specificity is thus imperative. In this talk, I will show that one can simply achieve this by manipulating H2O2 activation pathway on pristine CeO2 in well-defined shapes. This is because the coordination and electronic structures of Ce sites vary with CeO2 surfaces that (100) and (111) surfaces display unprecedented specificity toward POD-/CAT-like and HPO-like activity, respectively. The antibacterial results suggest that the latter surface can utilize H2O2 well to kill bacteria (cf. the former), which is promising for antibiofouling applications. This work is expected to guide the rational design of nanozymes with improved activity, reaction specificity, and H2O2 utilization.

Keyword: CeO2, surface understanding, catalytic mechanism, reaction specificity

最终交流类型: Oral

Colorimetric Detection of Nucleic Acids Based on Core–Shell Au@Pt Nanozyme for Mumps Virus Diagnosis

Jiano Liu
枣庄学院

Mumps is a common childhood infectious disease caused by the mumps virus. Although most cases of infection lead to a mild disease, orchitis, permanent deafness, and disability are some untoward effects of mumps. A laboratory diagnosis of mumps is based on detection of viral nucleic acid using polymerase chain reaction, isolation of the virus from saliva or spinal fluid, or serological confirmation. Nucleic acid amplification tests are highly recommended by the World Health Organization, and they are based on reverse transcription polymerase chain reaction (RT-PCR). However, RT-PCR is limited by the need for special reagents (fluorescent probe or DNA-binding dye) and relatively expensive fluorescence instrumentation. Therefore, the development of simpler DNA screening methods that do not require complicated instrumentation would be beneficial in facility-limited environments. In this study, we have developed a fast and convenient colorimetric detection method for mumps virus diagnosis that employs the peroxidase activity of core–shell Au@Pt nanozymes. By using the new technique, DNA samples can be analyzed by naked-eye detection within a few minutes. The highly sensitive peroxidase-like activity of core–shell Au@Pt nanozymes, along with their catalytic stability and robustness, can facilitate their utilization in biochemical assay and clinical diagnosis.

Keyword： nanozyme, core/shell nanostructures, nucleic acid detection, mumps virus, diagnosis

最终交流类型: Oral

Bifunctional botanicals@nanozymes for synergistic antibiotic-resistant bacterial treatment

董凯
吉林农业大学

Nowadays, bacterial infection has attracted widespread attention in public health and become a major global health problem. With the long-term widespread overuse of antibiotics, a large number of antibiotic-resistant bacteria have emerged and become a serious threat to healthcare systems. As an alternative strategy, nanozymes have become a new generation of antibiotics with exciting broad-spectrum antibacterial properties and negligible biological toxicity. However, their inherent low catalytic activity limits their antibacterial properties. In order to overcome these restrictions of single therapeutic modality, the synergistic antimicrobial method is encouraged to enhance the antimicrobial effect and weaken the side effect. Compared to antibiotics, botanicals are witnessing sharp popularity because of their infrequent adverse effects and the bioactive ingredients. Herein, we have reported a dual-modal antibacterial strategy based on botanicals@nanozymes for synergistic antibiotic-resistant bacterial treatment. In the bifunctional nanosystem, Berberine (BBR), an isoquinoline alkaloid, was chosen as the botanical antibiotic for combatting antibiotic-resistant bacteria. Zn single-atom (ZnSA) nanozymes were constructed by a pyrolysis-etching-adsorption-pyrolysis (PEAP) strategy. ZnSA nanozymes can effectively induce peroxidase-like activity in the presence of H2O2, thereby generating a large amount of hydroxyl radicals (•OH), which have a certain killing effect on antibiotic-resistant bacteria. Additionally, ZnSA nanozymes had large pores for effectively loading botanicals. With the results of antibacterial assays, the BBR@ZnSA nanozymes revealed the superior effectiveness of synergistic antibiotic-resistant bacterial treatment. Furthermore, the BBR@ZnSA nanozymes showed good biocompatibility. Based on the excellent sterilization performance and good biocompatibility, the BBR@ZnSA nanozymes could be a promising candidate for antibiotic-resistant bacterial treatment.

Keyword： Nanozymes, Botanicals, Dual Mode, Antibiotic-resistant Bacteria, Synergistic Sterilization

最终交流类型: Oral

Construction of nanozyme microenvironmental engineering and application of analytical sensing

赵怡琳
北京化工大学

Nanozymes are nanomaterial-based enzyme mimics, which are attractive for their excellent catalytic activities, stability, and cost advantages. Nanoceria (CeO2) is a highly important oxidation catalyst, and it has been explored as an oxidase mimic. Many nanozymes have a relatively low activity, including nanoceria. Since nanozyme reactions take place mainly on their surfaces, microenvironmental engineering could be useful for promoting activity.

We recently reported that the activity of nanoceria is significantly boosted by fluoride [1], and the turnover number increased from around 10 to near 300 in 10 min. This activity enhancement was attributed to the interactions between F− and cerium ions on the surface of CeO2, facilitating product desorption, generating more OVs and enhancing electron transfer. The use of CeO2 for the oxidation of common chromogenic substrates was also investigated at low pH, where its activity was greatly enhanced. [2] At very low pH conditions, the catalytic activity of CeO2 nanoparticles also significantly increased due to the weakened adsorption of oxidation products, increased concentration of oxygen vacancy, and enhanced electron transfer rates.

The development of nanomaterials with multi-enzyme activities (nanozymes) has attracted extensive attention. Herein, we rationally designed a pH-responsive hybrid

Fe3O4@CeO2 nanorod which simultaneously possesses high ALP and CAT activities for OPs removal and phosphorus recovery.. The addition of AA could significantly accelerate the CAT activity by promoting the surface Ce3+/Ce4+ and Fe2+/Fe3+ redox cycle of nanozymes. This nanozyme can degrade 91% parathion-methyl (MP) under 2 g/L Fe3O4@CeO2, 25 mM H2O2 and 4 mM AA. After recycled for 5 times, the degradation of MP is still up to 89%. In this strategy, multi-functional cascade nanozymes, coupled with in situ dephosphorization and catalytic oxidation, were used to recycle organic phosphate ester pesticides, providing theoretical support and technical accumulation for green, efficient, and cost-effective organic phosphorus wastewater recycling applications.

Keyword： Nanozyme, microenvironment, cascade reaction, multi-enzyme activities, biosensor

最终交流类型: Invited

A Nanozyme-based Electrode for Neural Recording

Xiaodong Zhang
天津大学

Implanted neural electrodes have been widely used to brain diseases that demand high sensitivity and biocompatibility at the tissue-electrode interface. However, current clinically-used electrodes cannot simultaneously meet both ends, which hinders effective recording of electronic signals. Herein, nanozyme-based neural electrodes by incorporating bioinspired atomically-precise clusters are developed, as a general strategy with heterogeneous design for multiscale and ultrasensitive neural recording via quantum transport and biocatalytic processes.1-3 Owing to dual high-speed electronic and ionic currents at electrode-tissue interface, the impedance of nanozyme electrodes is 26 times lower than that of state-of-the-art metal electrodes, and the acquisition sensitivity for local field potential is increased by ~10 times than clinical PtIr electrodes, enabling signal-to-noise ratio (SNR) of up to 14.7 dB for single-neuron recordings.4,5 Meanwhile, the electrodes provide more than 100-fold higher antioxidant activities and multi-enzyme mimicking activities, which effectively decrease 67% neuronal injury area by inhibiting glial proliferation and allowing sensitive and stable neural recording. In addition, nanozyme electrodes can considerably improve SNR and detection sensitivity of seizures, which is expected to achieve precise localization of seizure

foci in the clinic. The nanozyme electrodes designed herein are not only record but also extended to deep brain stimulation for treatment of neurological disorders.

Keyword： Neural Recording

最终交流类型: Oral

Single-atom Fe nanozymes coupling with atomic clusters as superior oxidase mimics for ratiometric fluorescence detection

鲁娜
Shanghai University of Engineering Science

Single atom metal-nitrogen-carbon (M-N-C) nanomaterials are recognized as a class of promising candidates alternatively to natural enzymes, but are still restricted by the limited catalytic activity. Tuning the geometric and electronic configurations of atomic active sites via coexistence of single atoms and atomic clusters provides a good avenue to prepare high-performance M-N-C catalysts. Herein, we report a model Fe-N-C catalyst integrating Fe single atoms with Fe atomic clusters on N-doped porous carbon (denoted as FeAC/FeSA-NC) synthesized by a ligand-mediated strategy that pyrolyzes Fe(II)-phenanthroline complexes assembled zeolitic-imidazolate-frameworks (ZIF-8@Fe-Phen). As expected, the as-prepared FeAC/FeSA-NC catalyst exhibits remarkable oxidase-mimicking activity by activating oxygen into the reactive oxygen species, superoxide radicals (•O2-). Density functional theory (DFT) calculations reveal that the coupling of Fe single atoms with Fe clusters contribute to lower activation energy, leading to the enhancement of catalytic activity. As a concept application, the FeAC/FeSA-NC nanozyme is employed for ratiometric fluorescence detection of acetylcholinesterase activity and organophosphorus pesticides (OPs) based on the inhibition effect of thiols on nanozymatic activity. The proposed ratiometric bioassay for OPs determination achieves an excellent linearity over 0.005 to 50 ng mL-1, and a low limit of detection of 1.9 pg mL-1. This work not only provides an effective strategy for rationally design of high-performance nanozymes, but also displays a broad prospect of nanozyme for biochemical sensing applications.

Keyword： Single-atom, atomic cluster, nanozyme, oxidase-like, ratiometric fluorescence biosensors

最终交流类型: Oral

Targeted and Microenvironment-Activated Platinum Nanoenzymes for Cell Activity Regulation

卿志和
University of Science and Technology

Nanozymes have enzyme-like activities based on the surface catalytic chemistry of nanomaterials. Compared to natural enzymes, nanozymes displayed many advantages, including high stability, easy synthesis and low cost. In the past years, we focused on the development of targeted and microenvironment-activated platinum nanoenzymes for cell activity regulation, and have made some progress in this field. For example, ultrathin platinum shell-coated AuNPs were developed to stably modify targeting ligands (functional nucleic acids), avoiding non-specific interference from biothiols. Compared to previous methods of changing the ligand chemistry, coating a Pt shell is more accessible, and previously developed methods for nanoparticles can be directly adapted. In addition, the stable AuNP@Pt nanoenzymes were used for cell activity regulation. An activatable nanozyme with targeting capability to simultaneously break the local pH and H2O2 limitations under physiological conditions was constructed: Aptamer-functionalized nanozymes, glucose oxidase, and hyaluronic acid constitute an activatable nanocapsule, which can be activated by bacteria-secreted hyaluronidase in infected wounds. The nanozymes bind onto bacteria through aptamer recognition, and glucose oxidation tunes the local pH down and supplements H2O2 for the in-situ generation of •OH on bacteria surfaces. The activity switching and enhanced antibacterial effect of the nanocapsule were verified in vitro and in diabetic wounds.

Keyword： nanozymes, platinum, chemodynamic sterilization, functional nucleic acids

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最终交流类型: Invited

Structural regulation and theranostic performance of piezoelectric semiconductor enzymes

杨飘萍
哈尔滨工程大学

Piezoelectric catalytic therapy has become a new research hotspot, as the polarization and built-in electric field generated in piezoelectric materials under external mechanical

forces separate electrons and holes, producing reactive oxygen species to kill tumor cells. However, the research of piezoelectric catalytic therapy is still in its infancy. Because the threshold of critical Gibbs free energy obtained is not enough to start the Redox, the treatment efficiency is still low. In order to improve the performance of piezoelectric materials, the research team has attempted various strategies, including introducing defects and oxygen vacancies: (1) A simple defect engineering strategy was used to design a BiO2 − x nanosheet rich in oxygen vacancies; (2) Design piezoelectric Bi2MoO6 nanoribbons for glutathione enhanced tumor sonodynamic therapy; (3) Developed phononic liquid type Cu3VS4 nanoparticles for tumor photothermoelectric therapy.

Keyword： semiconductor, pizeocatalytic, cancer therapy

最终交流类型: Invited

Nanozybiotics: Nanozymes-based biomimetic antimicrobial strategy

高利增
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Infectious diseases caused by microbes represent a global threat to human health. However, due to the abuse of antibiotics, antimicrobial resistance has evolved rapidly and led to the failure of antibiotics treatment. Thus, alternative antimicrobial strategies different to traditional antibiotics are urgently needed. Lysosomal enzymes-based bacteria killing plays a vital role in innate immune defense system, inspiring novel antimicrobial strategy. However, due to their low stability, potential immunogenicity, and high cost, natural enzymes have limitations in practical antimicrobial therapy. In recent years, many nanomaterials with enzyme-like activities (Nanozymes) have been discovered as a new generation of artificial enzymes and demonstrated highly antimicrobial effects against bacteria or viruses. To highlight the progress in the field of nanozymes-based antimicrobial strategy (Nanozybiotics), we summarized the antimicrobial mechanisms of action, versatile therapeutics and translational potentials of nanozybiotics in various infectious diseases. We believe that nanozybiotics will provide a new strategy by mimicking immune defense using nanozymes to combat antimicrobial resistance.

Keyword： Nanozybiotics, Nanozymes, Immune biomimetics, Antimicrobial resistance, Bacteria, Virus

最终交流类型: Keynote

Down-regulation of tumor interstitial pressure enhances intratumoral drug delivery and tumor therapy

高大威
燕山大学 环境与化学工程学院

The global incidence and mortality of tumors continue to rise, and the drug treatment effect is limited, mainly because the obstruction of lymphatic reflux leads to the interstitial high pressure within the tumor, making the delivery efficiency of drugs from the blood to the tumor is low, only 2% of drugs enter the tumor, and it is difficult to kill the deep stem cells, resulting in tumor recurrence and metastasis. Therefore, enhanced intratumoral delivery of drugs can kill deep stem cells more effectively, which is a bottleneck problem to be solved urgently in cancer therapy. Our team proposed a novel nanocatalytic treatment strategy based on catalytic decomposition of aquatic hydrogen or oxygen to reduce tumor interstitial high pressure and enhance the deep intratumoral delivery of drugs. This strategy utilizes photocatalysis/thermoelectric catalysis/piezoelectric catalysis to decompose water and enzyme degradation of interstitial proteins in combination to reduce the interstitial pressure of tumors, resulting in an effect similar to lymphatic reflux and enhancing the accumulation of drugs in tumors. Then through the coordination of photoheat, ultrasound, drugs and free radicals, the effective killing of tumor deep cells was achieved. The effect of nanocatalytic system on pressure was analyzed for tumors with different interstitial pressures, so as to achieve efficient delivery of drugs and effective treatment.

Keyword： tumor interstitial pressure; nano drug delivery system; catalytic water splitting

最终交流类型: Invited

Electrochemical analysis of single nanoenzyme particles

Yige Zhou
湖南大学

Nano-impact electrochemistry (NIE) allows the measurement of the electrochemical reactions at the individual particle level. Apart from serving as a powerful analytical tool, NIE exhibits distinctive intrinsic characteristics that differ from their ensemble counterparts on modified electrodes, including much enhanced mass transport, significantly reduced reaction time scale, and an intermittent reaction mode. In this presentation, I will discuss the study of two nanoenzymes, specifically LaNiO3 and Prussian Blue (PB) particles, at the single-particle level using NIE. Our findings demonstrate that NIE is able to alter the reaction selectivity of LaNiO3 catalyzed H2O2 reduction as compared to the ensemble-based approaches. Additionally, we have gained valuable kinetics information of PB, a material featuring multiple redox centers.

Keyword： nano-impact electrochemistry; nanoenzymes, reaction selectivity; multiple redox centers

最终交流类型: Invited

Near-infrared-IIb fluorescent nanozymes for imaging-guided treatment of Reactive Oxygen Species-Related Diseases

崔然
武汉大学

How to finely regulate the concentration of reactive oxygen species (ROS) in vivo, eliminating the negative effects of excessive ROS without affecting the normal physiological functions of cells, is of great significance for the treatment of diseases such as cancer, traumatic brain injury, and neurodegenerative diseases. Currently, the use of free radical scavengers to inhibit oxidative damage and neuroinflammation has shown promising prospects in related therapies. However, traditional neuroprotective strategies still face challenges in providing real-time information feedback for evaluating treatment outcomes.

This work constructs the nanoenzyme probes based on NIR-IIb fluorescent quantum dots by proposing original strategies, achieving efficient clearance of reactive oxygen species in vivo. The "high-temperature-driven" doping strategy successfully disperses Mn in a single-atomic form on the surface of NIR-IIb quantum dot crystals (Ag_2Te, PbS, etc.), constructing Mn single-atom catalysts (Mn/QD SAC) with fluorescence emission wavelength in the NIR-IIb window (1500-1700 nm)[1-3]. The highly single-atom dispersed Mn on the surface of quantum dots enables Mn/QD SAC to exhibit efficient catalytic activity in clearing reactive oxygen species.

The above-mentioned NIR-IIb nanoenzymes have advantages such as low background interference, deep penetration depth, and high signal-to-noise ratio in in vivo imaging. It can successfully open the "black box" in the treatment process of reactive oxygen species-related

diseases by dynamically monitoring the treatment status in real time with high spatial and temporal resolution. At the same time, it can effectively alleviate hypoxia, neuroinflammation, and neuroapoptosis mediated by reactive oxygen species, providing timely therapeutic feedback and guidance for precise treatment of tumor microenvironment hypoxia, brain neuronal secondary damage caused by insufficient oxygen supply after traumatic brain injury, and other related conditions[1-3]. This work provides new ideas and research foundations for real-time dynamic imaging-guided precise neuroprotection therapy and some reactive oxygen species-related diseases.

Keyword： NIR-IIb, nanoenzyme, ROS, imaging-guided

最终交流类型: Invited

Tumor Microenvironment Responsive Nanocomposites for Synergistic Therapy of Tumors

李春霞
山东大学

At present, some progress has been made in cancer treatment based on nanocatalysts, but it is still a huge challenge to achieve precise treatment for specific tumor microenvironment. Additionally, it is difficult to achieve a satisfactory therapeutic effect by a single treatment mode. We mainly focus on the construction and their bioapplicaiton of rare earth upconversion nanoparticles (UCNPs) and photothermal conversion nanomaterials. A variety of nanocomposites have been designed based on the characteristics of tumor microenvironment (TME) to overcome the above problem so as to achieve tumor synergistic therapy.

The related papers:

[1] M. Wang, M. Y. Chang, C. X. Li, J. Lin, et al. Adv. Mater. 2022, 34: 2106010.
[2] M. Y. Chang, Z. Y. Hou, C. X. Li, J. Lin, et al. Angew. Chem. Int. Ed. 2021, 60: 12971.
[3] P. Zheng, B. B. Ding, C. X. Li, J. Lin, et al. Angew. Chem. Int. Ed. 2022, 61: e202204904.
[4] P. Zheng, B. B. Ding, C. X. Li, J. Lin, et al. Chem. Eng. J. 2022, 450: 137967.
[5] P. Zheng, B. B. Ding, G. Q. Zhu, J. Lin, C. X. Li, Small 2023, 19: 2300370.

Keyword： tumor microenvironment, rare earth upconversion nanoparticles,tumor synergistic therapy

最终交流类型: Keynote

Antioxidant artificial-enzymes-armed probiotics for inflammatory bowel disease management

Xiaoyuan (Shawn) Chen
National University of Singapore, Singapore

The dysfunction of the intestinal mucosal barrier and dysregulation of gut microbiota may induce hyperactive immune responses, resulting in inflammatory bowel disease [1, 2]. The clinical therapies for IBD mainly concentrate on using drugs to manage the inflammatory symptoms. However, they suffer from unsatisfactory therapeutic outcomes and potential systemic toxicity, due to their metabolic instability, poor targeting, and limited ability for microbiota modulation. Despite the fact that probiotic therapy has been a promising option to solve the underlying causes, their resistance to oxidative stress narrows the therapeutic windows. To address these issues, here we designed antioxidant artificial enzymes-armed probiotics to reshape a healthy immune system in IBD for potential clinical translation [3]. The biocompatible antioxidant artificial enzymes could persistently scavenge elevated reactive oxygen species (ROS) and inflammatory factors; the eased inflammatory environment will improve the bacterium viability to rapidly reshape the intestinal barrier functions and gut microbiota (Fig. 1)

Keyword： Antioxidant artificial enzymes, probiotics, inflammatory bowel disease, microbiota dysbiosis

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最终交流类型:

Single-atom nanozymes construction and biological applications

刘成辉
西南民族大学

In this presentation, we first explore a typical hydrothermal synthesis strategy for SAzymes, and summarize the active centers and catalytic mechanisms of iron-based and platinum-based SAzymes, Then, we discuss the promising applications of SAzymes in biosensing applications and biomedical applications.

Keyword： Single-atom nanozymes

最终交流类型: Keynote

Biomimetic design of nanozymes for efficient anticancer therapy

刘又年
中南大学

The ever-increasing pursuit of biological context regulation platforms and the fallibility of enzymes' nature propel the exploration of applicable alternatives to long-term biological activity. Recently, nanomaterials with artificial enzyme-mimicking capability (nanozymes) have demonstrated potential for improving anti-cancer therapeutic efficacy via catalytic conversion of small metabolic molecules. However, the design of nanozymes for the catalytic conversion of physiological molecules, especially key signaling metabolites in tumor progression, is still highly desirable but challenging.

Recently, our research group has successfully designed a series of highly efficient nanoenzymes based on biomimetic design for anti-tumor therapy. i) A lactate oxidase nanoenzyme based on Co4N/C were developed by manipulating the coordination field and electronic structure around the N center. Co4N promotes the recognition of lactate substrates and the charge neutralization of intermediates, thus efficiently extracting the α-C−H and α-C−OH protons of lactate. It has been applied to remodel the highly lactate-rich tumor microenvironment to activate anti-tumor immune responses and inhibit lymph node metastasis of tumors (Fig. A). ii) A catalyst with Fe-Cu hetero-bimetallic active sites was synthesized on hollow nitrogen-doped carbon nanospheres (FeCuNC) as a catalytic nano-drug for cancer therapy. The Fe-Cu hetero-bimetallic sites in FeCuNC were more effective in catalyzing the cleavage of O-O bonds in H2O2 molecules compared to single iron sites. The study demonstrated that FeCuNC could accurately identify sentinel lymph node metastasis and effectively suppress tumor metastasis and recurrence (Fig. B

Keyword: Biomimetic design

最终交流类型: Keynote

Enzyme Evolution for Efficient Biosynthesis of High-value compounds

冯雁

上海交通大学

Synthetic biology has accelerated our ability to design and construct the novel pathways for biosynthesis. However, we still face great challenge caused by the shortages of suitable enzymes for the desired reactions. It is highly desired to reveal the complicated regulation mechanisms of enzyme and develop new strategies for designing the efficient molecular machine. Here, we provides several examples for biosynthesis of high-value compounds by engineering the efficient enzymes based on semi-rational design. The results showed that the precise control of enzyme functions could greatly enhance the adaptation of the artificial biological system.

Keyword： enzyme evolution, semi-rational design, synthetic biology

最终交流类型: Invited

Regulatory strategies for cerium nanozymes in biomedical applications

于超

重庆医科大学

Since 2007, when Yan Xiyun's team found that Fe3O4 nanoparticles have peroxidase-like activity, a large number of nanomaterials, such as metal nanoparticles, metal oxide nanoparticles, carbon-based nanomaterials and metal-organic frameworks, have been shown to function like natural enzymes. Nanozymes have the characteristics of stable structure, adjustable activity, and diverse functions, which have become potential valuable competitors of natural enzymes in many fields. Rapid valence transition and surface electron transfer are the action mechanisms of most nanozymes, suggesting that surface properties such as size, morphology, surface lattice, composition, modification and other intrinsic factors determine their enzymatic properties. However, external factors such as pH, temperature and ionic strength of solution can affect the catalytic activity of nanozymes. The study of nanoenzymes is not only to solve the limitations of natural enzymes and traditional artificial enzymes, but also to explore the hidden intrinsic biological functions in nanomaterials has become an emerging field of nanotechnology and biology. Cerium nanozymes have attracted extensive attention for their potential therapeutic effects on oxidative stress and inflammatory diseases due to their unique and numerous mimic enzymatic activities. Due to the coexistence and transformation of Ce3+ and Ce4+ on its

surface, it exhibits a variety of mimic enzymatic activities (such as superoxide dismutase, catalase, alkaline phosphatase, oxidase, etc.) and is highly efficient and renewable. Thus, it has shown potential application value in the treatment of tumors, refractory wounds, and cardiovascular diseases. However, how to effectively regulate the enzymatic activity of cerium nanozymes, drug co-loading, and targeted synergistic therapy are the key and difficult problems in current research. Therefore, our group has carried out a series of studies based on cerium nanozymes in order to lay a theoretical foundation for their further biomedical applications.

Keyword： Cerium nanozymes， superoxide dismutase, catalase，refractory wounds, cardiovascular diseases

最终交流类型: Invited

Nanozyme-based Personalized Health Monitoring and Treatment Assisted by Polymer-based Substrate

杜衍
中国科学院长春应用化学研究所

Nanozymes have made remarkable contributions in personalized health monitoring and treatment by enabling rapid and sensitive detection of molecular signals for individual health assessment. The importance of loading nanozymes onto a specific substrate material lies in facilitating their stable catalytic activity. The substrate provides a supportive environment that helps preserve the structural integrity and enzymatic function of nanozymes, ensuring their long-term performance. Additionally, the choice of substrate material can enhance the specificity of nanozymes by creating a tailored microenvironment that promotes selective interactions with target molecules. Thus, the strategic use of substrate materials holds significant potential in optimizing the stability and catalytic efficiency of nanozymes for various practical applications. This report demonstrates the application of some characteristic polymer-based substrate in supporting nanozymes to address critical healthcare challenges.

The first research emphasizes the use of polymer-based matrices in nanozyme-enhanced cosmetic contact lenses (CCLs) to combat ocular surface diseases (OSDs). These lenses, embedded with antioxidant nanozymes, effectively scavenge excess reactive oxygen species (ROS) on the ocular surface, providing a preventive effect against OSDs. Demonstrated efficacy in rabbits and rats exposed to high-risk conditions highlights the potential of polymer-based nanozyme-CCLs as powerful wearable biomedical devices.

In the second research, the focus lies on point-of-care alcohol detection using Pd@Pt core-shell nanoparticles in a poly(vinyl alcohol) aerogel matrix. This system enables rapid, sensitive, and selective alcohol detection in saliva and whole blood samples. The integration of Pd@Pt nanozymes within the poly(vinyl alcohol) aerogel enhances the reliability of the diagnostic system, facilitating its potential application in law enforcement and forensic contexts. The strategic use of polymer-based matrices ensures stable catalytic activity and enhances the specificity of nanozymes, making them promising candidates for diverse biomedical applications.

Keyword： nanozymes, reactive oxygen species, Prussian blue analogues, cosmetic contact lens, ocular surface diseases

最终交流类型:

Remote Regulation of Enzyme-Nanozyme Cascade Reaction Kinetics by Magnetic Actuation

和媛
西北大学

The design of smart catalysts with tunable activity by physical stimuli is of great importance for precise enzyme catalytic therapy. Magnetic nanomaterials can generate a nanoscale magnetothermal effect under the exposure to an alternating magnetic field (AMF), which provides an opportunity for the remote and precise control of enzymatic processes without elevating the solution temperature. Previously, our research group has built an in situ magnetothermal-spectroscopy platform to show (1) the POD nanozyme activity of iron oxide and (2) enzymes immobilized on magnetic nanoparticles can be real-time controlled by the magnetothermal effect of iron oxide, respectively. Here, we report two stories to show the enzyme–nanozyme cascade reaction kinetics can be remotely controlled by magnetic stimuli for improved enzyme catalytic therapy. In the first example, a series of nanohybrid Glucose oxidase (GOx) was prepared and the activities of GOx and POD nanozyme in these systems were shown to be differentially stimulated by AMF, leading to dramatically improved ROS production for more efficient tumor catalytic therapy. In the second example, nanohybrid Uricase (UOx) was prepared, and the CAT nanozyme activity of iron oxide nanoparticle was

shown to be modulated by AMF, providing a new way to switch on and off uricase activity for precise regulation of uric acid lowering therapy in gout.

Keyword： nanozyme; nanohybrid glucose oxidase; nanohybrid uricase; iron oxide nanoparticle; magnetic field

最终交流类型:

Publishing in Materials Science and Beyond with Wiley.

Babak Mostaghaci
Wiley

Publishing papers in reputable journals is a crucial step in the research cycle. In this talk, Dr. Babak Mostaghaci, the deputy editor of Advanced Materials and Editor-in-Chief of Advanced Intelligent Systems at Wiley-VCH, will share his insights on the manuscript processing workflow from submission to publication. He will also discuss the ethical aspects of publishing and provide tips on how to prepare your manuscript for submission and increase your chances of successful publication. The topics that will be covered include:

- How to select the most suitable journal for your submission
- What criteria editors and reviewers use to evaluate manuscripts
- How to enhance the visibility and impact of your research

The presentation will also introduce the Advanced family of journals and the latest materials science titles launched by Wiley.

Keyword： Publishing in Materials;Wiley

Topical Sessions =》 16.Young Scientist Forum of Nanotechnology

最终交流类型: Oral

Study on the Design and Dynamic Response Mechanism of Hydrogen Explosion Nano Proof Coating

Fei Liu
Nanjing Tech University

Hydrogen was officially recognized as a designable and widely used energy source at the end of the last century and has gradually attracted people's attention. Due to its high combustion heat, water as the combustion product, and the ability to produce hydrogen again, hydrogen energy has become a clean, efficient, and sustainable new type of zero carbon energy, which can be directly produced from seawater or solar energy. For the large-scale commercialization of hydrogen, ‘safety of storage, transportation and use’ is the primary premise. Whether the hydrogen production from seawater and solar early or the later hydrogen fuel usage and hydrogen energy vehicles, etc. are implemented based on this primary premise. Therefore, the design of hydrogen explosion nano proof coating and the research on its dynamic response mechanism are important guarantees for the safe transportation and efficient use of hydrogen energy. However, the research on the attenuation principle of impact stress waves and the dynamic response mechanism of combustion and explosion of coatings with different properties and anti explosion structures when high calorific value hydrogen gas undergoes combustion and explosion is insufficient at present.

At the same time, whether the explosion nano proof coating materials can effectively prevent its impact damage on surrounding objects is of importance. Therefore, the reasonable selection of coating materials with different properties and the structural design and overlapping use of coatings with different characteristics are one of the key scientific issues. This topic successively studies the impact resistance and high temperature resistance characteristics of coating materials with different properties, the attenuation of shock stress waves by coatings with different structures, and the dynamic response mechanism of explosion nano proof coatings to hydrogen combustion and explosion. Combined with finite element numerical simulation and outdoor model test, the optimal design of explosion nano proof coatings is proposed.

Keyword: Hydrogen explosive; Explosion nano proof; Coating; Dynamic response; Numerical simulation

最终交流类型: Invited

Vacuum evaporation for high efficiency large-area perovskite solar cells

易陈谊
清华大学电机系

Metal halide hybrid perovskite solar cells (PSCs) have the advantages of high power conversion efficiency (PCE) and low cost and have received great attention from the academia and industry. Large-area PSC fabrication methods compatible with industrial applications must be developed to enable commercialization. However, most of the reported high-efficiency PSCs were prepared by spin coating, which is only suitable for laboratory-scale devices. Moreover, solvents used in the solution process may be detrimental to the underlying functional layers and are harmful to the environment. In contrast, these drawbacks can be avoided by using vacuum evaporation. The precursors can be evenly and uniformly deposited on substrates, and the film thickness can be precisely controlled during the vacuum evaporation process, which is compatible with scalable fabrication. Vacuum evaporation is promising for the high-throughput fabrication of PSCs because of its solvent-free characteristic, precise control of film thickness, and compatibility with large-scale production. Nevertheless, the PCE of PSCs fabricated by vacuum evaporation lags behind that of solution-processed PSCs.

In this presentation, we will report on recent progresses in the production of high efficiency large area perovskite solar cells by a Cl-alloy–mediated sequential vacuum evaporation. We evaporated cesium iodide (CsI), lead iodide (PbI2), and lead chloride (PbCl2) to create a composite precursor film on which formamidinium iodide (FAI) molecules were deposited under precise control. The Cl-alloy–mediated vacuum deposition method can produce perovskite films with high crystallinity and homogeneity. Compared with the coevaporation process, the layer-by-layer sequential deposition method avoids the risk of cross-contamination by evaporating lead halide and organic ammonium salt separately in different vacuum chambers. An efficiency of over 24% has been achieved with negligible

difference for large-area and small-area devices. The evaporated PSCs show good stability with negligible decline in device performance after storage in dry air for more than 4000 hours. Moreover, the unencapsulated devices maintained 97% of their initial PCE after 1300 hours of storage in ambient air at a humidity of 35% and maintained 92% of the initial PCE after 450 hours of maximum power point (MPP) tracking under continuous light irradiation. Further, a molten salt strategy has been employed to improve the reproducibility of the evaporation process. Additionally, high efficiency flexible perovskite solar cells will also be discussed.

Keyword: Vacuum evaporation, high efficiency, large area, perovskite solar cells

最终交流类型: Invited

Charge Separation and Recombination Dynamics in Organics Photovoltaic Blends Studied by Ultrafast Spectroscopy

王睿
南京航空航天大学

Organic solar cells (OSCs) based on blends of electron donors and acceptors hold the advantages of flexibility, environment-friendly and low cost, which attracts numerous interests recently. Owing to the development of nonfullerene acceptors, the certified power conversion efficiency (PCE) of OSCs has exceeded 19%. Nevertheless, the PCEs of OSCs still lag behind their inorganic counterparts. This is mainly because of the existence of additional energy loss channels in OSCs, such as: 1) Additional driving forces are needed for efficient charge separation; 2) Charge recombination can form low-lying triplet states, causing non-radiative losses; 3) Excitations may be trapped during the power conversion, etc. To solve the problem, we first develop a high-precision broadband transient absorption (TA) spectroscopy equipped with the home-made fast double line cameras enabled by a field-programmable gate array (FPGA) control board. Utilizing the TA spectroscopy with improved sensitivity, we systematically study the excited-state dynamics in organics photovoltaic (OPV) blends. In model OPV systems, we find charge separation is mediated by intra-moiety delocalized excitations (i-EX) other than the local excitations in the hole transfer channel. Due to the enlarged electron-hole separation, the i-EX shows reduced binding energy, which can lower the driving forces needed for charge separation. In addition, we find

the non-radiative triplet loss channel is suppressed in OPV blends with fluoridized acceptors, which can be explained by the modified energy arrangement of singlet and triplet states at donor:acceptor interfaces supported by the quantum chemical calculation results. Moreover, we find a conformation dependent trapping loss channel of local excitations in all-polymer blends with the acceptor of N2200. Such a trapping loss can be effectively reduced by detuning the dielectric constant with additives. These findings suggest modifying the intra-moiety and interfacial intermolecular interactions to optimize charge separation and recombination dynamics may be a promising way to further improve the device performance of OSCs.

Keyword: Excited state dynamics, charge separation, charge recombination, transient absorption

最终交流类型: Oral

Strain engineering of 2D semiconductor materials

王聪
北京化工大学

Elastic strain engineering is a technique to regulate the electronic structure of materials by altering the relevant structure and mechanical properties of the materials. In the past decades, this technology has been widely applied in the semiconductor industry, in order to increase the electrical performance of the device by improving the carrier mobility of the silicon. However, the traditional semiconductor single crystal materials due to the limited strain that can be sustained, largely restricting the ability to regulate the electronic properties of semiconductor materials through elastic strain. Recently, two-dimensional layered materials have attracted considerable attention, which is characterized by a strong covalent bond within the plane, while the layers are only connected by very weak van der Waals force. Among the most remarkable two-dimensional (2D) materials are graphene, hexagonal boron nitride (h-BN), black phosphorus (BP) and transition metal dichalcogenides (TMDs) such as MoS2, WS2, WSe2, etc. These materials possess distinctive optical and electronic properties. More importantly, these 2D materials are generally able to endure greater elastic strain than bulk materials without damage. For example, most graphite materials will break when strained to 0.1%, but single-layer graphene can withstand 25% elastic strain. This makes 2D materials a promising field to explore in elastic strain engineering. Therefore, the strain engineering of 2D materials has a wide range of research prospects and potentials. In this report, I will report some recent research progress in strain engineering of 2D semiconductor materials and flexible optoelectronic devices to the teachers. These include: experimental evidence of nanoscale local strain modulation induced ferromagnetism in 2D ReSe2; strain engineering of band, excitonic properties of 2D GaSe and PbI2, realization of wide-spectrum light absorption and enhancement of light absorption efficiency by designing nanoscale wrinkled morphology, providing theoretical and experimental basis for the construction of high-performance solar cell devices; modulation of WSe2/WS2 heterojunction coupling properties and excitonic emission characteristics by applying strain on flexible substrates; Preparation of strain sensors based on two-dimensional GaSe and SnSSe, realizing characteristics of resistive, repeatable, and high strain sensitivity.

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Keyword: Strain engineering; 2D semiconductor materials; Flexible optoelectronic devices

最终交流类型: Oral

Dynamic Self-Assembly of Plasmonic Nanoparticles

刘一丁
西南石油大学

Plasmonic nanomaterials possess unique physical and chemical properties and are widely used in optical sensing, chemical detection and other fields. Their properties can be modulated by controlling their assembly structure. How to achieve precise positioning of assembly structural building blocks, construct stimuli-responsive dynamic regulation systems and realize their applications are the hotspots of research in this field at this stage. This presentation will report recent research by the author on the preparation and regulation of plasmonic nanomaterial assembly structures, including: (1) Preparation and mechanism study of gold nanoparticle colloidal self-assembly and gold-silver co-assembly structures with precise positioning of structural building blocks: previous studies on regulation of colloidal nanoparticle self-assembly mainly focused on tuning nanoscale interactions based on DLVO and related theories and methods. Our study revealed by tuning ligand conformation on plasmonic nanocrystals along with classical colloidal interactions, tailored colloidal nanoparticle assembly structures with precise positioning could be constructed. (2) Design and construction of programmed assembly-disassembly systems with structural feedback and self-oscillating assembly-disassembly systems of gold nanoparticles: development of nanoparticle self-assembly processes from passive stimuli-responsive towards active self-regulated processes will expand the application of colloidal assembly materials to complex biomimetic functions such as signal processing and adaption. Our study realized the above-mentioned self-regulated nanoparticle assembly paradigms by first constructed the reversible gold nanoparticle self-assembly units followed by introduction of coupled stimuli (both physical and chemical) which initiate feedback functions for the self-regulation processes. In both studies, the mechanism of the self-assembly processes were analyzed by both theoretical and experimental approaches. It is believed the above work provides theoretical and technical support for the in-depth intelligentization and application of plasmonic nanomaterials.

Keyword: plasmonic nanoparticles, nanoparticle self-assembly, stimuli-responsive colloidal materials, dynamic self-assembly, nanoparticle surface chemistry

最终交流类型: Invited

Determining Quasiparticle Bandgap of 2D Transition Metal Dichalcogenides with Femtosecond Mid-Infrared Spectroscopy

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The features of excitons formed in atomically-thin two-dimensional transition metal dichalcogenide (2D TMD) materials dominate their optical and optoelectronic response and nonequilibrium dynamics even at room-temperature. Accurately determining the quasiparticle bandgap E_g is of crucial importance for investigating their excitonic properties. For example, the exciton binding energy of a 2D TMD semiconductor is generally determined by the difference between its quasiparticle bandgap E_g and optical bandgap E_X. E_X can be easily obtained by measuring its photoluminescence spectrum. However, up to now, it is still full of challenges to experimentally determine the value of E_g for 2D TMDs. One commonly used method is scanning tunneling spectroscopy (STS), which suffers from the use of conducting substrates required for STS. Therefore, it is necessary to develop an effective experimental approach to determine the quasiparticle bandgap of the TMD samples prepared on nonconducting substrates under ambient conditions. Here, we develop a technique named as excitation-energy-scanning ultrafast infrared microspectroscopy to systematically study the excess energy dependent hot carrier relaxation dynamics in 2D TMD materials. The experimental results confirm that the ultrafast relaxation dynamics is strongly correlated with E_g. A good linear relationship between the carrier relaxation time and the excitation wavelength is observed for all measured monolayer (ML) and bilayer (BL) TMD samples, which allows us to determine their quasiparticle bandgaps as well as corresponding exciton binding energies. A carrier-optical-phonon scattering-mediated cascading-relaxation model is proposed, which can perfectly describe all the measured dynamics. As a result, the quasiparticle bandgaps as well as the corresponding exciton binding energies are precisely determined in four samples ML and BL $MoSe_2$, ML MoS_2, and BL $MoSe_2$. Our work reveals a general picture for the hot carrier relaxation dynamics and the carrier-phonon interactions in atomically-thin TMDs and offers a novel experimental approach in determining the quasiparticle bandgap of TMDs under ambient conditions.

Keyword: quasiparticle bandgap, 2D TMDs, femtosecond infrared spectroscopy, hot carrier relaxation dynamics, exciton binding energy

最终交流类型: Oral

Fluorescence anisotropy probes constructed on the basis of NIR-II quantum dots applications in complex matrix detection

刘婧
武汉大学

Fluorescence anisotropy (FA) analysis is a traditional analytical method that has been widely used in various biochemical analysis because of its separation-free, high-throughput. Fluorescence anisotropy values are positively correlated with the mass and volume of fluorescence molecules. Compared with the conventional FA detection in the visible region, the autofluorescence background interference of biological matrices in the near-infrared region (NIR) is significantly reduced, making it more suitable for the detection of biomolecules in complex matrices. The FA method in NIR has great potential for early diagnosis of diseases because of its strong anti-interference ability, high sensitivity, and separation-free. The second near-infrared window (NIR-II) fluorescence quantum dots (QDs) have the characteristics of good photostability and low spontaneous interference of substrates, which have a promising future in the detection of complex matrices. We constructed different FA detection probes based on Ag2Se QDs in the NIR-II for the detection of different biomolecules in complex matrices.

Studies revealed that the levels of small extracellular vesicle (sEV) programmed cell death-ligand 1 (PD-L1) may serve as a predictive biomarker for the clinical responses to immunotherapy (The particle size of sEV in the range of 50-150 nm). While, the currently available enzyme-linked immunosorbent assay (ELISA)-based quantitative analysis of sEV PD-L1 is tedious and time-consuming and have low sensitivity. The detection probe was constructed by combining small molecule aptamer that can specifically recognize PD-L1 to achieve an isolation-free, rapid and highly sensitive detection of sEVs PD-L1 in human plasma. It can detect amounts of PD-L1-positive sEVs in plasma samples that diluted more than 70 times. This method can differentiate samples from clinical oral squamous cell carcinoma patients (OSCCP) and healthy donors (HD) well, providing a new idea for the clinical detection of sEV PD-L1 levels in tumor patients. While, this FA strategy generally relies on signal changes caused by changes in molecular mass before and after binding between the probe and the test object to achieve detection of the target. Small molecules are difficult to detect because of their small masses, which do not induce significant signal changes upon binding to the probe. Thus, we further developed FA signal amplification strategies by nanomaterials enhance the FA signal by binding the probe to graphene oxide (GO) or streptavidin (SA), thereby enhancing the sensitivity of the assay. Adenosine triphosphate (ATP) is an important nucleotide (also known as adenosine triphosphate) that acts as a "molecular currency" for intracellular energy transfer, storing and transmitting chemical energy. The quantitative detection of ATP in human serum samples was achieved by combining graphene oxide with a fluorescent anisotropic probe that specifically recognizes ATP. ATP could be quantitatively detected in concentrations ranged from 3 nM to 2500 nM, with a detection limit down to 1.01 nM. DA is an important small molecule neurotransmitter that is closely associated with the development of many diseases. We combined SA with a FA probe that specifically recognizes dopamine (DA) to construct a biosensor that enables amplification of the detection signal, enabling rapid, separation-free detection of DA in human serum. The detection signal has a good linearity between 50 nM-3000 nM with a detection limit of 11.2 nM. The construction of GO and SA signal amplification device provides a new idea for the analysis of small molecule FA.

In summary, Near-infrared fluorescence anisotropy (NIR FA) analysis has the advantages of anti-interference, high sensitivity and separation-free, and has a greater potential for early diagnosis of diseases. By modifying different aptamers for NIR II QDs and combining them with different target substances, it is expected to achieve the detection of sEVs and small biomolecules in clinical complex matrix samples.

Keyword: NIR-II QD, Fluorescence anisotropy, Bioanalysis, Complex biological samples

最终交流类型: Oral

Theoretical Insight into Guest Adsorption and Transport in Porous Nanomaterials

征甲甲
国家纳米科学中心

Porous nanomaterials, such as metal-organic frameworks (MOFs), have recently attracted significant attention due to their potential applications in guest storage, selective

recognition, separation, and conversion. Among the reported porous nanomaterials, soft porous crystals (SPCs) are of particular interest due to their stimuli-responsive frameworks that enable unique guest adsorption and transport behaviors, such as gate-opening and non-equilibrium adsorption. Understanding the adsorption and transport of guest molecules in such dynamic crystals is essential to facilitate the further development of these materials for applications in challenging guest identification and separation. Various theoretical studies based on thermodynamics analysis, Monte-Carlo (MC) and molecular dynamics (MC) simulations have been carried out to understand guest adsorption and transport in SPCs. However, theoretical knowledge about those unusual guest adsorption and transport behaviors is still limited; for instance, it is not clear in what case the gate-opening and non-equilibrium adsorptions occur (or do not occur). For these purposes, a reliable computational method to describe the non-covalent host-guest interactions is essential. Here, we will introduce our recent theoretical studies on guest adsorption and transport in SPCs, taking several reported compounds as examples.[1-3] Using an ONIOM-type computational method that combines the density functional theory method (PBE-D3) for crystals and the post-Hartree-Fock methods for small clusters (Figure 1a), we were able to accurately calculate the binding energy and isotherm for gas adsorption into SPCs and provide an in-depth understanding on the gate-opening (Figure 1b) and non-equilibrium adsorption.

Figure 1. (a) Schematic representation for the periodic model and cluster model in the calculation of adsorption energy of guest molecules in MOFs. (b) Comparison between computational and experimental adsorption isotherms in a soft MOF.

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Keyword: MOFs, density functional theory calculations, host-guest interaction, guest adsorption and transport

最终交流类型: Invited

Mechanism of Controllable Nucleation and Growth of MoS2

马亮
东南大学

MoS2, as a representative example of two-dimensional (2D) semiconductors, has attracted great interest in extending Moore’s law beyond silicon owing to its atomic thickness, proper bandgap, and easy-to-integrate planar structure. The controllable growth of wafer-scale single crystal MoS2, as the prerequisite of industrial application, however, is still very challenging due to the symmetry mismatch with the epitaxial substrate. Based on theoretical simulations, we proposed a surface step-MoS2 interface-guided unidirectional nucleation mechanism for the epitaxial growth of MoS2 on c-plane sapphire. It is shown that properly orientated steps, in addition to lowering the surface symmetry, can break the formation energy degeneracy of antiparallel nucleation of MoS2 and give rise to only one thermodynamically favorable nucleation direction under the sulfur-rich conditions. On the other hand, the growth of multilayer MoS2 with controllable and uniform thickness is also very challenging. It is revealed by our calculations that monolayer MoS2 domains are thermodynamically much more favorable than multilayer ones on epitaxial substrates due to the competition between surface interactions and edge formation, leading accordingly to a layer-by-layer growth pattern and non-continuously distributed multilayer domains with uncontrollable thickness uniformity. We theoretically proposed a step-guided mechanism for the growth of uniform multilayer MoS2 on an epitaxial substrate. The steps with proper height on the sapphire surface can guide the simultaneous nucleation of multilayer MoS2 with aligned edges and uniform thickness and promote the continuous growth of multilayer MoS2 films. It is noted that, according to our simulations, the proposed mechanism can be reasonably extended to grow other 2D materials with controlled direction and uniform thickness on epitaxial substrates. With the proposed mechanisms, our experimental collaborators have successfully synthesized wafer-scale monolayer MoS2 single crystal and centimeter-scale uniform bilayer MoS2 films on the stepped sapphire substrate, where the performances of the fabricated MoS2 FETs are among the best of 2D semiconductor devices.

Keyword: 2D semiconductor, crystal growth theory, nucleation mechanism, interfacial thermodynamics, first-principles calculation

最终交流类型: Invited

Toward accurate and efficient microkinetic modeling in heterogeneous catalysis

陈征
复旦大学

While the multiscale approach has become the gold standard in modeling heterogeneous catalysis, increasing the fidelity and accuracy of each stage of the multiscale process is highly desired but challenged. As a key part of the multiscale approach, microkinetic models are required to bridge the gap between atomic scale properties and macroscopic performance. However, the accurate and efficient microkinetic method is still lacking. On the one hand, the efficient and widely used mean-field microkinetics can't accurately describe the intrinsic inhomogeneity of heterogeneous catalysis arising from adsorbate-adsorbate lateral interactions and nonuniform reaction sites on nanoparticale. On the other hand, while Kinetic Monte Carlo (KMC) on the explicit lattice can account for such inhomogeneity, the disparity in time scales of various processes usually makes brute force KMC simulations impractical. Recently, we have proposed a method, namely XPK, to extend the phenomenological kinetics for the accurate and efficient microkinetic modeling of heterogeneous catalysis. XPK is achieved through a hybrid between the diffusion-only KMC on the explicit lattice to evaluate the reaction propensities and later an implicit lattice KMC in the PK form to evolve the coverages and calculate the final rates. The accuracy and efficiency of XPK have been tested against the explicit lattice KMC by using model systems.

XPK has been successfully applied to various important systems, including syngas conversion on Rh(111) surface. We show that it is the dynamic and intermediate-specific local coverage that controls the activity and selectivity instead of the average coverage. The commonly used mean-field models fail to account for this dynamic and intermediate-specific local coverage change and thus fail to reproduce the experimental observations on the pressure-dependent selectivity changes. Our study provides new insights into how local surface coverage tunes the catalysis. Therefore, XPK is expected to be a powerful tool for understanding the catalytic phenomena and rational design of catalysts.

Keyword: microkinetics, KMC, time-scale separation, lateral interactions, syngas conversion

最终交流类型: Invited

Voltage Losses in Organic Photovoltaic Devices

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东华大学

Organic photovoltaic (OPV) devices possess unique properties, such as lightweight, cost-effectiveness, flexibility, and solution processability, which make them highly promising for applications in the fields of renewable energy and wearable electronic technologies. Currently, high-performance organic photovoltaic devices have achieved a power conversion efficiency (PCE) exceeding 20%, with an external quantum efficiency (EQE) of up to 90% and a fill factor (FF) over 80%. However, a contentious debate persists regarding whether the performance of organic photovoltaic devices can ultimately match that of silicon-based or perovskite-based photovoltaic devices. This debate arises primarily due to the existence of charge transfer states formed at the interface between the donor and acceptor materials in organic photovoltaic devices, which are required for the photo-generated excitons to split into free charge carriers. The presence of the charge transfer states introduces new recombination pathways for free charge carriers, leading to rapid charge carrier recombination and significant voltage losses, thereby limiting the open-circuit voltage (Voc) of the devices. Consequently, the key to further enhancing the performance of organic photovoltaic devices lies in reducing voltage losses and improving the open-circuit voltage.

In this presentation, we will discuss the key factors determining the open-circuit voltage of organic photovoltaic devices, the origin of radiative (Vr) and non-radiative voltage losses (Vnr), and the reasons for excessive voltage losses in organic photovoltaic devices. Specifically, we will present findings from our research group on the radiative voltage losses caused by the energy loss induced by the charge transfer process, the non-radiative voltage losses resulting from the diffusion of charge carriers to the minority contact, and finally, the non-radiative voltage losses associated with the rapid non-radiative decay of charge transfer states, which are influenced by the microstructure of the donor-acceptor active layer, the molecular structure of the donor and acceptor materials, and the electronic properties at the donor-acceptor molecular interface.

Keyword: photovoltaics, organic solar cells, charge transfer state, voltage losses, open-circuit voltage

最终交流类型: Invited

Characterization and Modulation of the Interlayer Interactions of 2D Materials

高扬
浙江大学

The interlayer van der Waals (vdW) interactions play a vital role in the emergence of the novel and extraordinary physical properties of two-dimensional (2D) materials and their vertical heterostructures. Therefore, precise and quantitative characterization and modulation of the vdW interlayer interactions in 2D materials are of fundamental importance in both scientific research and potential applications. In this presentation, I will first introduce a novel scanning probe microscopy (SPM) based methodology - Angstrom indentation (Å-I) which allows for Å-scale shallow indentation on 2D materials, so the vdW interactions can be extracted from the force-indentation curves without destruction. The interlayer elasticities of some typical 2D materials (graphene, graphene oxide) were successfully measured [1]. Furthermore, an ultrahard monolayer diamond structure driven from bilayer graphene by Å-I was observed. Local high pressure by atomic force microscopy (AFM) applied on epitaxial bilayer graphene on SiC(0001) induces interlayer sp^3 covalent bonds forming, eventually creating a novel monolayer diamond structure. The elastic modulus of the monolayer diamond was obtained via Å-I, which turns out to be 1.08 TPa, close to the value of cubic diamond. First principle calculations along with nano-hardness measurements demonstrate that the graphene-diamene phase transition is reversible and cannot be activated when the epitaxial graphene is thicker than 3 layers [2]. The second part of the presentation is focused on the graphene/h-BN heterostructure system. We used diamond anvil cell (DAC) to apply up to 10 GPa hydrostatic pressure to engineer the band structure of the graphene/h-BN moiré superlattices. High pressure compresses the interlayer spacing between the graphene and h-BN flakes, enhancing the interlayer interactions and the inversion asymmetry, thus tuning the band structure of graphene. We found that the primary Dirac gap of graphene in the large-twist-angle superlattices can be further enlarged from 30meV to 80 meV at 8.3 GPa, and the pre-closed secondary Dirac gaps were re-opened at 7 GPa [3].

Keyword: 2D material, van der Waals heterostructure, atomic force microscope, diamond anvil cell, high pressure

最终交流类型: Oral

Self-pumping dressing

时连鑫
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Capillary adhesion and anti-adhesion problems caused by the interfacial fluid layer are hot issues in the area of interfacial research. In recent years, we have developed a series of self-pumping textiles/dressings and wet adhesive fibers focusing on the problems of impeded healing caused by excessive exudate wetting and dis-attachment caused by the interfacial liquid layer. 1) We propose a biofluid "self-pumping" model and develop a self-pumping dressing with unidirectional transportation of wound exudates to promote overhydrated wound healing (Adv. Mater. 2019, 31 (5), 1804187); 2) We construct a bio-inspired "self-pumping" textiles with asymmetry wettability and structure, which effectively removes sweat from the skin surface and solves the problem of wet stickiness and coldness by the wetted conventional cotton textile (Adv. Mater. 2019, 31 (41), 1904113); 3) A series of self-pumping dressings based on aligned channels and fractal channels are developed to achieve rapid and continuous unidirectional transportation of wound exudates, promoting the healing wound, such as diabetic wounds and burns (Macromol. Rapid Commun. 2022, e2200814, Front. Bioeng. Biotechnol. 2023,11, 10.3389/fbioe.2023.1188782).4) Inspired by the wet adhesion and low-temperature toughness of spider silks, a series of core-sheath/side-by-side hydrophilic fibers are fabricated to achieve omni-wet adhesion on oil/water wetted surfaces and ultra-low temperatures tolerance (-196°C) for the storage of wet-adhesive materials at extremely low temperatures (Adv. Mater. 2021, 33 (14), e2007301, Nano Today 2023, 48, 101748).

Keyword: Self-pumping, Unidirectional Draining, Janus Materials, Wet Adhesion, Super-cold Tolerance

最终交流类型: Invited

Microenvironment Matters: Exploring the Toxicological Impacts of Nanomaterials and Microplastics in Health and Disease

彭国涛
同济大学

The safety assessment of nanomaterials has been extensively investigated over the past decades. However, there remains a need to further understand the intricate toxicological mechanisms operating within complex biological systems. Moreover, current nanotoxicological studies predominantly focus on healthy individuals, leaving a significant knowledge gap regarding the effects on compromised individuals. Here, we aimed to explore the toxicological impacts of 2D materials and microplastics within the context of the gut microenvironment in both health and disease conditions. Initially, we uncovered the mechanism by which graphene oxide induces immune responses via the aryl hydrocarbon receptor (AhR) signaling pathway [1]. Oral exposure to graphene oxide was found to modulate the composition of the gut microbiome in adult zebrafish, with notable distinctions between wild-type and ahr2-deficient animals. Furthermore, when combined with butyrate, graphene oxide was observed to elicit AhR-dependent induction of cyp1a and the homing of lck+ cells to the gut in germ-free zebrafish larvae. Single-cell RNA sequencing analysis provided additional evidence of the presence of innate lymphoid cell (ILC)-like cells in germ-free zebrafish [1]. Subsequently, we investigated the behavior of nanomaterials under inflammatory bowel disease (IBD) conditions. We induced an IBD-like phenotype in zebrafish larvae by exposing them to dextran sulfate sodium salt (DSS) for three days. Notably, subsequent exposure to nano- and microplastics revealed increased susceptibility in the IBD-like zebrafish, resulting in significant mortality. RNA-seq analysis further demonstrated that both nano- and microplastics induced similar effects, with metabolic processes and localization being the most enriched up- and downregulated GO processes. KEGG analysis revealed dysfunctions in ribosome activation and boosted oxidative phosphorylation, potentially contributing to cell death and zebrafish mortality (Unpublished data). Collectively, our findings underscore the critical role of the microenvironment in both health and disease settings, providing valuable insights into the toxicological impacts and underlying mechanisms of nanomaterials and microplastics.

Keyword: Compromised nanotoxicology, gut microbiome, immune responses, inflammatory bowel disease

最终交流类型: Invited

单原子 CO2 电化学还原催化剂选择性的根源探索与调控

李亚飞

南京师范大学

CO2 的电化学还原可以实现碳资源的回收利用，对实现“双碳”目标意义重大。单原子催化剂因为兼具均相和非均相催化剂的优点而成为近年来催化领域的研究热点。在众多类型的单原子催化剂中，金属-氮-碳(M-N-C)型单原子催化剂因为具有高原子利用率、高活性、高导电性等优点，是构建高效 CO2 电化学还原催化剂的优良候选材料。然而目前实验上报道的 M-N-C 型单原子催化剂的 CO2 还原产物几乎都是 CO，而另外一种两电子还原竞争产物甲酸(HCOOH)却很难得到。甚至一些具有很高甲酸选择性的金属催化剂，当以单原子的形式分散时，产物也以 CO 为主。另外一方面，CO 的电化学还原也是近年来的研究热点，但目前实验上用于 CO 还原的电催化剂大都是 Cu 基材料，很少有单原子催化剂用于 CO 还原的研究见诸报道。我们利用基于恒电位方法并结合真实溶剂模型的理论计算揭示了 M-N-C 型单子催化剂具有高 CO 选择性的内在根源，并阐明了在单原子催化剂上 CO 难以被深度还原这一问题背后的原因，并提出了相应的调控催化剂产物选择性的策略。

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Keyword: CO2 还原；电催化；选择性；单原子催化剂

最终交流类型: Invited

Surface and interface of nanomaterials characterized by in situ TEM

罗浪里

天津大学

In situ TEM techniques provide an ideal platform for the characterization of surface and interface phenomenon in functional nanomaterials including heterogeneous catalyst, energy storage and conversion materials. Ultrahigh spatial resolution coupled with real-time monitoring of chemical and physical processes, which are vital to decipher the underlying mechanisms. We demonstrate the ability of real-time high-resolution imaging at atomic scale under an in-situ gas-heating experiments would provide atomic insights for the surface and interfaces of thermal catalysts. Surface adsorption, activation under reaction gases have been directly observed, and unique structural motif relevant to specific reactions have been found.

Corroborated by theoretical calculation and simulation, we unveil the atomistic mechanisms governing these critical processes.

Keyword: In situ TEM, atomic-scale, heterogeneous catalysis

最终交流类型: Invited

Selective Protein Capture and Function Regulation Based on Stimuli-Responsive Spherical Nucleic Acids

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北京科技大学

Proteins participate in and regulate almost all cellular activities. In order to better understand the roles of specific proteins in pathophysiological reactions, it is critical to develop strategies that allow selective capture and functional regulation of proteins in complex living systems. Herein, by combining aptamer design with spherical nucleic acid (SNA) nanotechnology, we designed and constructed stimuli-responsive aptamer-SNA nanoplatforms which could achieve specific capture and controlled release of proteins of interest (POI) and demonstrated their applicability for protein function regulation in cells and living bodies. Furthermore, we validated that the aptamer-SNA nanoplatform was able to capture and modulate the function of POI in a cancer cell-selective manner through the introduction of enzyme-responsive module in the aptamer design. Besides, the enzyme-controlled methods could also be used for cell-selective sensing and imaging with enhanced signal-to-background ratio. In summary, such strategies provided new toolkits for protein capture and functional regulation with cell specificity and could promote the development of protein-based therapeutics.

Keyword: protein capture; function regulation; spherical nucleic acids; aptamer; enzyme

最终交流类型: Invited

The Nanostructured Materials for Natural Sunlight-Driven Photothermal Catalysis

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河北大学

Photothermal catalysis has the advantages of~100% sunlight absorption and high catalytic activity. However, the temperature of photothermal materials under low density natural sunlight irradiation is too low (generally below 100 ℃) to drive industrial catalysis, making it difficult to apply in practical applications.[1] Here, we design photothermal materials based on the gradient film extinction principle to achieve the synergy of efficient sunlight spectrum absorption and low infrared radiation, making the standard sunlight radiation temperature of photothermal materials reach 300 °C level,[2] which is three times of the corresponding temperature of traditional photothermal materials, and realizing the natural sunlight-driven photothermal CO_2 Methanation, CO oxidation, NO_x removal, VOCs combustion, etc. On this basis, the concept of heterogeneous photothermal materials is proposed to achieve the coupling of efficient sunlight spectral absorption and ultra-low infrared thermal radiation, which increases the standard solar irradiation temperature of photothermal materials to 350 ℃ level. Joint with the two-dimensional photothermal catalysts, the systems exhibit superior performances in natural sunlight-driven photothermal methanol,[3] ammonia hydrogen production,[4] CO_2 hydrogenation.[5]

Keyword: Photothermal catalysis, Hydrogen; CO2; Sunlight; Two-dimensional materials

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最终交流类型: Invited

Ultrafast electronic dynamics at MXene interface

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Plasmonic MXenes are of particular interest, because of their unique electron and phonon structures and multiple surface plasmon effects, which are different from traditional plasmonic materials. However, to date, how electron damping energy to lattice vibrations (phonons) in MXenes has not been unraveled. Here, we employed ultrafast spectroscopy to identify the energy transfer channels at MXenes interfaces. Distinctive from the well-known damping pathways, our results demonstrate a new energy damping channel, in which the

Ti3C2Tx plasmonic electron energy transfers to coherent phonons by nonthermal electron mediation after Landau damping, without involving electron-electron scattering. Moreover, electrons are observed to strongly couple with A1g mode and weakly couple with Eg mode. Our results provide new insight into the electron-phonon interaction in MXenes, which allows the design of materials enabling efficient manipulation of electron transport and energy conversion.

Keyword: MXene, Ultrafast dynamics, Spectroscopy

最终交流类型: Invited

Time-resolved imaging technique and applications

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We focus on the study of photoinduced carrier dynamics in perovskite optoelectronic materials by utilizing time-resolved techniques. We have developed an innovative time- and spatial- resolved imaging technique and applied it to the research of carrier dynamics in perovskite optoelectronic materials, including 1. By developing a new time-resolved imaging technique, We for the first time realized the direct visualization of carrier transportation dynamics in organolead halide perovskite nanowires and nanoplates. 2. By utilizing the unique time-resolved fluorescence imaging technique, we have realized the local carrier diffusion imaging in perovskite solar cell polycrystalline film, and revealed that large heterogeneity of carrier extraction efficiency at the perovskite grain electrode interface could be the major factor limiting the improvement of solar cell efficiency; We also realized manipulation of the properties of crystal edges in layered 2D perovskite single crystals and revealed long distance carrier transport beyond the limit of exciton in pure phase layered 2D perovskite single crystals. 3. We developed a new strategy to fabricate perovskite nanostructures, where the manipulation of carrier unidirectional transportation was realized. The research has provided insights for the development of highly efficient perovskite materials or structures and paved the way for their novel applications in optoelectronic devices.

Keyword: time-resolved fluorescence; time-resolved imaging; carrier dynamics; photoelectric conversion materials; perovskites

最终交流类型: Invited

Near-Infrared Nanoprobes for In Vivo Biomedical Applications

齐迹
Nankai University

Precision medicine requires noninvasive and accurate early diagnosis of diseases and appropriate treatments. Phototheranostics that are triggered or activated by photons hold great advantages in terms of real-time diagnosis with high sensitivity and in situ phototherapy with excellent spatiotemporal resolution and negligible toxicity to normal tissues. According to Jablonski diagram, there are several energy dissipation pathways after a chromophore is excited to the high-energy excited state by light. When the absorbed light is reemitted as low-energy photons, it provides fluorescence/phosphorescence imaging with high sensitivity. When the absorbed photons are converted into localized heat through vibrational deactivation to ground state, this process can be used for photoacoustic imaging and photothermal therapy of diseases. The electrons in the singlet excited state could also transfer to the triplet excited state to produce highly toxic reactive oxygen species for photodynamic therapy. However, these photophysical energy relaxation processes usually compete with each other, and it is preferable to maximize the energy dissipation as needed to boost the theranostic outcome.

We focus on the development of organic near-infrared (NIR) nanoprobes for in vivo biomedical applications. The photophysical energy transition processes and related optical imaging/therapy properties can be optimized by tuning the molecular structure and nanoaggregate state. Through rational molecular design, high-brightness and long-wavelength emission NIR-II molecular probes were obtained, which have been used for high-resolution and large-depth in vivo brain angiography and vascular disease detection in mice, rats, and monkeys. By making full use of the absorbed photon energy, high-performance phototheranostic and disease-responsive nanoprobes were developed for in situ detection, monitoring and treatment of important diseases such as tumor, arthritis, and encephalitis. We also synthesized molecular probes with tunable properties, and fabricated smart multifunctional agents for precise image-guided surgery and immunotherapy.

Keyword: nanomedicine, phototheranostics, near-infrared II, biomedical nanoprobe, aggregation-induced emission

最终交流类型: Invited

Carbon-based Memristive Materials and Devices

赵晓宁
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Carbon-based Memristive Materials and Devices

Xiaoning Zhao

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ABSTRACT

Memristor has emerged as a promising technology for memory and computing applications. Carbon materials are suitable as dielectric layer for memristor because of their remarkable electronic and thermal properties. Aiming at the key issues of the controllability of conductive channels for high density storage/high performance computing, we have developed carbon-based memristive materials and devices with long life, heat-resistant, multi-states, and low switching fluctuations.[1-5] In this report, we will introduce our research progress on carbon-based memristive materials and devices.

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Keyword: Memristor, carbon materials, conductive channel, memory, computing

最终交流类型: Invited

AlGaN-based solar-blind UV focal plane array imaging photodetectors: material growth, device preparation, and functional verification

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It is well known that solar radiation negatively affects the ability of the visible or infrared photodetector to capture target information. Fortunately, ozone in the stratosphere can filter out most of the solar radiation in the wavelength between 200 and 280 nm, thus forming a detection window without the background of solar radiation, called solar-blind ultraviolet band. Using this window, the fabricated solar-blind ultraviolet photoelectric imaging detectors have essential applications in national defense and national economic construction, such as missile approach warning, leakage monitoring of ultra-high voltage transmission lines, ozone concentration monitoring, non-line-of-sight secure communication, and so on. Under this application background, Group-III nitride alloy semiconductor AlxGa1-xN possessing with the advantages of direct wide bandgap, high optical absorption coefficient, and high chemical stability, is considered to be ideal material for developing high-performance solar-blind UV photodetectors.

Herein, we report the development of a 320×256 hybrid AlGaN-based solar-blind UV focal plane array (FPA) photodetector from material growth, array preparation and hybrid integration to functional verification in detail, which has excellent reference significance for the manufacture of the AlGaN-based solar-blind UV imaging sensor. The whole process starts with the preparation of a high-quality, crack-free AlN template by MOCVD, followed by the growth of polarization-enhanced p-i-n structure high Al content AlGaN-based photosensitive material. Then, combined with standard optoelectronic processes, a 320×256 FPA of back-illuminated solar-blind photodiodes is fabricated. Finally, followed by hybridizing to a matching Si-based CMOS read-out integrated circuit (ROIC) chip, the obtained FPA photodetector is imaging verification to evaluate its performance.

Keyword: Photodetector, focal plane array, AlGaN-based material, MOCVD

最终交流类型: Oral

Accurate and controllable organic photovoltaic materials and their devices

Dan Deng
National Center for Nanoscience and Technology (NCNST)

有机太阳电池由于其轻薄柔，可大面积制备，易于实现建筑一体化等优势而备受关注。近年来，具有高电致发光效率的非富勒烯受体的发展将聚合物太阳电池的能量损失降低至 0.5 eV 以下和器件性能提升至 19%。但是聚合物合成的不可控性，导致材料批次性差异大，大批量生产制备困难。

近年来，我们一直致力于开发分子量精准可控的小分子光伏材料，提出的高结晶性和高相容性分子设计策略缓解了小分子电荷输运和激子扩散长度相互制约，提出的热聚集敏感性低的致密性材料设计策略将全小分子非辐射能量损失降低至 0.2 eV 以下器件性能提升至 17%以上。基于小分子的电荷输运过于依赖材料的有序堆积，导致形貌难以调控，因此我们结合小分子结构精准可控和聚合物存在链内输运优势发展了新型共轭结构的大尺寸二聚体寡聚物，结合相应的小分子和聚合物，探讨了新型大尺寸寡聚型受体材料在激子性质、电荷性质、氯仿溶剂加工和非卤溶剂加工、能量损失、低能量损失下电荷产生效率，以及稳定性等关键性能和参数的独特优势.

Keyword: 精准可控，形貌调控，分子设计，有机太阳能电池，器件性能

最终交流类型: Invited

Role of ferroptosis in metabolic associated fatty liver disease induced by SiNPs and the intervention effect of melatonin

段军超
首都医科大学

The large-scale production, widespread application, and potential environmental release of silica nanoparticles (SiNPs) have led to increased exposure opportunities for the population and increased cumulative risk in organisms. SiNPs can cause hepatotoxicity and disorders of liver lipid metabolism, but the underlying mechanism has not been fully elucidated. In this study, C57BL/6J mice and L-02 cells were used to illustrate the effects of

SiNPs on liver function and hepatotoxicity, explore the molecular mechanism of metabolic associated fatty liver disease (MAFLD) induced by SiNPs via ferroptosis signal pathway, and evaluate the effect of melatonin antioxidant action on SiNPs-induced liver lipid metabolism disorder. The results showed that SiNPs caused liver damage and lipid accumulation. L-02 cell activity decreased, mitochondria and intracellular Fe2+ accumulated, and lipid peroxidation repair ability was impaired. Melatonin can alleviate the tissue/cell damage and antioxidant capacity decline caused by SiNPs. In addition, the rate-limiting enzyme ACSL4 knockout of polyunsaturated fatty acid synthesis reduced the level of intracellular Fe2+, moderated lipid peroxidation, and finally weakened ferroptosis caused by SiNPs. Our data indicated that SiNPs induced ferroptosis through ACSL4, leading to MAFLD. Melatonin acted as an antioxidant and provided repair for oxidative damage to cells.

Keyword: Silica nanoparticles, Ferroptosis, ACSL4, Hepatotoxicity, Metabolic associated fatty liver disease

最终交流类型: Invited

Nanopore and DNA nanotechnology based single-molecule sensing

陈凯凯
中国科学院大学

Nanopore technology has emerged as an attractive label-free method for single-molecule detection and sequencing. Its applications extend beyond DNA sequencing, as nanopore sensors have proven effective in detecting various biomolecules. The detection is achieved by monitoring the ionic current through the nanopore during the translocation of molecules which partially blocks the nanopore. Acquiring an accurate understanding of the translocation dynamics is an essential step in the quantitative analysis of polymer structure, we use synthetic nanopores and nanostructured DNA molecules to directly measure the dynamics of driven polymer transport through a nanopore. We show that the combination of nanopore technology with DNA nanotechnology allows for specific, multiplexed detection of DNA, RNA, and protein molecules. This feature is advantageous for applications such as diagnostic testing, as it allows for the detection of multiple targets in a single assay. Furthermore, nanopore sensing exhibits the capability to detect molecules at low concentrations, enabling sensitive and direct detection. In addition to its diagnostic potential, we also demonstrate that

nanopore is promising in the field of DNA data storage. By encoding digital data in DNA carriers attached with DNA nanostructures, and subsequently reading and decoding the data using nanopores, single-molecule sensing with nanopores can be employed for next-generation DNA storage.

Keyword: Nanopore, DNA nanotechnology, single-molecule method, biophysics, transport

最终交流类型: Oral

Multivalent Engineering of Exosomes with Activatable Aptamer Probes for Specific Regulation and Monitoring of Cell Targeting

刘文静
Beijing Tuberculosis and Thoracic Tumor Research Institute, and Beijing Chest Hospital, Capital Medical University.

Reconstituting and probing exosome-cell interactions is critical for elucidating exosome-related cell biology and advancing their diagnostic and therapeutic potential. We report here an exosomal engineering strategy to achieve controlled regulation of exosome-cell interactions with activatable sensing capability. The approach relies on membrane-protein directed, programmable DNA self-assembly to construct a DNA polymeric scaffffold with multivalent display of structure-switchable aptamer sensing probes on exosome surfaces. The engineered exosomes exhibit enhanced cancer cell targeting ability compared to exosomes modified with monovalent aptamers. Furthermore, the anchored aptamer probes could be activated by specifific membrane protein targeting, followed by structural switching to report an output flfluorescence signal, thus allowing dynamic monitoring of exosome-cell interactions both in vitro and in vivo. We envision this will provide a complementary tool for specifific regulation and monitoring of exosome-cell docking interactions and will advance the development of exosome-based biomedical applications.

Keyword: exosome, multivalent, activatable Aptamer, structure-switchable

最终交流类型: Oral

In vivo therapeutic effects of small molecule-drug conjugates enhanced by Fc grafting

台万一
武汉大学

Small molecule-drug conjugate (SMDC) shows great potential as a new class of targeted chemotherapeutic agents to tackle cancer. However, its in vivo therapeutic effect is compromised by its poor pharmacokinetic parameters. Herein we describe an approach that enables the precise conjugation of SMDC on N-terminus of the Fc protein to produce a SMDC-Fc bioconjugate (Fc1070) with superior specificity, affinity and potency to tumor cells. In vivo, Fc1070 exhibited an antibody-like pharmacokinetic profile with a long circulation half-life (t1/2 = 79 h) and pro-liver clearance pathway, that is distinct from the parent SMDC (t1/2 = 0.5 h and renal clearance). Intravenous injection of Fc1070 can eliminate the tumor with a single dosing of 7 mg/kg. Coupled with a predefined ligand toolbox, this approach allows the fast generation of other SMDC bioconjugates on demand, thus extending the format easily to other tumor targets. This may provide a general approach for the development of SMDC with enhanced therapeutic properties

Keyword: Drug conjugates; MMAF; Small molecular ligand; Blood circulation; Fc protein

最终交流类型: Invited

Specific Interactions Based Drug Loading Strategies

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Drug carriers have been commonly used for drug control release, enhancing drug efficacy and/or minimizing side-effects. However, it is still difficult to get high loading efficiency when encapsulating super hydrophilic drugs with narrow therapeutic index, such as many neurotoxins. Increasing the carrier proportion can improve drug loading in a certain degree, while the burst released drug when the formulation enters the body may cause overdose side-effects. Moreover, high-dose carriers themselves may increase the metabolic burden of the body. Hence, new drug carriers and/or loading strategies are urgently needed to promote the applications of these drugs. This topic will introduce drug loading strategies

based on specific interactions (between drugs and carriers) and will discuss the challenges and perspectives of these strategies. This work is expected to provide alternative inspirations for the delivery of hydrophilic drugs.

Keyword: Specific interaction, drug loading, super hydrophilic drugs, Bioinspired design

最终交流类型: Invited

Application-oriented SERS Detection Chips: Design, Manufacturing, and Functionalization

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The molecular detection technology based on surface-enhanced Raman scattering (SERS) using noble metals has significant advantages such as high sensitivity, rapid response, and fingerprint recognition. However, despite more than 50 years of research on SERS and the miniaturization, integration, and intelligence of Raman spectroscopy instruments, there are very few practical applications of rapid detection based on the SERS effect. Although the reasons are complex and comprehensive, the lack of noble metal SERS substrates with characteristics such as super sensitivity, high stability, and specificity is an important factor. In order to achieve on-site rapid SERS detection, we have carried out innovative design and mass production of gold and silver noble metal nanostructures, and functionalized the substrate surface specifically to adapt to complex on-site environments, thereby achieving high selectivity detection of various target molecules in complex matrices.

Keyword: SERS, surface-enhanced Raman scattering, noble metal SERS substrate, rapid on-site detection

最终交流类型: Invited

Polymeric nanocarriers for tumor precision diagnosis and targeted therapy

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Tumor is a top risk to public health. However, less effectiveness has been achieved by conventional anticancer drugs, thus, developing novel strategies to deal with cancer is

important. Polymeric nanocarriers have demonstrated high potential for delivery bioactive compounds to tumors with improved therapeutic outcomes. Base on the specific pathological features in tumor microenvironment, we have developed series of stimuli-responsive polymeric nanocarriers for tumor-aimed drug delivery. At one hand, we have synthesized tumor hypoxia and pH-responsive nanocarriers, which could diagnosis ultrasmall tumors at early stage, and detect primary and metastatic tumors in different tumor models by magnetic resonance imaging. It could further predict the responses to radiotherapy and immunotherapy by imaging the hypoxia levels in tumors, and improve the immunotherapeutic outcomes by normalizing tumor microenvironment. On another hand, we have synthesized stimuli-sensitive nanocarriers, which could delivery drugs for treating breast tumors, melanoma and esophageal tumors by stimulating antitumor immune responses, to further prevent distant and metastatic tumor development. In all, polymeric nanocarriers could alert the tumor targeting performance, diagnosis and inhibiting tumors with improved therapeutic outcomes and survival rates.

Keyword: Polymeric nanocarriers; Tumor; Diagnosis; Therapy; Immunotherapy

最终交流类型: Oral

Molecular carbon nanomaterials: From cellular redox regulation to next generation therapy

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Extracellular environment is an important part of cell microenvironment. The abnormality of redox in extracellular environment is closely related to the occurrence and development of tumor and other major diseases. Therefore, the regulation of redox homeostasis in the extracellular environment has important research significance and application value for the treatment of major diseases. However, the regulation of extracellular environment still faces many challenges. For example, the components of extracellular environment are complex, and the effect of regulating a single component cannot meet the needs of efficient treatment of diseases. Based on this, we propose a redox regulation strategy in extracellular environment for major disease therapy. By utilizing the properties of fullerene nanomaterials in regulating biological redox, we have developed a variety of therapeutic strategies for tumor and metabolic diseases by using fullerene nanomaterials to regulate the

redox in extracellular environment, revealing its regulatory mechanism, and realizing safe and efficient therapy for tumor and metabolic diseases.

Keyword: carbon nanomaterials, redox homeostasis, extracellular environment, disease therapy

最终交流类型: Invited

CRISPR/Cas Powered Cancer Theranostics

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南京大学

Clustered regularly interspaced short palindromic repeats (CRISPR) and CRISPR-associated protein (Cas) system has been considered an outstanding ‘gene scissors’ that is efficiently utilized as a tool for gene editing across the biomedical landscape [1-3]. Herein, we present a conceptual approach for the design of orthogonally NIR-light activatable CRISPR-Cas13d nanoprodrug by introducing a green light-activatable Pt(IV) prodrug and UV light-activatable Cas13d gene editing tool into the orthogonal emissive core/multi-shell UCNPs [4]. The Pt(IV) prodrug was rational designed by covalent coupling of oxaliplatin-based Pt(IV) complex to the Rose Bengal (RB) photosensitizer. Such a design specifically triggers the activation of prodrugs under 980-nm light irradiation, thus rapidly releasing parent drugs through Pt-O bond cleavage and generating fluorescence imaging probes concurrently with reactive oxygen species, such as singlet oxygen. On the other hand, CRISPR/Cas13d gene editing system is constructed by assembling a RNA-guided Cas13d ribonuclease with a MRP1-targeted sgRNA, which is caged by a single-stranded oligonucleotide incorporating three photocleavable linkers. Under 808-nm light irradiation, the UV light emitted by UCNPs could break PC linkers and activate the CRISPR/Cas13d system to cleave intracellular MRP1 mRNA, leading to efficient downregulation of membrane MRP1 protein and thus drug resistance attenuation. To provide cancer-targeting delivery as well as improve the in vivo stability of the nanoprodrug, it was encapsulated into a cyclic RGD peptide moieties (cRGD)-functionalized phospholipid, termed as URL. We demonstrated that URL maintained excellent orthogonal emission behaviors under 808 and 980 nm excitations, allowing wavelength-selective photoactivation of oxaliplatin prodrug-induced chemo-photodynamic therapy and Cas13d-mediated gene editing. Moreover, in vivo studies demonstrated that such an orthogonally activatable nanoprodrug can promote the

activation of Pt(IV) prodrug and ROS generation and massively induce on-target drug accumulation with the help of Cas13d-mediated drug resistance attenuation, delivering an ultimate chemo-photodynamic therapeutic performance in efficiently eradicating primary tumors and preventing further liver metastasis.

Keyword: CRISPR-Cas13d, prodrugs, spatiotemporal control, multidrug resistance, chemo-photodynamic therapy

最终交流类型: Invited

Stabilization of terahertz dual-comb sources

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In the terahertz (THz) frequency range, the electrically pumped quantum cascade laser (QCL) offers the possibility of realizing a compact dual-comb source due to its semiconductor-based chip-scale configuration. Although dual-comb operation of THz QCLs has been experimentally demonstrated, a full stabilization of THz dual-comb sources is still challenging due to the extreme complexity of locking elements. In this work, two stabilization methods of THz QCL dual-comb source are presented. The first stabilization method is a relative phase locking by employing a phase-locked loop (PLL). In this method, only one dual-comb line is firmly locked. However, it is shown that the phase noise of other dual-comb lines is significantly reduced. The other method is a self-reference stabilization technique. Without using any external locking components, one dual-comb line is filtered out and it is beaten with the whole dual-comb signal, which eliminates the common carrier offset frequency noise and reduces the dual-comb repetition frequency noise. It is experimentally demonstrated that the self-reference technique can significantly improve the long-term stability of the dual-comb signal. A record “maxhold” linewidth of 14.8 kHz (60 s) is obtained by implementing the self-reference technique, while without the self-reference, the dual-comb lines show a “maxhold” linewidth of 2 or 3 MHz. The method provides the simplest way to improve the long-term stability of THz QCL dual-comb sources, which can be further adopted for spectroscopic measurements.

Keyword: Terahertz, quantum cascade laser, frequency comb, dual-comb

最终交流类型: Invited

Research on stable and safe perovskite solar cells

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Because of their unique properties, the PCE of PSCs has risen considerably over the last decade, from 3.8% to 26%. The key factors restricting its commercialization have gradually shifted from the pure pursuit of efficiency to the long-term operational stability of the devices and the problem of lead leakage. This report presents some previous interfacial modifications to improve the PCE and stabilities. Then, various effective lead chemical adsorptions were shown.

Keyword: perovskite;solar cell; stability; lead leakage

最终交流类型: Invited

Hybrid Plasmonic Effect Enhanced Light Detection Based on Low Dimensional Materials

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The plasmon resonance effects are found in metals, metal oxides and emerging two-dimensional materials etc. Such effects have been used in many types of micro devices, including light emitting devices, photodetectors, solar cells, lasers and so on. Hybridization of plasmonic nanostructures with photodetection materials is a topic of broad and increasing interest particularly owing to the broadening of the detection spectral range beyond the materials' bandgap, which can potentially overcome some of the intrinsic limitation that conventional photodetection devices face. Moreover, the emerging plasmonic materials has offered an attractive platform to tune the fundamental principles of electronic and optoelectronic properties, with the ultimate goal to realize high performance optoelectronic devices like photodetectors. In this talk, I will introduce our recent progress on the synthesis of novel plasmonic materials and their potential application for efficient photodetection. We will show that by carefully combing the proper materials, the hybrids can show unexpected properties far surpass that of a single material, especially, the high photodetection performance covering a broad wavelength range paves the way for future applications in remote sensing, biological imaging and environmental monitoring and so on.

Keyword: Plasmon resonance, photodetection, broad wavelength range, low dimensional materials

最终交流类型: Invited

Holographically activated biopolymer nanoprobe for high-contrast tumor MR imaging

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Applying contrast agents (CAs) to increase signals in tumors specifically is considered an extensively applied approach among clinically relevant diagnostic modalities such as magnetic resonance imaging (MRI). Smartly improving tumor contrast has been widely explored to visualize tumors from surrounding healthy tissues through stimuli-responsive probes, enabling enhanced sensitivity and accuracy in response to subtle physiopathologic alterations such as tumor acidity, hypoxia, glutathione (GSH), and enzymes. However, many intracellular physiopathologic alterations (e.g. 1-10 mM GSH or lysosomal pH) only occur within subcellular organelles, whereas it is difficult to activate probe retained in GSH- or acidity-deficient tumor stroma, and undesired distribution of probes in normal tissues might compromise their tumor contrasts. A major challenge remains in robustly activating CAs for holographic imaging in the whole tumor, together with suppressed background noise.

In recent years, our group from the College of Pharmaceutical Science, Soochow University focused on the construction of multi-modal imaging probes for cancer diagnosis (Adv Mater, 2015, 27, 3874-3882; Adv Mater, 2015, 27, 5049-5056; Adv Mater, 2016, 28, 5923-5930; ACS Nano, 2017, 11, 1848-1857; Theranostics, 2017, 7, 764-774; Biomaterials, 2018, 154, 248-260; Small, 2018, 14, 1802905; J Control Release, 2021, 329, 997-1022; J Control Release, 2022, 350, 761-776). Based on the previous research, this team further cooperates with Dr. Zhen Jiang’s group in the Second Affiliated Hospital of Soochow University to develop a holographically activatable nanoprobe caging manganese tetraoxide for tumor-selective contrast enhancement in magnetic resonance imaging (MRI) through cooperative GSH/albumin-mediated cascade signal amplification in tumor and rapid elimination in normal tissues, thus achieving precise tumor malignancy detection, surveillance and surgical guidance (Figure 1).

Keyword: Biomedical polymers, Biological supramolecular carriers, Carriers and controlled release materials, Responsive carrier materials

最终交流类型: Invited

Degradation mechanism and stability improvement strategy of perovskite photovoltaic cells

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Ion dissociation has been identified to determine the intrinsic stability of perovskite solar cells (PVSCs), but the underlying degradation mechanism is still elusive. Herein, by combining highly sensitive sub-bandgap external quantum efficiency (s-EQE) spectroscopy, impedance analysis, and theoretical calculations, the evolution of defect states in PVSCs during the degradation can be monitored. It is found that the degradation of PVSCs can be divided into three steps: 1) dissociation of ions from perovskite lattices, 2) migration of dissociated ions, and 3) consumption of I− by reacting with metal electrode. Importantly, step (3) is found to be crucial as it will accelerate the first two steps and lead to continuous degradation. By replacing the metal with more chemically robust indium tin oxide (ITO), it is found that the dissociated ions under light soaking will only saturate at the perovskite/ITO interface. Importantly, the dissociated ions will subsequently restore to the corresponding vacancies under dark condition to heal the perovskite and photovoltaic performance. Such shuttling of mobile ions without consumption in the ITO-contact PVSCs results in harvesting–rest–recovery cycles in natural day/night operation. It is envisioned that the mechanism of the intrinsic perovskite material degradation reported here will lead to clearer research directions toward highly stable PVSCs.

Keyword: Perovskite solar cells, Sub-bandgap EQE, Ion migration, Ion consumption, Stability

最终交流类型: Oral

Single small extracellular vesicle physical measurement for non-invasive tumor diagnosis

朱凌
国家纳米科学中心

Extracellular vesicles are cell-derived membranous vesicles that transfer molecular information for intercellular communication. They participate in tumor progression and metastasis and are diagnostic markers for tumors. The analysis of molecular information and physicochemical properties of extracellular vesicles helps to elucidate the mechanism of tumor development, providing essential information for the in vitro diagnosis of tumors. Extracellular vesicles are highly heterogeneous. Different subtypes of extracellular vesicles show different diagnostic values. Single-vesicle characterization helps to study the heterogeneity of extracellular vesicles, which is conducive to the development of accurate diagnosis of tumors. However, the nanoscale size of extracellular vesicles makes single-vesicle characterization challenging. Here, we utilize atomic force microscopy (AFM) and near-field infrared (nano-FTIR) spectroscopy to study the physical properties and protein secondary structures of single extracellular vesicles for the in vitro diagnosis of tumors. We develop a model based on nano-indentation on AFM to analyze the mechanical properties of single vesicles and prove that the stiffness, bending modulus, and osmotic pressure of extracellular vesicles are related to tumor malignancy. We investigate protein fingerprint spectra of single extracellular vesicles in nano-FTIR and demonstrate that the proportion of protein secondary structures in extracellular vesicles are related to tumor malignancy. We further demonstrate that extracellular vesicles' mechanical properties and protein secondary structures can sensitively detect tumors and evaluate tumor metastasis in breast cancer patients. These studies provide techniques and information for understanding cancer development at the single-vesicle level. They also provide a solution for in vitro accurate diagnosis of tumors.

Keyword: small extracellular vesicle, atomic force microscopy, nano-FTIR, tumor diagnosis

最终交流类型: Invited

Design, Synthesis and Properties of Small Molecule Photovoltaic Materials

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Taizhou University

To solve the problem of phase separation in organic solar cells, series of small molecule photovoltaic materials were designed and synthesized, including small molecule donors, small molecule acceptors and small molecule additives, which were applied to organic solar cell to significantly optimize the phase separation morphology, so as to achieve the purpose of efficiency improving. Design and synthesize liquid-crystal small molecule donors such as BTR, BTR-Cl, L2, and gradually regulate the crystallinity of materials based on the molecular structure, to significantly improve the effciency of small molecule solar cell and set several records for the highest efficiency of the all small molecule solar cells ; Design and synthesize series of oligothiophene based small molecule donors, optimize the phase separation morphology based on halogenated elements and conjugate length, and finally prepare oligothiophene based all small molecule solar cells with an efficiency of 16% ; Design a series of volatile small molecule additives, significantly optimize the phase separation morphology and prepare a double-layer organic solar cell with an efficiency of 18.4% ; Design and synthesize several novel small molecule acceptors and increase the efficiency of single organic solar cell to 20%.

Keyword: organic solar cells; small molecule donors; small molecule acceptors; small molecule additives;

最终交流类型: Invited

Precision diagnosis and treatment of tumor guided by Near-infrared II fluorescence imaging

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Surgery and drug therapy are the preferred treatment options for most tumors. However, there are still clinical challenges that need to be addressed, such as the difficulty in early detection of hidden lesions and achieving on-demand drug administration. The key problems to be solved are how to achieve intraoperative tiny tumor detection with high specificity and sensitivity, and how to clarify the pharmacokinetic and pharmacodynamic characteristics of drugs to achieve accurate drug delivery. In this study, we focused on NIR-II fluorescence imaging and developed new strategies for nano-bio interface regulation, signal amplification, and fluorescence activation. We constructed a targeted quantum dot-peptide self-assembly probe system to effectively amplify the fluorescence signal of the detection target and achieve highly sensitive detection of tiny and hidden tumor metastases without vascularization. Additionally, we constructed activatable NIR-II probes with a selective

response to target molecules to achieve highly sensitive and specific detection of tumor-related markers. Furthermore, we established a new visualization method for in vivo nanodrug tracking, drug release, and efficacy evaluation to guide the precision of tumor drug therapy. The research mentioned above provides a foundation for the accurate diagnosis and treatment of major clinical diseases and offers new ideas for future studies.

Keyword: Near-infrared II region, Tumor diagnosis and treatment, In vivo imaging

最终交流类型: Invited

Stability of Organic Solar Cells: Degradation Pathways of Materials and Devices

杜晓艳
山东大学

Organic photovoltaics (OPV) is a promising renewable energy source for a decentralized power supply. With significant advances in the development of novel materials in recent years, lab-cells with power conversion efficiencies (PCEs) > 19% have been achieved with several material systems in combination with non-fullerene acceptors (NFAs), which further enhances the potential for real applications. Stabilizing OPV is critical for commercialization of this technique. Identification of degradation mechanisms will contribute to reveal strategies through materials design and device engineering for highly efficient and stable OPVs. In this talk, intrinsic materials photo-stability, microstructure as well as interface related device stability for polymer solar cells based on NFAs will be discussed.[1-7] Considering strong processing-dependent device performance and photostability, evaluating the potential of organic photovoltaic materials and devices for industrial viability is a multi-dimensional large parameter space exploration. High-throughput experimentation offers huge opportunities for accelerating materials discovery and development for renewable energy. Recent results on integrating high-throughput methods in OPV research will be discussed.[8]

Keyword: Organic Photovoltaics, Non-fullerene acceptors, Stability, High-throughput

最终交流类型: Invited

高效有机光伏材料与叠层太阳能电池

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中国科学院化学研究所

在有机太阳能电池领域，非富勒烯受体材料逐渐取代了富勒烯衍生物成为有机光伏的热点，并大幅推动了有机太阳能电池光电转化效率的提升。一方面由于非富勒烯受体材料在可见及近红外区具有宽而强的吸收，同时器件表现出低的能量损失有利于实现高的开路电压和更充分的太阳光谱吸收，另一方面非富勒烯受体的光吸收特性和电子能级可以通过分子修饰轻易调节，可以充分利用和发挥有机材料具有的结构多样性, 为叠层电池光伏材料提供了更多的选择。在有机太阳能电池中，将具有互补吸收光谱的两个或更多个本体异质结电池堆叠形成串联叠层电池结构，可以有效地收获更宽范围的太阳光谱并且减少了较高光子能量的量子损失。这种电池结构已被广泛应用于传统无机太阳能电池，考虑到有机半导体窄吸收峰的独特特性，叠层电池会有更有效的提升。叠层电池通过隧穿结连接层串联连接的子电池组成，该中间层用作电子空穴/复合层，理想的串联光伏电池开路电压为各个子电池的开路电压的总和，而不会损失光生载流子与填充因子。相对于富勒烯衍生物类受体，新型 A-D-A 类受体具有可调的吸收光边带和前线轨道能级的优势，通过拓宽共轭和增强分子电荷转移，一系列具有近红外吸收的受体被设计和合成出来，表现出了非常优异的性能。

Keyword: 有机太阳能电池，近红外吸收，叠层太阳能电池

Nanoprobe in MicroRNA Analysis

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Accurate imaging of molecular in cells and living bodies is a hotspot in the field of biomedicine, and it is a significant tool to obtain biochemical information directly. Using cells and living bodies as models, we design highly efficient imaging nanoprobes to develop new principles, methods and tools for in situ accurate imaging of nucleic acids. Owing to the excellent physicochemical properties, nanoparticles (NPs) have great prospects in biosensors and precision medicine. By combining the nanotechnology and nucleic acids isothermal amplification technique, we have developed a series of methodologies for miRNA imaging in

vitro and in vivo. For example, a specific target miRNA-triggered chain displacement signal amplification system was constructed by rationally designing the initiation position of chain displacement. A sensitive intracellular enzyme-free signal amplification system was developed for miRNA detection via designing chain displacement driving mode. By rationally designing the chain displacement reaction space, the improved reaction speed of intracellular signal amplification was realized.

For example, we describe a multiplexed error-robust combinatorial fluorescent label-encoding method, termed fluorophores encoded error-corrected labels (FluoELs), enabling multiplexed miRNA imaging in living cells with error-correcting capability. The FluoELs comprise proportional dual fluorophores for encoding and a constant quantitative single fluorophore for error-corrected quantification. Both are embedded in 260 nm core–shell silica nanoparticles modified with molecular beacon detection probes. The FluoELs are low cytotoxic and could accurately quantify and spatially resolve nine breast-cancer-related miRNAs and evaluate their coordination. The FluoELs enabled a single-cell analysis platform to evaluate miRNA expression profiles and the molecular mechanisms underlying miRNA associated diseases.

Keyword: Nanoprobe，miRNA Biosensor，Theranostic platform

最终交流类型: Invited

Size controllable single-crystalline Ni-rich cathodes for high-energy lithium-ion batteries

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Single-crystalline Ni-rich (SCNR) cathode with a large particle size can achieve a high energy density and safety over the polycrystalline counterparts. However, synthesis of large SCNR cathodes (>5μm) without compromising electrochemical performance is very challenging due to incompatibility between Ni-rich cathodes and high temperature calcination. Herein, we introduce Vegard’s Slope as a guidance to rationally select sintering aids, and successfully achieved size-controlled SCNR cathodes, the largest of which can be up to 10 μm. Comprehensive theoretical calculation and experimental characterization show that sintering aids continuously migrate to the particle surface, suppress sublattice oxygen release and reduce the typical exposed facets energy, which promote grain boundary migration and

elevate calcination critical temperature. The dense SCNR cathodes fabricated by packing of different size SCNR achieve the highest electrode press density of 3.9 g cm^{-3} and a highest volumetric energy density of 3000 Wh L-1. The pouch full cell demonstrates a high energy density of 303 Wh kg^{-1}, 730 Wh L^{-1} and 76% capacity retention after 1200 cycles. SCNR cathodes with an optimized particle size distribution can meet the requirements for both the EVs and portable devices. Furthermore, the principle for controlling the growth of SCNR particles can be widely applied to synthesize other materials for Li-ion, Na-ion and K-ion batteries.

Keyword: Lithium-ion batteries；Ni-rich cathodes； Single-crystalline

最终交流类型: Invited

Organic Neurmorphic Materials and Devices

马伟
西安交通大学

By integrating sensing, memory and processing functionalities, biological nervous systems are energy and area efficient [1]. Emulating such capabilities in artificial systems is, however, challenging and is limited by the device heterogeneity of sensing and processing cores. Here, we present a universal solution to simultaneously perform multi-modal sensing, memory and processing using organic electrochemical transistors. The device has a vertical traverse architecture and a crystalline–amorphous channel that can be selectively doped by ions to enable two reconfigurable modes: volatile receptor and non-volatile synapse. As a volatile receptor, the device responses to multiple stimulus such as ions and light, and as a non-volatile synapse, it is capable of 10-bit analogue states, low switching stochasticity and ＞10^4 s state retention. Homogeneous integration of such devices enables functions such as conditioned reflex and real-time cardiac disease diagnose via reservoir computing, illustrating the promise for future edge AI hardware.

Keyword: Organic Materials, OECTs, X-ray Scattering

最终交流类型: Invited

Photophysics of Molecular Aggregates: Computational Methods and Applications

任佳骏
北京师范大学

The photophysical processes of molecular aggregates have been widely investigated in both molecular materials and biological systems, including relaxation of excited state radiatively and non-radiatively, energy transfer, etc. Excited-state electronic processes are influenced mainly by two factors: electronic coupling and electron-vibration coupling, leading to a quantum many-body problem that is notoriously challenging to accurately simulate. In this presentation, I will discuss our recent developments in time-dependent density matrix renormalization group (TD-DMRG) methods for solving electron-vibration coupling models related to molecular aggregates. Through various illustrative examples, I will demonstrate that TD-DMRG is a numerically exact, scalable, and robust method. Furthermore, I will present our recent research on excitonic coupling effects in non-radiative processes of molecular aggregates. Our findings reveal that with an increase in excitonic coupling, the effective strength of electron-vibration coupling decreases, resulting in the suppression of non-radiative decay processes. This violates the widely known energy gap law, that the non-radiative decay rates increase as the energy gap reduces. However, with further increase in excitonic coupling, the factor related to energy gap reduction dominates again, and the behavior conforms to the conventional energy gap law. This non-monotonic behavior is robust in both dimeric and one- and two-dimensional stacked molecular aggregates. Additionally, the extent of this reduction in non-radiative decay rates is influenced by factors including aggregate size, dimensionality, and temperature. We find that the excitonic coupling that minimizes non-radiative decay rates typically occurs at around half of the reorganization energy.

Keyword: molecular aggregates, photophysics, DMRG, nonradiative decay

最终交流类型: Invited

Freestanding low-dimensional single-crystalline semiconductors

蒋杰
浙江大学

Low-dimensional single-crystalline semiconductors have unique physical properties that are different from bulk materials due to the confined electronic state wave function in at least one dimension and the exigent surface effect. The freestanding form of these materials brings new science and technology due to their flexibility, light weight and easy integration. The speaker is committed to develop new defect-controlled fabrication technology and physical property tuning methods of freestanding low-dimensional single-crystalline semiconductors, explore new physical phenomena, and study new mechanisms. The speaker has made some achievements: observing giant pyroelectricity in nanomembranes and revealing dimensionality effect of phonon dynamics; fabricating defect-controlled halide perovskite epitaxial film via remote heteroepitaxy and revealing its dislocation-carrier dynamics relationship; inventing a phase change material-based new strategy to generate controllable strain gradient, achieving flexo-photovoltaic effect and room-temperature electrically switchable spin states in two-dimensional semiconductors, and revealing strain gradient/electrical field-transport/band structure relationship. These achievements could stimulate fundamental study in freestanding nanomembranes and inspire technological development for flexible optoelectronic applications in sensing and energy harvesting.

Keyword: low-dimansional semiconductor; freestanding nanomenbrane; epitaxy; pyroelectricity; optoelectronics

最终交流类型: Invited

On-surface chemistry of spatial molecules on metal surfaces

高洪营
天津大学

The on-surface chemistry is an interdisciplinary frontier area between physics and chemistry, which has attracted a wide academic interest and been highly active in recent years. The on-surface chemistry of spatial molecules have also been intensively studied,

which are generally more difficult than the flat aromatic systems in the characterization by STM, nc-AFM and XPS techniques. Herein, I would like to introduce three experimental works: 1, The planarization of Pt-complexes; 2, The on-surface chemistry of spatial diamantane molecules to build up covalent diamantane chains; 3, The host-guest chemistry of spatial 18-crown-6-ether molecule.

Keyword: On-surface chemistry, Spatial molecule, Host-guest chemistry.

最终交流类型: Invited

High-Precision Design and Processing of Thick Electrode

田瑞源
吉林大学

Li ion battery has been widely used in various key areas of national economy as one of the most developed energy storage technologies. However, it can’t meet the demands for future applications in electrical vehicles and large-scale energy storage energy, which is limited by the theoretical specific capacity of materials. To drastically increase areal capacity and thus energy density, we focus on high-precision design and processing of thick electrodes by quantifying the factors limiting the performance. We developed and built physical models and equations to quantitively study the effects of physical properties of composited films on the charge transport and rate performance of batteries. With the above achievements, the physical properties of thick electrodes are precisely controlled, obtaining high energy and power density batteries.

Keyword: Thick electrode；Physical modeling；Limiting factors；Rate performance；High energy/power density；

最终交流类型: Invited

Multiscale simulations of organic phosphorescent materials

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Phosphorescence generally refers to the radiative transition of triplet excitons, commonly found in metal complexes containing heavy atoms. Due to its high exciton utilization efficiency and long lifetime, phosphorescence is highly favored in optoelectronic devices and bioelectronics. In contrast, organic molecules have weak spin-orbit coupling, making it difficult to generate triplet excitons, and these excitons are easily quenched by oxygen, temperature, and moisture, making it generally impossible to observe room-temperature phosphorescence (RTP) in organic molecules. Recently, RTP has been discovered in some molecular aggregates, challenging the traditional understanding. However, the mechanism underlying the connection between molecular aggregates and phosphorescence performance remains unclear. To address this issue, we employed theoretical computational chemistry methods to elucidate the intrinsic correlation between molecular configuration, aggregation morphology, and excited-state dynamics at the molecular and electronic scale. We identified the key parameters affecting phosphorescence properties, established a theoretical model dominated by the excitation state components ($n\pi^*$, $\pi\pi^*$) governing phosphorescence performance, and developed molecular descriptors (γ, β) to characterize phosphorescence efficiency and lifetime. Furthermore, we proposed a theoretical mechanism to suppress electron-vibration coupling and enhance phosphorescence performance. Based on theoretical research and experimental collaboration, we designed ionic phosphorescent materials, overcoming the challenge of balancing high efficiency and long lifetime.[1-6]

Keyword: organic phosphorescence, excited-state dynamics, multiscale simulations

最终交流类型: Invited

Chemical Biology Tools for Achieving Precise Spatiotemporal Regulation and Sensing at the Cellular Interface

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Biomolecules that are expressed on the plasma membrane of cells play a critical role in cellular behavior and communication. These molecules interact with each other and with compartments in the local microenvironment to regulate important biological functions such as signal transduction, metabolic processes, cancer metastasis, and autoimmune response. Therefore, the ability to synthetically engineer the cell membrane with diverse functional molecules provides a promising strategy to better understand and control a variety of biological processes. Many different functional moieties, including synthetic protein complexes, nucleic acids, polymers, and inorganic materials, have been incorporated to impart specific functions on the cell membrane. These materials have enabled a broad range of applications, such as drug delivery, intracellular sensing, cell-based therapeutics, and tissue engineering. However, most efforts to apply artificial functions to cells are limited to the external surface due to the lack of synthetic tools to engineer the intracellular side, which hinders many biosensing and biomedical applications. Inspired by the natural extracellular vesicle fusion process, we have developed a fusogenic liposomal construct (FLip) to achieve robust functionalization on both the external and internal cell leaflets via a liposome fusion-based transport (LiFT) strategy [1]. This approach can engineer cell membranes in a spatially controlled manner, allowing for the creation of anisotropic membrane structures with two bioorthogonal functionalities, enabling applications such as programmed signaling pathways, detection of intracellular metabolites, and bioorthogonal catalysis [2]. Our work is an initial proof-of-concept study that lays the foundation for engineering both sides of the cell membrane with high spatial control, significantly expanding the capabilities to study, mimic, and manipulate the biochemical functions on the plasma membrane, particularly the interior surface. Importantly, the LiFT strategy we report is facile and generalizable, providing a potentially straightforward route to incorporate diverse functionalities onto the cell membrane by incorporating corresponding fusogenic vesicles.

Keyword: Cell membrane engineering, inner leaflet modification, functional DNA sensor, spatiotemporal control, biosensing and bioregulation

最终交流类型: Invited

Nano-functionalization of Polymer Sponges and Their Applications

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Polymer sponges, known for their unique porous structure and excellent mechanical properties, have found extensive applications across various fields and have become essential in our daily lives. By combining sponges with emerging nanomaterials featuring innovative functionalities and enhanced performance, the potential for further expanding the application scope and increasing the value of polymer sponges is highly promising. This report focuses

on the fabrication of nano-functionalized sponges and explores their potential applications. Addressing key scientific challenges such as regulating electronic transport networks and achieving efficient separation of multiphase fluids, we have successfully developed a series of high-performance nano-functionalized sponges tailored for applications in flexible electronics and oil-water separation. These achievements not only offer novel solutions for flexible electronics and oil-water separation challenges but also provide crucial theoretical and technical support for innovatively designing and preparing materials based on sponges.

Keyword: sponges, nano-assembly, flexible electronics, oil-water separation

最终交流类型: Invited

储钾负极材料与原位透射电镜解析

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发展高能量密度、高功率密度和长循环寿命二次电池是当前国内外前沿研究热点，也是能源电化学材料研究的核心。先进电极材料开发是实现高比能二次电池的关键前提，这迫切需要对现有电极材料进行优化并探索新型高性能电极材料，同时借助清晰、精确的先进实验表征手段对新机理、新材料和新设计进行深入探讨，以形成系统的科学认识；特别是采用先进原位表征手段精准解析电极材料在工况下的动态演化行为与劣化失效机制，从而在更深层次上理解电池中各类构效关系和电化学反应机制，为电极材料和化学电源的设计与优化提供科学依据。

本报告将重点针对储钾关键负极材料在工况下的微观结构动态演化与宏观电化学性能间的构效机制这一关键科学问题，以原位显微与谱学表征为研究手段，结合理论模拟，深入解析关键电极材料在工况下化学、物理特性的动态演化机制，阐明材料微观结构与宏观电化学性能间的构效关系，进而“自下而上”地指导多种高性能复合负极材料的构筑，以期为解决目前钾离子电池中存在的瓶颈问题提供新的研究思路

Keyword: 储钾负极；原位透射电镜；钾离子电池材料；反应机理

最终交流类型: Invited

Radiofrequency-Activated Pyroptosis of Gold Nanocluster for Cancer Immunotherapy

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Pyroptosis is gasdermin-mediated programmed necrosis that exhibits promising potential application in cancer immunotherapy, and the main challenge lies in how to provoke specific pyroptosis of tumor cells. Here, radio-frequency (RF) responsive biGC@PNA with a precisely stoichiometric ratio of Au (I) ion and Au(0) atom is reported to elicit caspase 3/GSDME-N mediated pyroptosis of tumor cells by its RF-heating effect. In vitro/in vivo assay on 4T1 tumor cells indicates RF-activated pyroptosis of tumor cells elicits robust ICD effect, enhancing the synergistic antitumor efficacy of biGC@PNA with decitabine, significantly suppressing tumor metastasis and relapse by provoking systemic antitumor immune responses. Utilizing RF-activated pyroptotic immune responses, biGC@PNA efficiently enhances the antitumor efficacy of αPD-1 immunotherapy under RF irradiation and provides a promising strategy for improving cancer immunotherapy by the non-invasive RF field with highly clinical transformation potential.

Keyword: Pyroptosis; Radiofrequency; immune response