Catalytic Enantioselective Photoredox Reaction of Carbonyl Compounds

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Visible-light induced radical reaction has been regarded as advantageous and attractive approach for the development of efficient and selective synthetic methodology. To develop efficient enantioseletive photoredox catalysis, organocatalyst or chiral Lewis acid catalyst has been used as a cooperative catalyst with photosensitizer. We have studied COBI (chiral oxazaborolidinium ion) catalyzed visible-light photoredox radical reaction with aldehydes and ketones. Compared to the previous results affording 1,4-addition products, the reaction between α,β-unsaturated aldehyde and α-silyl amine in the presence of COBI catalyst provided 1,2-addition products in good to excellent yields and with high enantioselectivities. We discerned that this photocatalysis could also be applied to the ketone substrate to give chiral 1,2-amino tertiary alcohols. We also demonstrated the first case of a chiral Lewis acid-assisted ternary EDA complex initiating an enantioselective photoredox reaction of α-aminoalkyl radicals to α, β-unsaturated aldehydes and ketones. The chiral Lewis acid-assisted ternary EDA complex provided 1,2-addition and 1,4-addition products with high yields and enantioselectivities.

Recently, a visible-light-driven catalytic tandem Giese addition/homolytic aromatic substitution (HAS) reaction was developed. Using COBI catalyst and a photosensitizer, α-aminoalkyl radicals reacted with α,β-unsaturated carbonyl compounds to afford tetrahydroquinolines (THQ)s with two stereocenters in a single step. This method provides high yields (up to 97%) and excellent enantioselectivities (up to 99% ee, single diastereomer) under mild conditions.

Keywords: enantioseletive, photoredox, cooperative catalyst, oxazaborolidinium ion, α-aminoalkyl radical,

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Asymmetric Synthesis via Bioinspired Peptide-Phosphonium Salt Catalysis

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The Wang Group focuses on the rational design of bioinspired P(V)-based chiral organocatalysts and ligands to enable novel synthetic methodologies, elucidate reaction mechanisms, and construct bioactive molecular architectures. In this presentation, we will highlight our recent advances in developing enzyme-inspired peptide-phosphonium salt (PPS) catalysts—a class of multifunctional asymmetric promoters that synergistically integrate peptide chirality with phosphonium activation. Key applications of these PPS catalysts will be demonstrated through the enantioselective synthesis of pharmaceutically relevant heterocycles, including stereochemically complex frameworks inaccessible via conventional approaches (Fig. 1)[1]. Furthermore, mechanistic insights derived from experimental studies and computational modeling will be discussed to rationalize the observed stereocontrol and catalyst-substrate interactions.

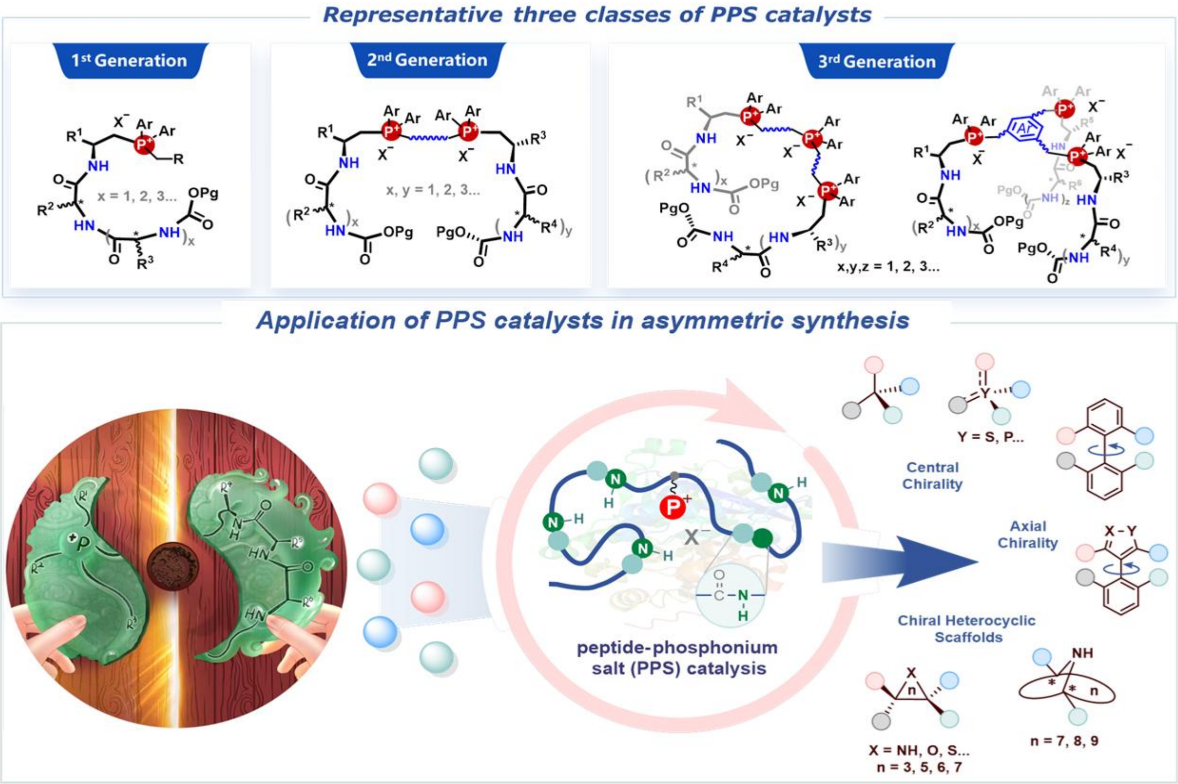

Fig 1. PPS catalysts and their applications.

Keywords: bioinspired PPS catalysis, organic synthesis, weak-bond synergy, reaction mechanism, bioactive molecules

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Catalytic Construction of Terpenoids from Isoprene

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Terpenoids are a class of natural products that widely exist in organisms and have isoprene units, accounting for about 60% of the known natural products. In biosynthesis, most of these thousands of terpenoids are derived from two C5 synthetic building blocks: dimethylallyl pyrophosphate (DMAPP) and isopentenyl pyrophosphate (IPP). Inspired by the biosynthesis of terpenoids, we carried out the precise divergent catalytic conversion of isoprene to construct natural or unnatural terpenoids.[1] This strategy has the following difficulties: 1) isoprene is not activated, and its reactivity is relatively low; 2) isoprene has four reaction sites, taking the coupling of arene and isoprene as an example, there are six possible addition methods. Further isomerization of the double bond will yield up to 14 regioisomers 3) In addition, hydroarylation of linear or cyclic dimer from isoprene could produce theoretically more than 150 isomers. Given these challenges on the chemo-, regio-, and stereoselectivity control in the catalytic conversion of isoprene, we developed a variety of regulatory strategies to address those issues based on the principle of transition metal catalysis: 1) Mechanism regulation; 2) Metal regulation; 3) Ligand regulation; 4) Additive regulation.

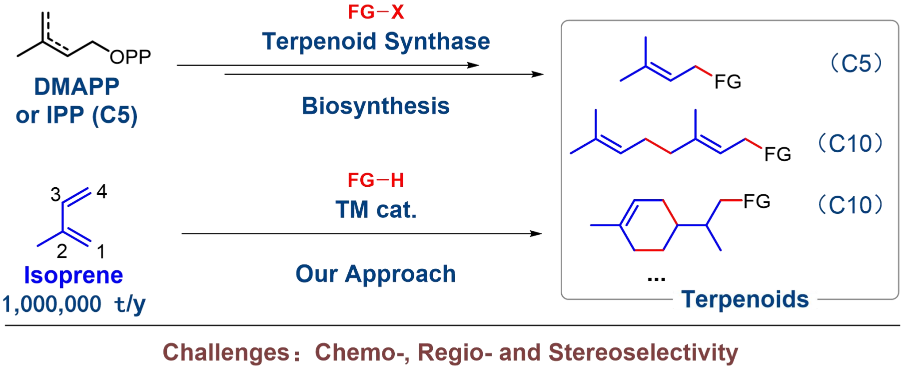

Figure 1. Catalytic Construction of Terpenoids from Isoprene

Keywords: Terpenoid, Isoprene, Transition metal catalysis

Reference

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Organocatalytic Enantioselective Nucleophilic α-Functionalization of Carbonyl Compounds

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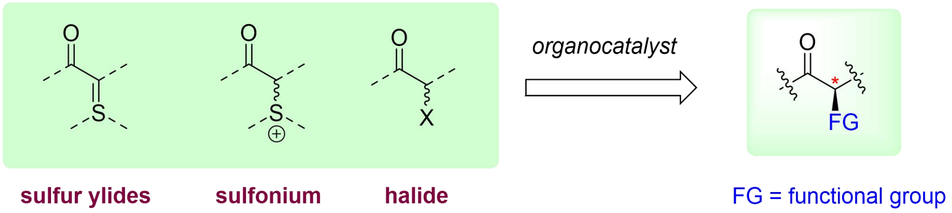
ABSTRACT

α-Chiral carbonyl compounds, particularly those bearing an α-heteroatom functional group, are highly important in drug development and asymmetric synthesis. While tremendous efforts have been devoted to the asymmetric electrophilic functionalization of carbonyl compounds via enolate intermediates, asymmetric nucleophilic α-functionalization has been less achieved. In particular, general protocols for the efficient construction of a tertiary α-stereogenic center of monocarbonyl compounds, such as ketones, have been limited developed. The challenges are partly associated with difficult stereocontrol, particularly in acyclic carbonyl substrates, and easy racemization of such labile stereocenters under relatively strong acidic and basic conditions.

α-Carbonyl sulfur ylides are a family versatile species that can serve as safe surrogates for diazo carbonyl compounds. However, they have been less-explored for asymmetric transformations, particularly for H-heteroatom bond insertion reactions. Our preliminary studies indicated that, in the presence of a chiral Brønsted acid catalyst, protonation of such sulfur ylides leads to the formation of sulfonium intermediates that can undergo enantioconvergent nucleophilic substitution. The chiral counter anion is responsible for effective stereocontrol, thereby representing a new approach to the asymmetric synthesis of α-chiral carbonyl compounds. Inspired by this process, we further extended this chemistry to the use of their synthetic precursors, such as sulfonium salts and even α-halocarbonyl compounds, for more direct asymmetric functionalization at the α-position using diverse nucleophiles. These processes provide a metal-free complement to the previously established metal-based systems.



Figure

Keywords: chirality, fluorination, chlorination, organocatalysis, carbonyl compounds

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Covalent Metal−Organic Frameworks

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Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), as emerging porous crystalline materials, have attracted remarkable attentions in chemistry, physics and materials science. MOFs are constructed by metal clusters (or ions) and organic linkers through coordination bonds, while COFs are prepared by pure organic building blocks via covalent bonds. Owing to the nature of linkages, MOFs and COFs have their own shortcomings. Typically, the relatively weak bond strengths of coordination bonds lead to poor chemical stability of MOFs, which limits their practical implementations. On the other hand, due to the strong covalent bonds, COFs exhibit rather higher stability under harsh conditions compared to MOFs. However, the lack of open metal sites restricts their functionalization and application. Therefore, it is hypothesized that the "cream-skimming" of MOFs and COFs would address these drawbacks and produce a new class of crystalline porous material, namely covalent metal-organic frameworks (CMOFs), with unprecedented structural complexity and advanced functionality.

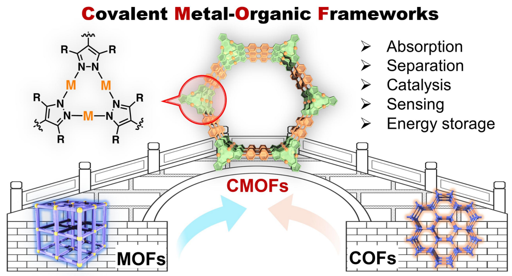

Fig 1 CMOFs: Fusion of Covalent Organic Frameworks and

The CMOFs reveal a new synthetic approach for the preparation of reticular materials, and synergize the advantages of MOFs and COFs, containing metal active sites ensuring various interesting properties, and covalent linkages that allow rather high chemical stability even under harsh conditions. In the past few years, our group has specifically focused on the development of general synthetic strategies for CMOFs by networking coinage metal (Cu, Ag and Au) based cyclic trinuclear units (CTUs)[1] with DCC. The CTUs exhibit trigonal planar structures and can be functionalized with reactive sites, such as -NH_2 and -CHO, that can further react with organic linkers to afford CMOFs. Notably, CTUs also features interesting properties including metallophilic attraction, π-acidity/basicity, luminescence, redox activity and catalytic activity, which can be incorporated into CMOFs. Therefore, we envision that CMOFs would be promising platforms not only for the development of novel reticular materials, but also for potential applications in many research fields including gas absorption/separation, sensing, full-color display, catalysis, energy and biological applications.[2]

Keywords: Covalent Organic Frameworks, Metal−Organic Frameworks, reticular chemistry, catalysis, separation

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Tissue Mimetic Membranes for Healing Augmentation of Tendon–Bone Interface in Rotator Cuff Repair

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With the aging of the society, the prevalence of skeletal diseases continues to grow, particularly those that cannot heal spontaneously, like critical-sized defects and interface tissue deficiencies. These conditions place a huge burden on healthcare system and society. Hence, there is a pressing demand for advanced regenerative biomaterials that can enhance healing outcomes and restore the normal functions of affected tissues. By harnessing the advantages of magnesium (Mg) in skeletal development, a range of Mg-containing bioceramic colloids has been created and assembled into polymer fibers to generate bioactive guided tissue regeneration membranes through colloidal electrospinning, which demonstrate exceptional regenerative capacity and great potential for real-world applications.

Recently, we develop a hierarchically organized membrane that mimics the heterogeneous anatomy and properties of the natural enthesis and finely facilitates the reconstruction of tendon–bone interface. A biphasic membrane consisting of a microporous layer and a mineralized fibrous layer is constructed through the non-solvent induced phase separation (NIPS) strategy followed by a co-axial electrospinning procedure. Cationic kartogenin (KGN)-conjugated nanogel (nGel-KGN) and osteo-promotive struvite are incorporated within the membranes in a region-specific manner. During *in vivo* repair, the nGel-KGN-functionalized microporous layer is adjacent to the tendon where intends to suppress scar tissue formation at the lesion and simultaneously heightens chondrogenesis. Meanwhile, the struvite-containing fibrous layer covers on the tubercula minus to enhance the stem cell aggregation and bony ingrowth. Such tissue-specific features and spatiotemporal release behaviors contribute to an effective guidance of specific defect-healing event at the transitional region, further leading to the remarkably promoted regenerative outcome in terms of the fibrocartilaginous tissue formation, collagen fiber alignment, and optimized functional motion of rotator cuff. These findings render this novel biomimetic membrane as an effective clinical solution to address the interface tissue deficiency at rotator cuff and even other transitional regions in sports medicine.

Keywords: Tissue mimetic membrane, Mg-containing ceramic colloids, colloidal electrospinning, bi-lineage bioinducible effect, tendon–bone healing

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Enzyme catalysis-mediated RAFT polymerization

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The research work of our group on enzyme-catalyzed initiation and regulation of Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization will be presented. This method exhibits characteristics such as mild conditions, environmental friendliness, oxygen tolerance, high polymerization efficiency, and high livingness. In conventional thermally initiated approaches, the concentration of radical initiators rapidly decays as polymerization progresses. In contrast, the enzyme-catalyzed initiation method enables continuous generation of radicals with relatively stable concentrations. By adjusting the components of the enzyme-catalyzed system, the radical concentration can be maintained at a relatively low level, which not only sustains the progression of polymerization but also reduces side reactions and enhances polymerization livingness. We have developed a series of cascade catalytic strategies, successfully synthesizing multi-block polymers and ultra-high molecular weight polymers.

Synthesis and Self-Assembly of Designer Polymer-Ligated Nanocrystals

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Nanocrystals demonstrate a broad range of intriguing properties that depend sensitively on their size and shape. In this talk, I will discuss the synthesis of a set of star-like, bottlebrush-like, and worm-like block copolymers, and their use as nanoreactors for crafting an array of designer polymer-ligated nanocrystals (NCs). These NCs include 0D nanoparticles, 1D nanorods, and shish-kebab NCs. Notably, the permanent tethering of polymers of interest on the NC surface imparts their self-assembly and disassembly on demand for applications in plamonics, controlled release, catalysis, etc.

Circularly polarized luminescence of Chiral supramolecular assemblies

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ABSTRACT

Chirality is a unique feature of nature, manifesting at various hierarchical levels from subatomic and molecular to supramolecular, nanoscopic, macroscopic, and galactic scales. Supramolecular chirality plays a bridging role from molecular to macroscopic chirality. In this talk, I will focus on how various chiral nanostructures, such as helical nanotube, nanotwist, nanotoroid and Möbius strips, could be generated through non-covalent interaction based designed chiral molecules. On the other hand, by coupling chiral or topological nanostructures with the luminescent molecules, circularly polarized luminescence (CPL) is generated. While isolated small molecules can be designed to show CPL, supramolecular assembly is an important way to amplify the performance of the chiroptical properties of the materials. Starting from the molecular design, the talk will discuss how to enhance the CPL performance of the materials from the perspectives of non-covalent interactions between molecules, coupling between chromophores and chiral elements, molecular arrangement and confinement in nanoassemblies.

Keywords: Supramolecular assemblies, chiral topology, chiral nanostructure, circularly polarized luminescence,

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Library Synthesis of Sequence-Controlled Copolymers and Stereoregular Polymers

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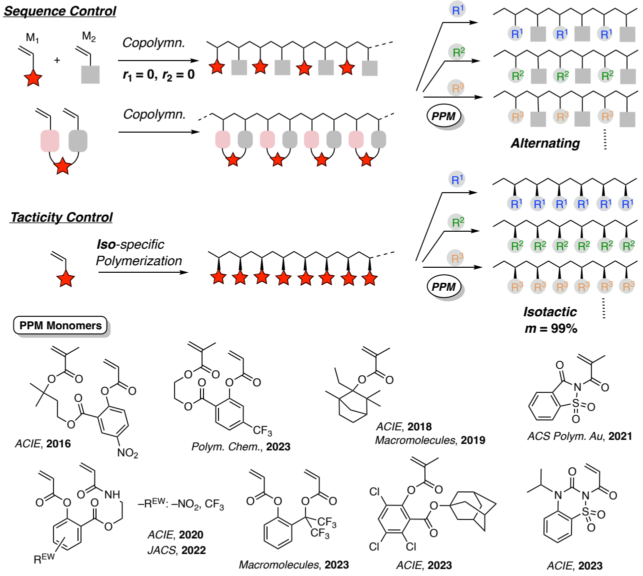
ABSTRACT

We have designed pendant-transformable monomers to control alternating copolymerization and stereospecific polymerization. A library synthesis of sequence-controlled or tacticitiy-controlled polymers was then achieved via quantitative post-polymerization modification. Our efforts were also directed to the evaluation of the physical properties seeking the maximal material performance of the (co)polymers via comparison with the corresponding random copolymers and atactic polymers.



Figure

Keywords: Sequence/Alternating/Tacticity/Post-Polymerization Modification/Radical Polymerization

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Shielding Pt/γ-Mo_2N by Inert Nano-overlays Enables Stable H_2 Production

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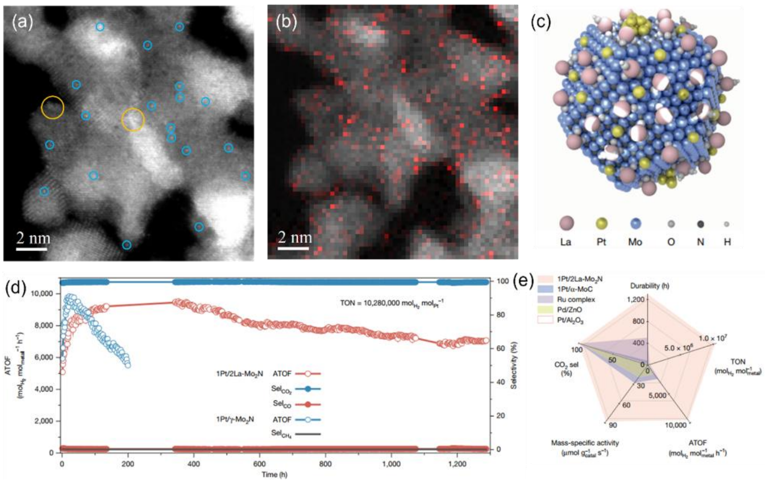
ABSTRACT

The use of reactive supports to disperse metal species is crucial for constructing highly efficient interfacial catalysts, by tuning the competitive reactant adsorption/activation pattern in supported metal catalysts into a non-competitive mechanism. However, these reactive supports are prone to deterioration during catalysis, limiting catalyst lifespan, frustrating their potential practical applications. New strategies are needed to simultaneously protect reactive supports and surface metal species without compromising the inherent catalytic performance. Herein, we report a new strategy to augment the structural stability of highly active interfacial catalysts by employing inert nano-overlays to partially shield and partition the reactive supports' surface (Figure 1). Specifically, we demonstrate that atomically dispersed inert oxide nano-overlays on a highly active Pt/γ-Mo_2N catalyst can block the redundant surface sites of γ-Mo_2N responsible for surface oxidation of this reactive support and the resulted deactivation. This strategy yields an efficient and highly durable catalyst for hydrogen production via methanol reforming (MR) reaction with a mere 0.26 wt% Pt loading, exhibiting a record-high turnover number (TON) of 15,300,000 and a superb apparent turnover frequency (ATOF) of 24,500 $mol_{H2}\cdot mol_{metal}^{-1}\cdot h^{-1}$. This innovative approach showcases the prospects of reducing noble metal consumption and boosting longevity, which could be applied to design effective and stable heterogeneous catalysts.



Figure

Keywords: heterogenous catalysis, hydrogen production, rare earth element, methanol steam reforming

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Precise tailoring of catalyst structure toward catalytic reforming for hydrogen production with zero CO_2 emission

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ABSTRACT

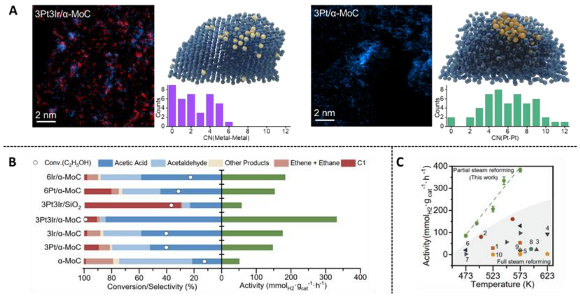
Carbon-neutral hydrogen production is essential for the sustainable chemical industry of the future, addressing both environmental and economic challenges. This study introduces a novel thermal catalytic method for the partial reforming of ethanol into hydrogen and acetic acid with near-zero carbon dioxide emissions, offering a more energy-efficient alternative to conventional reforming processes.

The reaction is enabled by a highly effective catalyst composed of atomic platinum (Pt1) and iridium (Ir1) species supported on a reactive alpha-molybdenum carbide (α-MoC) substrate. This innovative catalyst achieves a remarkable hydrogen production rate of 331.3 millimoles per gram catalyst per hour at 270°C, along with an acetic acid selectivity of 84.5%. The use of atomic Pt1 and Ir1 species ensures high catalytic activity, while the alpha-molybdenum carbide substrate enhances reactivity and durability under operating conditions. This combination allows for efficient ethanol conversion with minimal byproducts and reduced energy consumption compared to standard reforming methods.

A key advantage of this process is its near-zero carbon dioxide emissions, making it highly sustainable and aligning with global efforts to reduce greenhouse gas emissions. The lower energy requirements further enhance its viability for industrial applications, presenting an opportunity to produce hydrogen—a clean energy carrier—and acetic acid—a valuable chemical feedstock—simultaneously.

Techno-economic analysis highlights the potential profitability of scaling up this technology for industrial use, demonstrating its feasibility as a dual-purpose solution for hydrogen and acetic acid production. By significantly reducing the carbon footprint associated with hydrogen production, this method addresses both environmental and regulatory demands while offering economic benefits.

In summary, this study presents a groundbreaking pathway for sustainable hydrogen production through partial ethanol reforming, combining high efficiency, reduced emissions, and economic viability to meet the growing demand for carbon-neutral solutions in the chemical industry.



Figure

Keywords: heterogeneous catalysis, hydrogen production via reforming, structure-performance relationship, ethanol reforming, green hydrogen production

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Design of New Heterogeneous Zeolite-Based Catalysts for Efficient Conversion of Small Molecules

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ABSTRACT

Conversion of small molecules such as natural gas, CO, and CO_2 into value-added chemicals has been paid much attention recently towards a carbon-neutral future. In this talk, we briefly summarized our recent results for conversions of methane to methanol, syngas to light olefins, propane to propene, and reforming of CO_2 with methane to CO over new heterogeneous zeolite-based catalysts. When AuPd alloy nanoparticles were fixed within aluminosilicate zeolite crystals, followed by modification of the external surface of the zeolite with organosilanes, the catalyst allowed diffusion of hydrogen, oxygen, and methane to the catalyst active sites, while confining the generated peroxide there to enhance its reaction probability. In this case, at 17.3% conversion of methane and 92% methanol selectivity were achieved. When the isolated B was introduced into MFI framework, the catalyst exhibited high activity and selectivity in the oxidative dehydrogenation of propane (ODHP), which is a key technology for producing propene from shale gas. When Ni nanoparticles were fixed with an aluminosilicate zeolite catalyst, it was enhanced hydrogen spillover to favour the reduction of CO_2, which promoted the reducibility of methane relative to conventional dry reforming of methane (DRM), even to 2.9 mol of CO_2 per mol of CH_4.

Keywords: zeolite, efficient conversion, small molecules, energy utilization, heterogeneous catalysis

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Precise control of the microenvironment metal active sites in zeolites for catalytic conversion of alkanes and alkenes

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ABSTRACT

Single metal atoms and metal clusters have attracted much attention thanks to their possibility as heterogeneous catalysts. However, the generation of stable single atoms and clusters on a solid support is still challenging. In recent years, we have reported a general strategy for the generation of single metal atoms and subnanometer metal clusters with exceptionally high thermal stability, formed within purely siliceous zeolites (MFI, MEL and MWW etc.) during the growth of the zeolite crystallites. These subnanometer metal species are stabilized in the zeolite, even after treatment in either oxidative or reduction atmospheres up to 650 ^{o}C.

In the first example, we have shown that subnanometer Pt species are finely dispersed in MCM-22 crystallites. These encapsulated subnanometer Pt species show higher activity than Pt nanoparticles for propane dehydrogenation reaction and more importantly, higher stability during the reaction-regeneration cycles. Furthermore, using Pt@MCM-22 material as a model system, we have studied the evolution of Pt single atoms and clusters during reduction-oxidation treatments and under reaction conditions by ETEM. The states of metal species are dependent on the temperature and atmosphere. The high stability of the encapsulated metal clusters is achieved through the confinement effect between the metal species and the zeolite framework, which is visualized by HAADF-STEM and iDPC-STEM imaging technique.

In our second example, we will show the preparation of subnanometer Pt and Pt-based bimetallic sites encapsulated in MFI zeolite for dehydrogenation of light alkanes (ethane and propane). Thanks to the rigid zeolite framework surrounding the Pt species, the Pt clusters remain stable under the alkane dehydrogenation conditions and can be almost fully recovered after a facile regeneration procedure. Our detailed studies show that the particle size and chemical composition of the Pt species have profound influences on the catalytic performances, highlighting the importance in precise controlling the atomic structures of the metal active sites confined in zeolites.

Finally, we will discuss the synthesis of subnanometer Rh catalyst confined in MFI zeolite for hydroformylation of linear α-olefins for preparation of linear aldehydes. The zeolite framework surrounding the Rh clusters can serve as the inorganic ligand which modulated the structural configuration of the intermediates, yielding an exceptionally high l/n ratio in the aldehyde products. The optimal catalyst outperforms the reported supported Rh catalysts and also match the best homogeneous Rh catalysts. This example infers the promise of modulating the microenvironment of subnanometer species confined in zeolites for organic transformations.

Keywords: zeolite, metal clusters, alkane dehydrogenation, olefin hydroformylation

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From Green Chemistry to Clean Water: Synthesis and Applications of Stable Covalent Organic Frameworks

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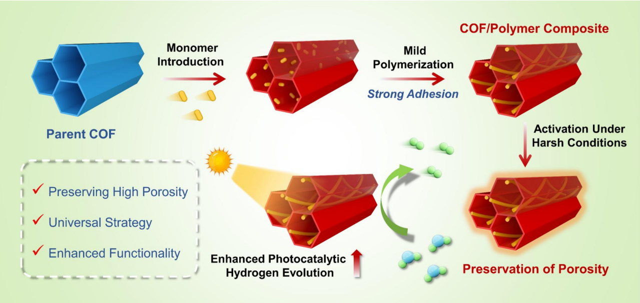
ABSTRACT

The quality of covalent organic frameworks (COFs) is vital for their applications, yet structural damage during activation remains a major challenge. This presentation introduces two innovative strategies to synthesize high-quality COFs with enhanced stability and functionality.

The first strategy utilizes functional polymer guests, such as polydopamine (PDA), to stabilize COF structures. Polymers act as supportive pillars, preventing pore collapse and maintaining high porosity and crystallinity. For instance, the TAPB-TA/PDA composite achieves a 16-fold increase in surface area compared to its parent COF. The reinforced structure also enhances photocatalytic hydrogen evolution by improving charge carrier transport. Molecular dynamics simulations confirm that PDA oligomers reinforce COF walls through van der Waals interactions, preserving structural integrity.

The second approach employs a self-sacrificing guest method, where salt guests are incorporated into COF pores to provide structural support during activation. Upon heating, the salts decompose into gases, yielding highly pure COFs without residual guests. This method produces twelve SG-COFs with superior crystallinity and porosity, demonstrating exceptional performance as adsorbents for per- and polyfluoroalkyl substances (PFAS).

Together, these approaches- polymer stabilization and self-sacrificing salts-address key challenges in COF synthesis, enabling high-quality frameworks with expanded applications in environmental remediation, catalysis, and beyond.



Figure

Keywords: covalent organic frameworks, self-sacrificing guest method, polymer stabilization, structural integrity, environmental remediation

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Quantitative Study of the Stability of Colloidal Metallic Nanoparticles at an Atomic Level

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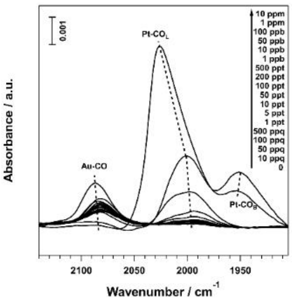
ABSTRACT

Understanding and controlling electrochemical interfaces at atomic and molecular levels have transformed electrochemistry into a science with clearly defined fundamental principles, leading to significant impact on various electrochemical systems and devices. Although the principles guiding the activity of electrochemical reactions are quite well established, the driving forces that control stability are still poorly understood. Here, we achieve in situ monitoring of the early stages of Pt, Pd, and Ni dissolution using the operando attenuated total reflectance surface enhanced infrared absorption spectroscopy (ATR-SEIRAS). Our unique operando ATR-SEIRAS method provides femtogram sensitivity levels that, in combination with other techniques, provide otherwise inaccessible information about the dissolution of colloidal metallic nanoparticles with different shapes in acidic environments, and thus deliver a more sensitive approach to understanding the structure-stability relationships of colloidal metallic nanocatalysts at an atomic level.



Figure

Keywords: surface-enhanced infrared absorption spectroscopy, structure-stability relationship

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Research on Metal Substrate-Boron Composite Catalysts for Propane Oxidative Dehydrogenation

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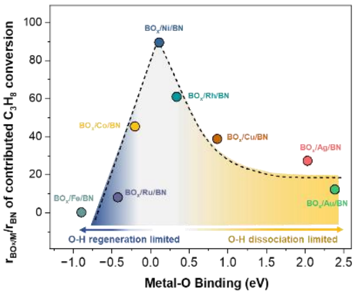
ABSTRACT

Propylene, a key chemical feedstock, is experiencing continuous growth in demand. Among the various technologies for propylene production, propane oxidative dehydrogenation (ODHP) stands out due to its thermodynamic advantages and exceptional resistance to coking. Boron-based non-metallic ODHP catalysts currently exhibit excellent propylene selectivity, with ethylene as the main by-product, rather than deep oxidation products such as CO_x. As a result, these catalysts offer significant economic advantages and better application prospects compared to traditional metal oxide and carbon-based catalysts. The ODHP reaction on boron-based catalysts follows a surface-gas phase coupled free radical mechanism, where the continuous generation of highly active surface B-O· and gas-phase ·OOH free radicals is driven by the dissociation and regeneration cycle of BO-H groups in hydroxyl-functionalized boron sites. However, the high dissociation energy of the O-H bond makes it difficult to efficiently generate B-O· and ·OOH free radicals at low temperatures, preventing the initiation of the free radical chain reaction. Therefore, effectively activating the boron hydroxyl O-H bond to enable efficient initiation of free radicals and cyclic regeneration of active sites at low temperatures is crucial for improving the low-temperature catalytic performance of boron-based catalysts.This study introduces a strategy for constructing metal substrate-boron composite catalysts, utilizing the hybridization of the d-band of the metal substrate with the p-orbital of the O atom in BO-H to modulate the geometric and electronic properties of the overlayer BO_x. The aim is to activate the boron hydroxyl group under mild conditions. Transition metals such as Fe, Co, Ni, Cu, Ru, Rh, Ag, and Au were selected as sublayer metals, and $M@BO_x/BN$ catalytic systems with tunable metal sublayers were synthesized. Experimental results reveal that the intrinsic activity of BO_x/M correlates with the metal-oxygen binding energy, in line with the Sabatier principle, where an intermediate M-O binding energy enhances ODHP catalytic activity. Thus, the M-O binding energy serves as a descriptor for the performance of $BO_x/M/BN$ catalysts in propane oxidative dehydrogenation. By fine-tuning this binding energy, the low-temperature catalytic performance of boron-based catalysts can be significantly improved. This research offers new insights for the design and development of low-temperature boron-based ODHP catalysts.



Figure

Keywords: propylene, ODHP, boron-based catalyst, substrate-boron composite catalyst

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Synthesis and energy storage applicarions of heteroatom-doped porous Carbons

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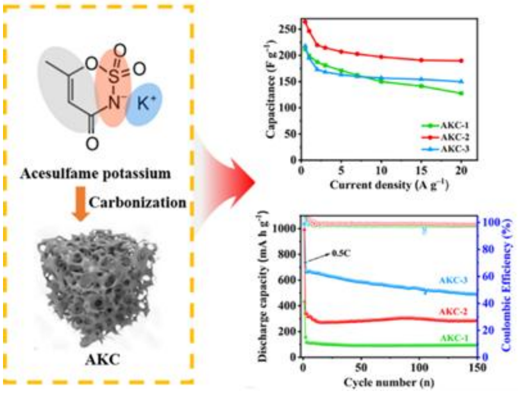
ABSTRACT

Organic potassium salts have emerged as a highly potential class of carbon precursor materials, triumphantly surmounting the flaws of traditional porous carbon preparation methods. The drawbacks typically consist of an extremely time - consuming preparation process, a high degree of complexity, the presence of corrosive substances, and exorbitant costs. Under high - temperature conditions, organic potassium salts can trigger the generation of potassium carbonate, potassium oxide, and metallic potassium. This chemical transformation significantly contributes to the formation of a dense pore structure inside the material.In this specific research, acesulfame potassium (AK) was chosen as the precursor material. The potassium ions, along with nitrogen and sulfur elements inherently present in acesulfame potassium, simplify the high - temperature carbonization process. Through this process, nitrogen - and sulfur - doped porous carbon with a complex and well - developed pore structure has been fabricated.Owing to the combined influence of a large specific surface area, an optimized pore structure, and nitrogen - sulfur co - doping, acesulfame potassium - derived carbon (AKC) has demonstrated excellent performance in both supercapacitors and lithium - sulfur batteries. Overall, this study puts forward a novel synthesis strategy for preparing dual - heteroatom - doped porous carbon, aiming to achieve high - performance applications in energy storage systems.



Figure

Keywords: heteroatom-doping, hierarchical porous carbon, energy storage

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Salen Complex−Derived Metal Sulfide/Carbon Nanocomposites

for Advanced Energy Storage Applications

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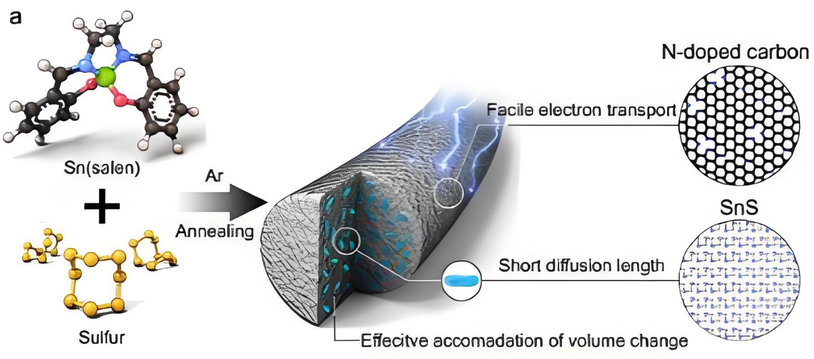
ABSTRACT

Among conversion-reaction materials, metal chalcogenides stand out for their exceptional theoretical capacities. Metal sulfides exhibit particular advantages over oxides, demonstrating smaller voltage hysteresis and higher energy efficiency due to weaker metal−sulfur bonding. However, their practical application faces challenges including poor electrical conductivity and significant volume variation during sodiation/desodiation cycles. This study presents an innovative materials design strategy utilizing salen complexes as precursors to overcome these limitations. The unique tetradentate Schiff−base structure of salen ligands enables strong chelation with transition metals, forming stable complexes. During pyrolysis, the nitrogen−rich ligands facilitate in situ nitrogen doping, creating a defect−rich carbon matrix that simultaneously enhances ion transport kinetics and provides additional sodium storage sites, thereby improving electrochemical performance. A facile solvothermal method was used to synthesize metal salen complexes, followed by direct sulfurization with sulfur powder, enabling the one−step fabrication of metal sulfide/nitrogen−doped carbon (MS/N−C) nanocomposites with tunable morphologies and carbon architectures. When applied as anodes for lithium− and sodium−ion batteries, MS/N−C nanocomposites exhibited excellent rate capability and long−term cycling stability. The nanoscale dimensions of MS/N−C effectively shortened Na^+ diffusion pathways, enhanced ionic migration efficiency, and mitigated volume expansion during cycling. Additionally, the carbon matrix acted as a structural buffer, confining the volume changes of metal sulfides and further improving cycling stability.The combination of these features significantly positions salen−derived materials as a promising platform for next−generation energy storage systems. This work provides both fundamental insights into materials design and practical pathways for developing high−performance battery electrodes.



Figure

Keywords: lithium−ion batteries; anodes; salen complex, N-doped carbon

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Single-Atom Electrocatalysis Driven by High-Energy Metastable Structures

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ABSTRACT

Nanoclusters or nanoparticles possess numerous low-energy metastable structures that drive their structural evolution; therefore, it is essential to consider the contributions of these low-energy metastable structures in nanocatalysis. In contrast, the structures of stable single-atom catalysts (SACs) typically lack low-energy metastable structures, leading to dominance by their lowest-energy configurations, thereby providing a straightforward structural basis for their structure-activity relationships. However, our theoretical study has revealed that high-energy metastable structures (HEMSs) in SACs can deliver exceptionally high catalytic activity. Even at trace concentrations, these HEMSs can dominate the catalytic performance of SACs. Consequently, HEMSs may play a critical role in single-atom catalysis and should not be overlooked. Furthermore, our theoretical investigations have demonstrated that in electrocatalysis involving high energy input, HEMSs in SACs can be promoted, thereby driving high catalytic activity.

Keywords: single-atom catalysis, high-energy metastable structures, electrocatalysis

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Atomically Dispersed Mo/Ni Alloy Catalyst for Partial Oxidation of Methane

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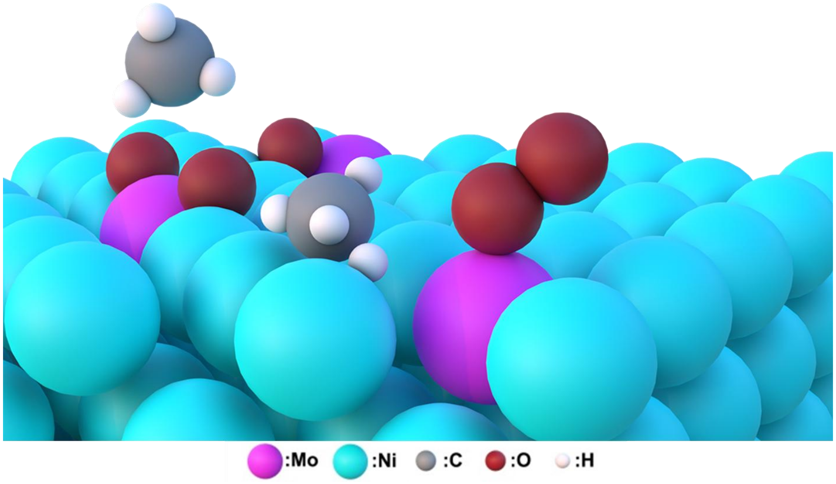
ABSTRACT

The catalytic partial oxidation of methane (POM) presents a promising technology for synthesizing syngas. However it faces severe over-oxidation over catalyst surface. Attempts to modify metal surfaces by incorporating a secondary metal towards C–H bond activation of CH4 with moderate O* adsorption have remained the subject of intense research yet challenging. Herein, we report that high catalytic performance for POM can be achieved by the regulation of O* occupation in the atomically dispersed (AD) MoNi alloy, with over 95% CH_4 conversion and 97% syngas selectivity at 800 °C. The combination of ex-situ/in-situ characterizations, kinetic analysis and DFT (density functional theory) calculation that Mo-Ni dual sites in AD MoNi alloy afford the declined O_2 poisoning on Ni sites with rarely weaken CH_4 activation for partial oxidation pathway following the combustion reforming reaction (CRR) mechanism. These results underscore the effectiveness of CH_4 turnovers by the design of atomically dispersed alloys with tunable O* adsorption.



Figure

Keywords: single-atom alloy, partial oxidation of methane, hydrogen, methane reforming, XAFS

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Defective Layered Double Hydroxide Based Nanostructured Photocatalysts for Nitrogen Fixation

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ABSTRACT

The activation and conversion of nitrogen is a major challenge in both basic and applied research. Industrial nitrogen fixation requires severe reaction conditions of high temperature and high pressure, and at the same time will emit a large amount of greenhouse gases causing serious environmental problems. Photocatalytic nitrogen fixation is considered as a promising artificial nitrogen fixation technology. At present, the performance of photocatalytic nitrogen fixation still needs to be further improved, and it is urgent to develop low-cost and efficient photocatalytic materials. Layered double hydroxide (LDH)-based nanomaterials have attracted much attention due to their advantages of easy structure regulation and simple preparation. In recent years, by creating defect sites on the surface of LDH-based materials, our research group has achieved enhanced adsorption and activation of N_2 reactants, thus significantly improving the photocatalytic nitrogen fixation performance.

Keywords: photocatalysis, defect, nitrogen fixation, layered double hydroxide

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Electroreduction of CO_2 into Important Fuels and Chemicals

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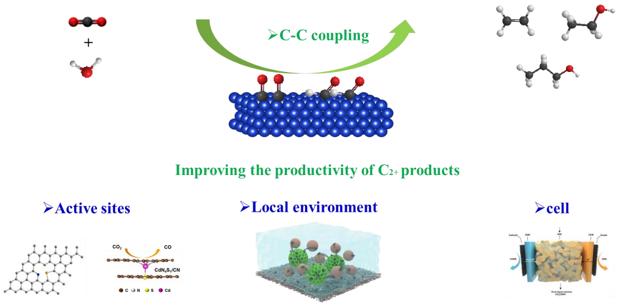
ABSTRACT

Electroreduction of CO_2 into important fuels and chemicals has good application prospects in the utilization of renewable energy and carbon emission reduction, but there are still many challenges to be addressed. In recent years, we carried out in-depth and systematic research on the key issues faced in the preparation of high-value fuels and chemicals through the electroreduction of CO_2 and H_2O, such as poor selectivity for multi-carbon alcohols, limited gas mass transfer, and unclear understanding of catalytic sites and mechanisms. A series of multifunctional catalysts were designed and prepared to achieve high selectivity of multi-carbon alcohols by regulating factors such as the adsorption, coverage, and local microenvironment of intermediates. A novel gas diffusion catalyst layer was designed and constructed to realize high-selectivity and high-activity electroreduction of CO_2. By integrating various in-situ techniques and theoretical calculations, the matching and synergistic effect mechanisms between catalytic sites were elucidated.



Figure

Keywords: CO_2, electroreduction, green chemistry

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Design of Heterogeneous Catalysts for Precise Conversions of Lower Alkane and C1 Molecules

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ABSTRACT

The heterogeneous catalyst is typically composed of an active phase, a support and one or several promoters. This conventional type of catalysts has played pivotal roles in the chemical industry. Under the current pursuit of precision catalysis, which demands precise control over the active site and reaction pathways, the development of new strategies for catalyst design has become imperative. Here, I present our catalyst-design strategies of dynamic control of confined single-atom catalysis for propane dehydrogenation and relay catalysis for syngas conversion to C_2 oxygenates.Propane dehydrogenation (PDH) is one of the most attractive heterogeneous catalytic reactions, with a simple reaction mechanism mainly involving the C-H activation. However, fast catalyst deactivation due to the coke deposition, induced by the C-C cleavage and deep dehydrogenation, remains a significant challenge. Rhodium is the most active metal towards C-H activation, but Rh-based catalysts typically exhibit poor PDH performance. We successfully designed and constructed a highly efficient and ultrastable Rh single-atom catalyst by leveraging zeolite-confinement effect and the dynamic migration of indium species under reaction conditions. The catalyst stability exceeds 1200 h in PDH, with a propylene yield of >60% at 600 °C. No catalyst deactivation was observed for the conversion of pure propane at 550 °C over 6000 h. Syngas (CO/H_2), a sustainable C1 feedstock derivable from either fossil resources or renewables, has attracted significant attention as a key platform. Despite remarkable advances in the conversion of syngas to lower olefins over the past decade, selective synthesis of a C_2 oxygenate from syngas, a reaction with complex mechanisms containing multiple intermediates and complex reaction networks, has been less successful. We demonstrate that relay catalysis is a promising methodology for designing catalyst to control such complex reactions. Constructing a relay system by integrating methanol carbonylation with its upstream and downstream reactions, such as syngas-to-methanol and acetic-acid hydrogenation, shows promise for selective synthesis of C_2 oxygenates from syngas. By designing and constructing a dual-site heterogeneous carbonylation catalyst that operates efficiently at a lower CO/CH_3OH ratio, we successfully overcame the conversion-selectivity trade-off in syngas conversion to C_2 oxygenates via relay catalysis. The selectivity of acetic acid or ethanol reached 90% at single-pass CO conversions of 30-40%.

Keywords: catalyst design, single-atom catalysis, relay catalysis, propane dehydrogenation, syngas conversions

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An unsung hero in electrocatalysis

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ABSTRACT

Electrocatalysis at the electrode-electrolyte interface is fundamentally governed by electron transfer across the electric double layer (EDL), highlighting a crucial mechanistic link between electrocatalytic properties and EDL structure. A central question in this field is the role of alkali metal cations at this interface, commonly known as the “cation effect”. This presentation will outline our ongoing research aimed at uncovering the fundamental principles underlying the cation effect in several important electrochemical reactions in aqueous environments. Using advanced *in situ* analytical techniques, we have discovered that alkali metal cations are not merely spectators, as traditionally believed, but actively influence the kinetics and mass transport in electrocatalysis. The identity and concentration of the alkali metal cation is critical in modulating electrocatalytic activity and selectivity, as well as affecting electrode stability. We will present a mechanism of cation-coupled electron transfer and its potentially interesting role in alkaline hydrogen evolution reactions. By gaining a deeper understanding of how alkali metal cations affect electrocatalysis, we aim to propose a novel conceptual framework for improving electrocatalytic processes.

Keywords: electric double layer, electrocatalysis, cation effect, cation-coupled electron transfer, *in situ* spectroscopy

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Developing Better Rechargeable Aluminum Batteries: Materials and Interfaces

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ABSTRACT

Rechargeable aluminum batteries (RABs) are regarded as important candidates for the next-generation energy storage technology due to their high theoretical capacity, low cost and environmentally friendly characteristics. However, its practical application still faces the following core challenges: unclear Al storage mechanism of key materials, insufficient structural stability leading to capacity attenuation, severe dendrite growth and interface corrosion of the Al anode, and poor compatibility between the electrolyte and the electrode interface limiting the cycle life. To address these issues, our group has focused on the following work: 1) To overcome sluggish carrier ions insertion/de-insertion kinetics and volume expansion in conventional cathode materials, we have optimized the structural design of sulfides, oxides, and layered compounds combined with theoretical calculations. Additionally, innovative liquid-state redox cathodes and bimetallic synergistic systems have been developed. By leveraging multi-ion reaction mechanisms and constructing three-dimensional conductive networks, carrier transport pathways are optimized, breaking the limitations of traditional cathodes to achieve high specific capacity, high energy density, and long-term cycling stability. 2) To resolve the narrow electrochemical window and interfacial side reactions of conventional electrolytes, a strategy of mixed electrolytes and additives is proposed. By regulating the components of the electrolyte and the double electric layer structure at the interface, side reactions are suppressed and ion transport efficiency is enhanced, achieving a high voltage window, wide temperature range and low cost. 3) To address the issues of dendrite growth and local corrosion in Al anodes, through surface modification and homogenization deposition strategies, the Al deposition/dissolution behavior is regulated to construct a stable solid electrolyte interface (SEI) layer, aiming to achieve dendrite-free, corrosion-free, and low-polarization long-cycling metal anodes. The above works, through multi-dimensional collaborative optimization of materials-systems-interfaces, have laid the foundation for the practical application of the efficient energy storage mechanism of RABs. In the future, it is necessary to further explore high-performance electrode materials, highly stable electrolyte systems and multi-scale interface dynamic regulation strategies to promote their advancement towards the field of high-safety and low-cost commercial energy storage.

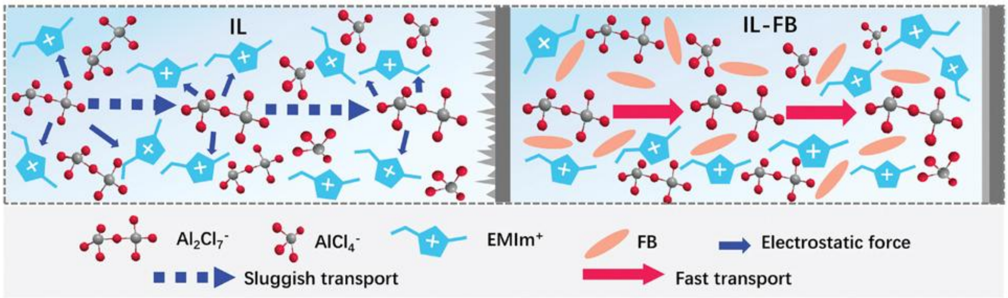

Figure 1 Schematic illustration of the solvent structure in the IL and IL-FB

Keywords: rechargeable aluminum batteries, electrode materials, electrolytes, interfaces

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Biomass-derived Electrochemical Energy Storage Materials

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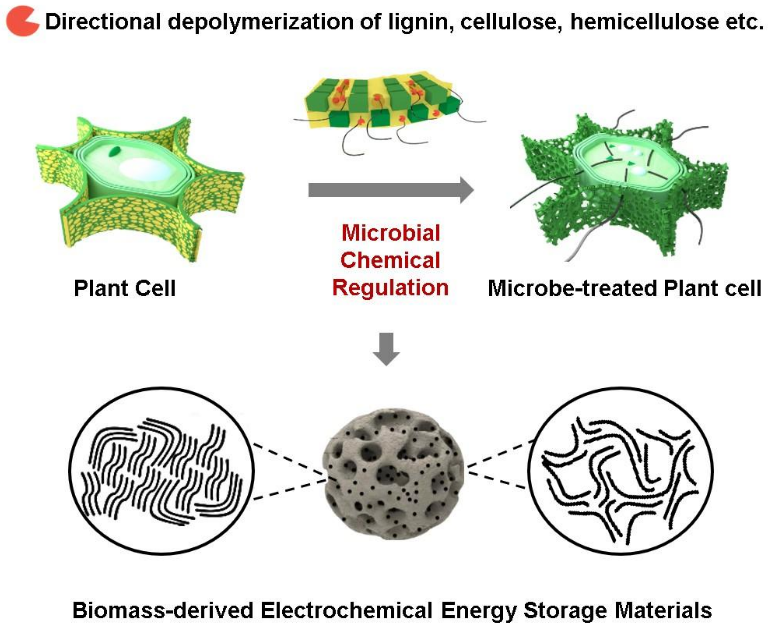
ABSTRACT

Biomass and its derivatives, featuring unique pore structures and rich functional groups, can meet the demands of emerging energy storage materials. Their applications in lithium-ion batteries, supercapacitors, etc., pave the way for sustainable energy development. For instance, coconut shell-derived biochar from Kuraray Co., Ltd. has shown its great potential in commercial hard carbon. Nevertheless, the regulation of microstructures and surface-interface properties for biomass-derived carbon faces challenges in excessive acid-base treatment and low efficiency. Meanwhile, the applications of biomass-derived materials in electrochemical energy storage mainly focus on carbon materials prepared by high-temperature pyrolysis. To address the above problems, we proposed a mild microbe-assisted biosynthetic approach to specifically adjust the raw components and textures of biomass through enzymatic reactions. As expected, a series of high-performance biomass-derived electrode and functional materials have been successfully synthesized, holding great promise for revolutionizing the application and innovation of secondary batteries and effectively harnessing biomass resources to contribute to the development of energy storage technologies.



Keywords: biomass, microorganisms, metallic lithium (sodium), secondary batteries

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Pickering Droplet - based Mimetic Cell Factory and Synthesis of Fine Chemicals

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Current industrial synthesis of organic chemicals predominantly relies on multi-step catalytic processes, which are inherently associated with significant separation requirements, high energy consumption, and suboptimal space-time yields. In the context of carbon neutrality objectives, there exists a pressing need for fundamental process redesign. The biomimetic droplet-cell factory paradigm, employing stabilized Pickering emulsion droplets to emulate cellular architecture and functionality, enables the precise organization of multiple catalytic systems within confined micro-nano compartments. This approach harnesses renewable energy inputs to drive chemical transformations while achieving spatiotemporal integration of consecutive reaction steps, thereby enhancing the efficiency of molecular/electron transfer processes and material conversion. This presentation systematically examines the developmental trajectory of biomimetic cell factories, critically evaluates existing scientific challenges and technological limitations, and provides a rigorous justification for employing Pickering emulsions as the foundational platform for constructing droplet-based biomimetic reaction systems. We elaborate on advanced methodologies for engineering micro-nano interfacial architectures and compartmentalized spaces within emulsion droplets, analyze the interfacial/spatial catalytic phenomena and microenvironmental modulation characteristics of these biomimetic systems, and demonstrate their practical implementation in continuous-flow asymmetric synthesis of chiral compounds and biocatalytic CO_2 conversion. Finally, we propose future research directions for advancing droplet-based biomimetic cell factory technology.

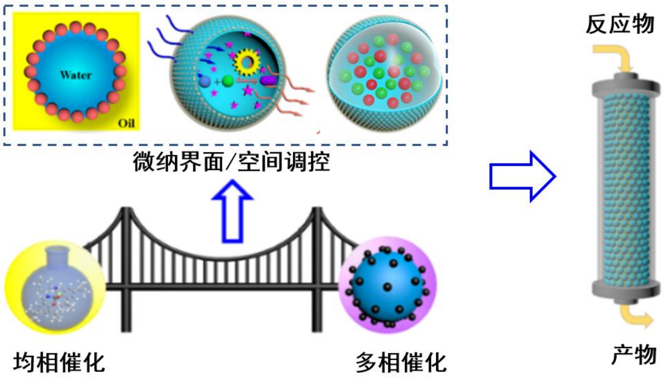

Figure. Schematic diagram of continuous-flow synthesis of fine chemicals in Pickering emulsion droplet fixed-bed reactors.

Keywords: pickering emulsion, continuous flow, micro-nano space, biocatalysis

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Metal nanoclusters: An ultrasmall system for energy conversion

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ABSTRACT

Atomically precise metal nanoclusters protected by ligands, which exhibit unique atomic stacking configurations, quantum confinement effects, enriched catalytically active sites, and discrete energy band structures, have garnered significant attention across diverse fields including photothermal therapy, photoluminescence, photocatalysis, and electrocatalysis. These nanoclusters are emerging as a novel platform to address critical challenges in energy harvesting, energy conversion, and environmental remediation. The physicochemical properties of metal nanoclusters can be precisely tailored through ligand design strategies. Here, we propose a ligand engineering approach to construct atomically precise photothermal nanomachines capable of achieving efficient light-to-heat conversion at the nanoscale.

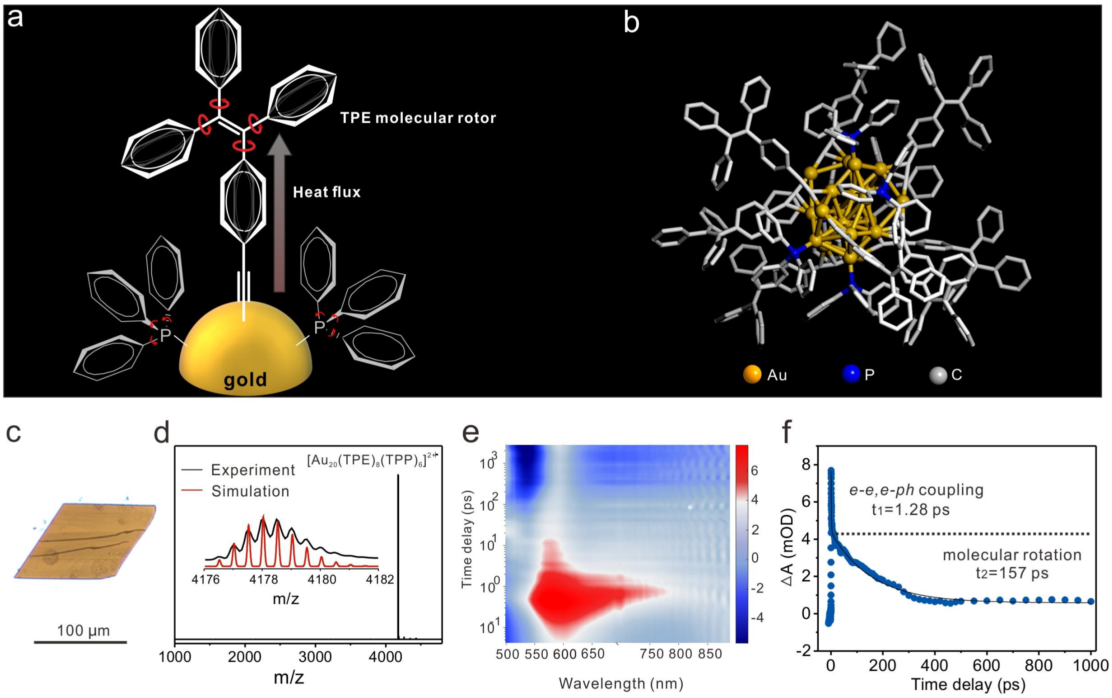

Figure: Design and characterization of an atomically precise photothermal nanomachine

Keywords: gold nanocluster, metal nanocluster, nanomachine, photothermal conversion, photothermal therapy

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Nondestructive In Situ X-ray Absorption Spectroscopy Analysis for Electrochemical Materials and Device

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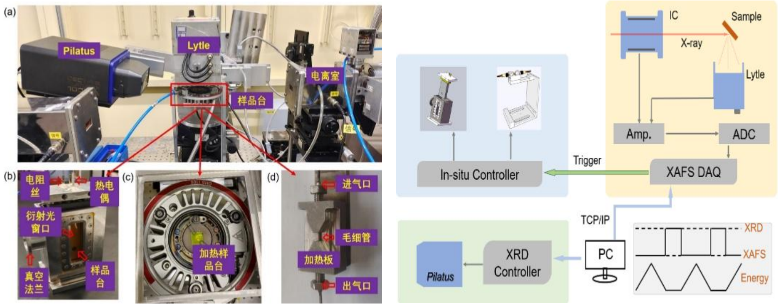
ABSTRACT

Electrochemical materials and device play a crucial rule for powering portable electronics, electric vehicles, large-scale energy storage systems, and so on. Enhancing the electrochemical performance hinges on a deep understanding of their operational and degradation mechanisms, necessitating advanced characterization method. In situ X-ray absorption spectroscopy is among the most important nondestructive analytical tool, providing local structure evolution during electrochemical reaction. Combined with X-ray diffraction (XRD) and integrated versatile in situ sample cell, we can simultaneously characterize the short- and long-range-ordered structure of materials, studying the electrocatalytic reaction mechanism, functional material growth process and their stability et al. By bridging the gap between advanced characterization techniques and electrochemical technologies, this presentation will aim to guide the iteration of new materials and stability prediction of devices.



Figure

Keywords: in situ, nondestructive, electrochemical, X-ray absorption spectroscopy

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Progress and Prospects in Theoretical Chemistry of Rare Earths

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ABSTRACT

Rare earths are important strategic resources in modern industries, and rare earth science and technology have important applications in the fields of chemistry, materials, energy, environment and medicine. With the development of quantum mechanics, relativistic mechanics and computational science, the theoretical chemistry of rare earths has made important progress [1-3], laying a theoretical foundation for the design and application of rare earth molecules and materials. In this talk, we will review the status of the development of rare-earth theoretical chemistry, introduce the recent advances in computational chemistry in the field of rare earths [5-6], and provide an outlook on the direction of future research.

Keywords: rare earth elements, quantum mechanics, relativistic effects, theoretical chemistry

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Electrode Interface Degradation and Electrolyte Chemistry in Sodium-Ion Batteries

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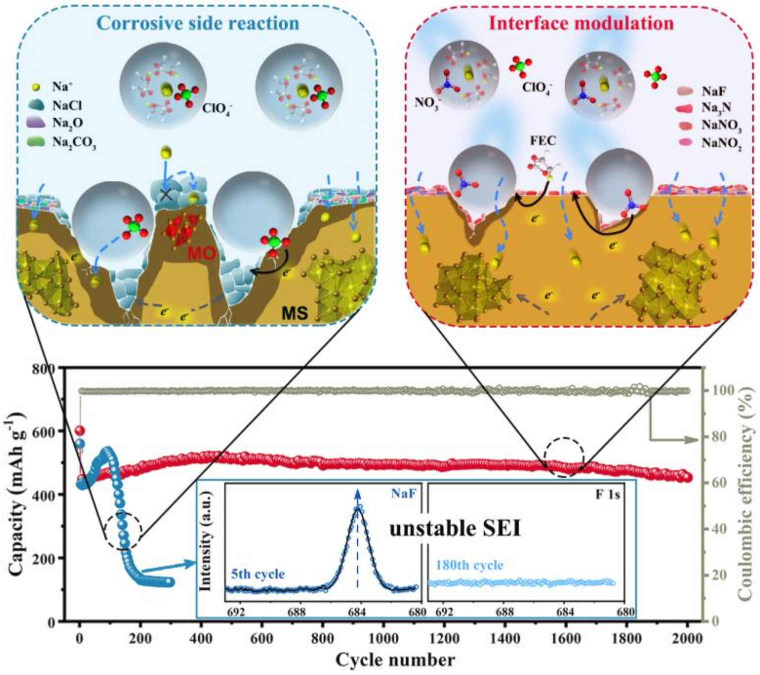
Our research team has been dedicated to studying the electrode-electrolyte interface in sodium-ion batteries, aiming to uncover the underlying causes of battery failure in cathode, anode, and electrolyte systems. We have proposed solutions from the perspectives of solvent chemistry modulation and solid electrolyte interphase (SEI) film engineering. In layered sodium manganese oxide cathode materials, we put forward a "NaF penetration-transition metal dissolution" synergistic failure model and designed a $ROSO_2Na/NaF$ composite SEI protective film. For carbon-based metal sulfide anodes, we found that ClO_4^- induces low-conductivity SEI film and revealed a chemico-mechanical coupled failure mechanism. By optimizing anion coordination to build a NaF/Na_3N SEI structure, the battery can achieve stable cycling up to 2,000 cycles. We also explored the oxidation decomposition pathway of ether solvent molecules, primarily driven by nucleophilic attack, and established an anion-mediated solvation reconstruction mechanism. This expanded the stable working voltage window from 3.9 V to 4.8 V (vs. Na^+/Na). Overall, these findings provide novel pathways for constructing highly efficient and stable interfaces in sodium-ion batteries from the interfacial chemistry perspective.



Keywords: Sodium-ion batteries, interface degradation, solid electrolyte interphase (SEI), electrolyte chemistry, solvent chemistry

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Battery Innovation Empowered by Lithium Bond and Artificial Intelligence

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ABSTRACT

Lithium bonds, analogous to hydrogen bonds, exhibit unique properties due to lithium’s weak metallic nature, offering exciting potential for lithium battery applications. This talk will delve into the concept of lithium bonds, exploring their underlying chemistry and how they can be harnessed to design new battery material combing with emerging artificial intelligence and further improve battery performances. Specifically, solid electrolytes combined with high-voltage Li-rich Mn-based cathodes and anode-free cell designs hold significant promise for high-energy-density and high-safety systems. However, challenges such as interfacial oxygen escape and unstable anode morphology continue to hinder their widespread applications. To address these issues, we have developed a fluoropolyether-based solid polymer electrolyte featuring a novel anion-rich solvation structure, which stabilizes the interface and enhances cycling stability. The resulting pouch cell demonstrates an ultra-high energy density (>600 Wh/kg) and excellent safety under a nail penetration at a full charge condition, advancing solid-state battery technology and paving the way for safer, higher-energy systems.

Keywords: lithium bonds, high-energy-density, solid polymer electrolyte

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Design electrolyte solvent molecule for energy-dense lithium batteries

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ABSTRACT

Since its commercialization in the 1990s, lithium-ion batteries have been widely used in mobile devices, electric vehicles and other fields. In order to satisfy the further demand of batteries such as fast charging, low temperature tolerance, high energy density, the research of electrolyte has attracted more and more attention in recent years. The electrolyte not only plays the role in the transport of lithium ions in the battery, but also has an important impact on the stability of the electrode - electrolyte interphase, as well as the improvement of the battery's fast charge and low temperature performance. Up to now, how to find a balance between the electrode/electrolyte interphase and the kinetics of electrolyte bulk is a difficult issue in electrolyte research.

This report focuses on how lithium ion coordination structure affects the ionic transport and interfacial dynamics on electrode surface. Based on the ion transport characteristics and the solvation structure, the “hopping” or “vehicle” transport behavior dependent on the electrolyte solvent was proposed, in which hopping mechanism was revealed to exhibit the best fast charging performance. Then, in the lithium-ion battery system, through molecular design, the traditional five-membered ring coordination structure of Li-ion was replaced by four-membered ring coordination, and the binding energy was thus largely reduced due to the weaker electron donating ability of methyl group, which resolved solvent co-intercalation of traditional ether electrolyte towards graphite anode and improved the low temperature performance of the batteries. In lithium metal battery system, a series of six-membered ring coordinated ether solvents were designed and synthesized, which could achieve more anion participation in Li-ion coordination ascribing to steric effect. Through fluorine atom substitution, the solvation ability was further regulated. It was found that fluorine substitution could improve the transference number of lithium ion, accelerate the kinetics of charge transfer, and elevate the Coulombic efficiency of lithium metal stripping/platting. In summary, the long cycling performance and interfacial charge transfer kinetics of Li-ion batteries and Li metal batteries can be effectively adjusted by designing the molecule structure of electrolyte solvents.

Keywords: coordination structure, Li-ion batteries, lithium metal batteries, electrochemical interphase

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Electrochemical Isotope Effects in a Lithium-Sulfur Battery

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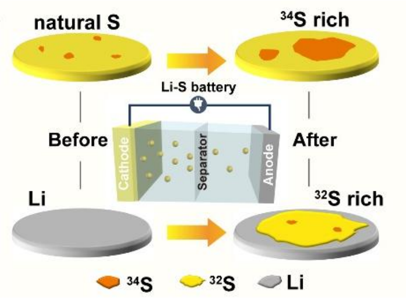
ABSTRACT

Isotope effect refers to the differences in physical and chemical properties between isotopic atoms (or molecules) of the same element, which originates from nuclei-related differences including nuclear mass and nuclear spin. Although basic physiochemical properties are governed by nuclear charge, isotopes exhibit noticeable isotope effects under certain circumstances. Currently, the isotope effects in electrochemical systems are often overlooked. Here, we initially investigate electrochemical isotope effects in lithium-sulfur batteries, and unveil the differences of electrochemical behaviors between stable isotopes of sulfur ($^{32}S/^{34}S$). Provided with the same octatomic ring structure, the cyclo-$^{34}S_8$ molecules form stronger S-S bond than cyclo-$^{32}S_8$, and are more prone to react with Li. The soluble Li polysulfides generated by the Li-^{34}S conversion reaction show a stronger cation-solvent interaction yet a weaker cation-anion interaction than the counterparts generated by the Li-^{32}S reaction, which facilitates quick solvation of polysulfides yet hinders their migration from the cathode to the anode. Consequently, the Li-^{34}S cell shows improved cathode reaction kinetics at the solid-liquid interface and inhibited shuttle of polysulfides through the electrolyte, so that it demonstrates better cycling performance than the Li-^{32}S cell. The suppressed cathode-anode crosstalk in the Li-^{34}S battery also accounts for reduced heat generation at the Li-anode surface, so that it demonstrates improved battery thermal safety. Based on the inhibited shuttle effect of the ^{34}S-based polysulfides, a new electrochemical separation method for $^{34}S/^{32}S$ isotope is proposed using Li-S battery. This electrochemical separation method demonstrated a separation ratio one or two magnitudes higher than the conventional methods via chemical exchange or distillation, which brings new opportunities to low-cost manufacture, utilization and research of chalcogen isotopes.



Figure

Keywords: lithium-sulfur battery, stable sulfur isotope, isotope effect, isotope separation

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Development of High-Performance Electrode Materials for Next-Generation Batteries: Insights from *Operando* Imaging

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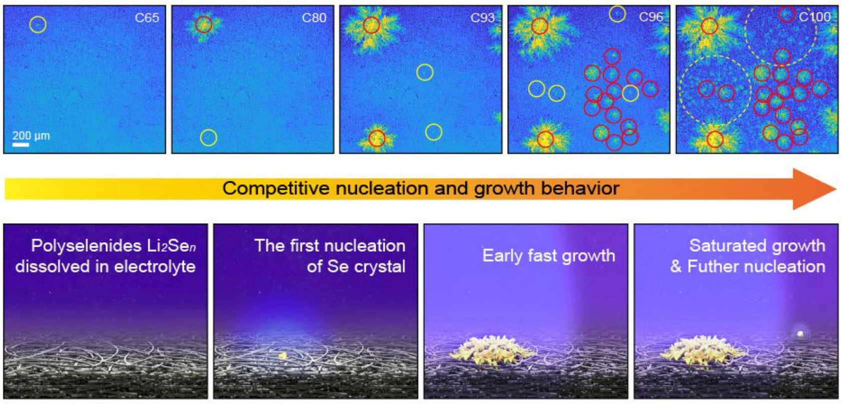
ABSTRACT

Lithium-ion batteries (LIBs) are widely used in devices like smartphones, laptops, and electric vehicles due to their high energy density and efficiency. However, as technology advances, the demand for even higher energy storage capacity is growing, and LIBs are increasingly unable to meet these needs. This highlights the urgent need to explore alternative battery technologies that can either supplement or replace LIBs to support future energy requirements. A key challenge in developing next-generation batteries is understanding the complex electrochemical reactions that occur during the charge and discharge cycles. Gaining a deeper understanding of these reactions is essential for designing more efficient and reliable energy storage systems. This presentation will focus on the reaction mechanisms in post-lithium-ion batteries, particularly the use of advanced operando imaging techniques. While lithium metal anodes and sulfur cathodes show promising theoretical capacities, their practical use is limited due to poorly understood and intricate reaction pathways. Operando microscopy is an emerging tool that allows real-time observation of structural and chemical changes within battery electrodes, offering valuable insights into the dynamic processes that affect battery performance. This technique enables researchers to visualize how materials behave during cycling, which is crucial for improving battery efficiency and lifespan. Ultimately, the goal of this research is to advance the development of next-generation batteries. By unraveling the electrochemical mechanisms and gaining a clearer understanding of material behaviors, researchers can design more efficient and reliable energy storage systems to meet the increasing global demand for advanced technology and sustainable energy solutions.



Figure

Keywords: lithium metal anode, Sulfur cathode, operando imaging

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Solvent-Mediated Regulation of Thermodynamics and Kinetics in Electrocatalytic Reactions

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ABSTRACT

Electrocatalytic reactions primarily occur at the electrode/electrolyte interface, where the solvent plays multiple critical roles in this interfacial system. As a reaction medium, the solvent not only modulates the micro-environment of the electrode interface but also directly participates in proton and electron transfer processes, thereby significantly influencing the thermodynamic and kinetic behaviors of the reaction. From the perspective of solvent engineering, we systematically investigated the regulatory mechanisms of solvent properties on electrocatalytic reactions: by designing solvent systems to alter the molecular configuration of ionomers, thereby adjusting the adsorption behavior of intermediates and the hydrogen bond network structure on the electrode surface; constructing multi-component solvent systems to modify the ion distribution characteristics in the electric double layer, enabling precise control over key steps such as adsorption, diffusion, and mass transfer during the reaction; and mediating the proton-electron coupled transfer process through electrolyte system design to achieve selective regulation of reaction pathways. This report will focus on elucidating how solvent system design enables precise control over electrocatalytic reaction pathways by modulating ionomer configurations, optimizing electric double-layer structures, and mediating charge transfer processes. Furthermore, it aims to establish a universal theoretical framework for solvent effects, providing new insights for the design of highly efficient electrocatalysts.

Keywords: Solvent effect, electrocatalysis, interface, thermodynamics, kinetics

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Functional Gel Materials Derived from Glycolysis Products of waste PET

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ABSTRACT

Polyethylene terephthalate (PET) has become the fifth most widely produced synthetic plastic. With its extensive use, the accumulation of waste has made the chemical recycling of PET a research hotspot. Currently, the recycling rate of post-consumer PET waste is only 1/3, while the remainder is disposed of through landfilling or incineration, leading to resource wastage and environmental pollution. Compared to reprocessing, products derived from plastic waste can save 50% to 60% of energy. Therefore, promoting the green closed-loop recycling of post-consumer PET, extending its lifecycle, and facilitating the development of a circular economy are crucial. In this study, we utilized the glycolysis process of PET to incorporate building blocks with rigid aromatic rings and hydrogen-bonding active sites into gels, resulting in a series of high-value materials such as ionicgels, eutectogels, and hydrogels. The abundant benzene ring structures and the double network system within the PET building blocks endow the gels with excellent mechanical properties, outstanding conductivity, and numerous binding sites. This enables the fabrication of high-performance gel-based electronic skin and adsorbent materials. This research offers a simple and cost-effective solution for the high-value utilization of PET.

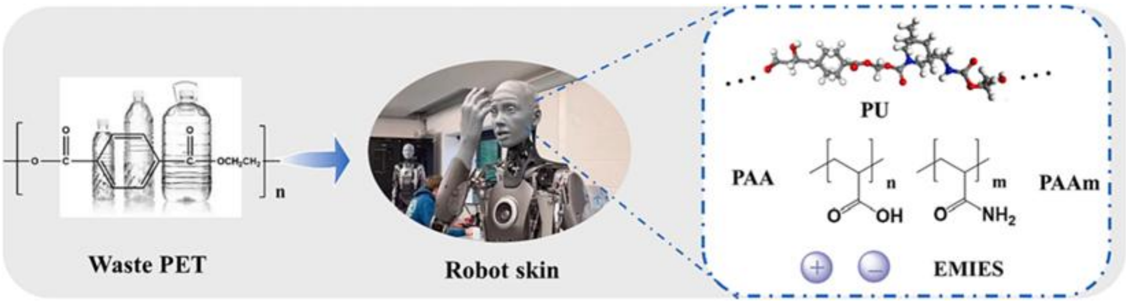

Figure Schematic diagram of PET conversion into ionicgels

Keywords: PET, valorization, gels, e-skin, adsorbent

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Designing Li-rich Ni-based cathodes for Li-ion batteries

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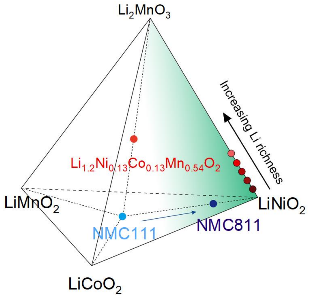
ABSTRACT

The current exploration of high-energy-density cathode materials is ongoing along two routes. The first concerns the so-called Li-rich materials, $Li_{1+x}M_{1-x}O_2$ (M denotes transition metal hereafter), with additional Li ions partially replacing M ions at the transition metal layer. They can provide exceptionally high capacities (>250 mA h g^{-1}) stemming from anionic redox phenomenon, a paradigm-shift concept that is receiving worldwide attentions. However, this class of materials are plagued by their common shortcomings such as voltage hysteresis and voltage fade brought forward by the anionic redox, and their prospect of practical use remains unclear unless these bottlenecks are overcome.

In parallel, the community is also striving on another strategy - the so-called Ni-rich (or high-Ni) oxides with either the $LiNi_xCo_yMn_{1-x-y}O_2$ (NMC) or $LiNi_xCo_yAl_{1-x-y}O_2$ (NCA) compositions with x typically equal or larger than 0.8. They are derived from $LiNiO_2$ and are generating great interest owing to their high capacities (> 200 mA h g^{-1}) and high working potentials (~3.8 V). However, these Ni-rich electrodes are suffering from mechanical, electrochemical and thermal stability issues that, in some extent, limit their commercial use. Therefore, our society is in dire need of new strategies for circumventing such weaknesses while keeping or even increasing the cathode capacity.

Here, we combine these two concepts to obtain Li-rich Ni-based oxides in pursuit of more practical high-energy-density cathodes. We developed a series of Li-rich Ni-rich oxides cathode based on high-valent TM ions, such as $Li_{1.09}Ni_{0.85}Mo_{0.06}O_2$, as well as cathodes that have medium Ni content like $Li_{1.12}Ni_{0.64}Mn_{0.24}O_2$. We systematically investigated their structure, electrochemistry and redox mechanisms that may provide insights for future cathode design.



Figure

Keywords: Li-ion batteries, cathodes, layered oxides, Li-rich, anionic redox

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AI-Assisted Study on Solid-State Electrolytes for Lithium Batteries

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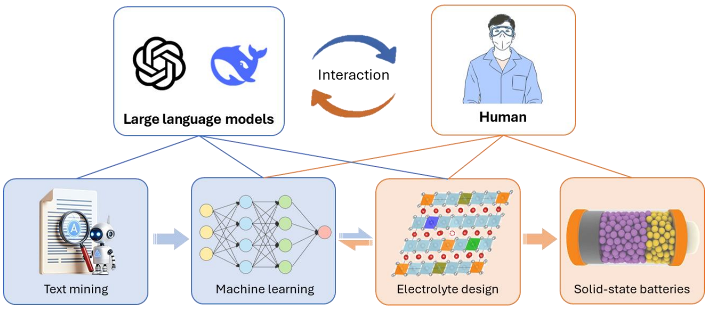
ABSTRACT

Solid-state lithium batteries (SSLBs) represent a transformative advancement in energy storage, offering enhanced safety and energy density over conventional liquid electrolyte systems. However, the development of high-performance solid-state electrolytes (SSEs) with superior ionic conductivity and electrochemical stability, particularly against lithium metal anodes, remains a critical challenge. Concurrently, artificial intelligence (AI), encompassing machine learning (ML) and large language models (LLMs), has emerged as a powerful tool to accelerate material discovery and optimization, creating great opportunities for the development of SSLBs.

Our study integrates domain-specific chemistry with AI to explore novel SSEs, focusing on three interconnected research aspects. First, a chemistry-informed ML framework is developed to design multi-anion-doped lithium halide SSEs. By embedding experimental information into feature engineering and machine learning, the model identifies SSE compositions that balance high ionic conductivity and stability against lithium metal, which has been a long-standing difficulty for halide SSEs. Second, a multi-agent LLM system is engineered to explore lithium oxyhalide SSEs. LLM agents collaborate to process literature through text mining, propose candidates through data analyzing, and predict properties through machine learning, leading to the discovery of a LiTaOCl-type of SSEs, which exhibit exceptional ionic conductivity and battery performance. Third, an intelligent mining platform combining LLMs and representation learning is developed to screen metal-organic framework (MOF) databases for SSE candidates. This approach identifies MOF-derived electrolytes with tunable Li^+ migration channels, achieving competitive ionic conductivities and electrochemical performances.

Collectively, our work demonstrates the synergistic potential of AI and materials science in addressing complex challenges in SSLBs. The developed frameworks not only advance the understanding of SSE design principles but also establish a paradigm for accelerated, data-driven discovery of next-generation battery materials, paving the way for safer, high-energy-density energy storage systems.



Figure

Keywords: solid-state lithium batteries, artificial intelligence, large language models, lithium halide electrolytes, metal-organic framework

Electrolyte architecting for aqueous batteries: playground for molecules

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ABSTRACT

Rechargeable aqueous batteries are being widely studied for their potential application in static energy storage as a high-safety alternative to the current lithium based batteries. The key challenges are relatively low energy density due to limited thermodynamic voltage window and short cycle life due to metal anode instability. Despite the tremendous progress in fundamental understanding and battery performance, mitigating the formidable challenges of metal dendrites, corrosion, and electrode instability, especially for large batteries, is still the holy grail. In this talk, I will discuss our recent progress in aqueous Zn and Sn batteries, showcasing our synchronous electrolyte strategies tailored for metal anodes and halogen cathode.

Keywords: aqueous Zn batteries, dendrites, hydrogel, zinc-iodine battery, electrolyte engineering

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Cheminformatic Methodologies toward Sustainable Electrocatalytic Synthesis of Chemicals and Fuels

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ABSTRACT

Exploiting the chemical sensitivity of nanomaterials that can be transformed into electrical signals, we have employed integrated and comprehensive on-chip signaling and electrochemically based cheminformatic approaches as new tools for the mechanistic study of key electrochemical interfacial processes in the research of materials, clean energy and sustainable synthesis. In specific, we have developed an on-chip electrical transport spectroscopy (ETS) for directly probing, via nano-electrochemical and nano-electronic approaches, the electrochemical surfaces of metallic nanostructures under *in operando* catalytic conditions. This study defines a novel on-chip characterization strategy, as an alternative to the traditional spectroscopic techniques, for *in situ* chemical signaling. In addition, different experimentally-derived electro-descriptors were developed for the machine-learning investigations of various chemical synthetic methodologies.

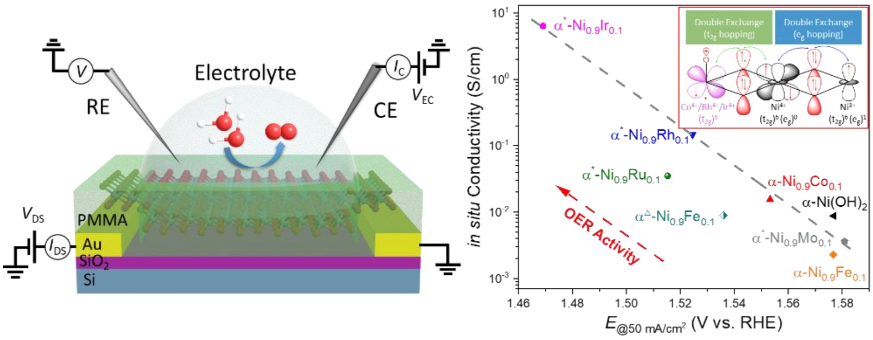

Figure 1 On-chip electrochemical and electrical transport measurements: an emerging platform

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Rechargeable Metal-Sulfur Batteries

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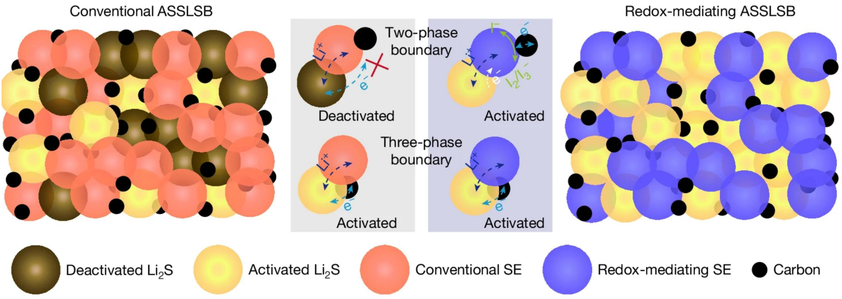
ABSTRACT

Rechargeable batteries are one of the key elements in promoting renewable energy utilization and transportation electrification, which are critical for carbon neutralization. Sulfur is an earth abundant element that is cheap and can offer high redox capacity, and therefore can have great potential to serve as an electrode material for rechargeable batteries. This talk summarizes our research progress on (1) liquid electrolyte design for lithium-sulfur battery, (2) solid electrolyte design for all-solid-state lithium-sulfur batteries, and (3) low-cost and highly safe aluminum-sulfur battery based on molten salt electrolytes. The emphasis is on the foundational chemical principles for designing high-performance sulfur batteries, strategies to tune the chemical reactions and the materials approaches to achieve such strategies, and examples of how to establish high-performance sulfur batteries.



Figure

Keywords: lithium-sulfur battery, solid-state battery, aluminum-sulfur battery

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Ionic Liquids Based High Safety Electrolytes for Rechargeable Batteries

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ABSTRACT

Developing high-performance lithium batteries is an important challenge and a major national strategic demand faced by the current academic and industrial communities. The high conductivity, wide electrochemical window, and flame retardancy of ionic liquids determine their inherent advantages in the field of electrochemistry. Our research group has been engaged in the design of ionic liquid functional electrolytes and the development of new electrochemical energy storage systems, mainly including new mechanisms for electrolyte-electrode interfaces, new strategies for electrolytes functionalization, and large-scale preparation and industrial applications of electrolytes. We have designed and developed a series of new electrolyte materials, which have been applied to lithium-ion batteries, solid-state batteries, sodium ion batteries, zinc ion batteries, etc, Provide important support for improving the performance of related energy storage devices.

Keywords: ionic liquid, electrolyte, interface, lithium ion battery, solid state battery

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High voltage solid polymer electrolyte

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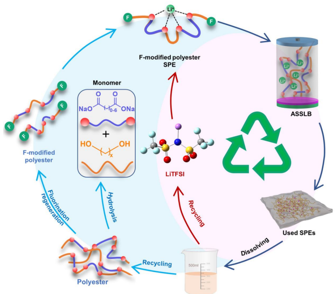
ABSTRACT

Solid polymer electrolytes own the advantages of high flexibility, seamless interfacial contact and low cost, but are limited by the relatively low ionic conductivity and narrow electrochemical window. To reveal the relationship between polymer structure and electrochemical performance, a series of linear poly-esters were prepared and demonstrated that the molecular asymmetry is critical for the ionic conductivity. To improve the ionic conductivity and maintain a high voltage stability, a family of ether-free polyacrylates were prepared with carbonate as Li^+-coordinating pendant, which show a high polymerization degree of 100% in the Li-metal containing cells and possess a high voltage stability even when matching 4.6V $LiCoO_2$ and 4.8V lithium-manganese-rich oxide. In addition, to make the solid-state batteries more sustainable, the recycling strategy of solid-polymer electrolyte and high value Li-salt was also explored.



Figure

Keywords: solid state batteries, polymer electrolyte, high voltage, electrolyte recycling

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Advanced Phosphate Cathodes for Sodium-Ion Batteries

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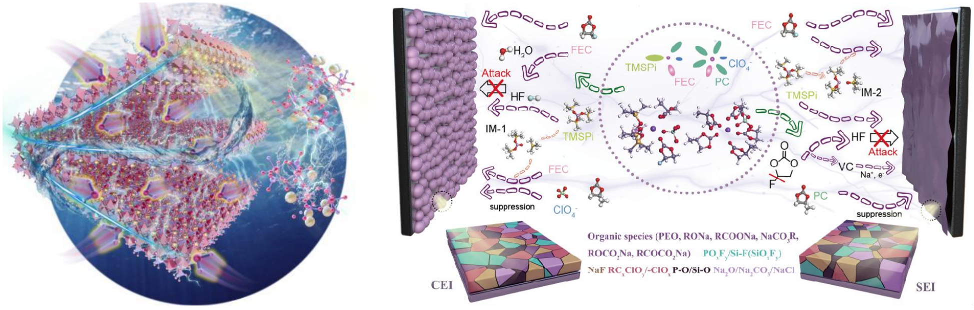
ABSTRACT

The electrode materials, especially the cathode materials, play a key role in the storage characteristics of the alkali metal ion batteries such as sodium-ion batteries based on the "rocking chair" energy storage mechanism. As one of the typical materials, phosphate cathode materials with covalent framework still encounter some challenges, such as poor electronic conductivity, low operating voltage, and insufficient practical cycle life. This report will focus on the design of phosphate cathode materials in sodium-ion batteries for high voltage and energy density, long cycle life, excellent rate and wide temperature range through lattice regulation (high entropy, high electronegativity anion substitution, hydroxyl radicals/H_2O molecules synergistic enhancement of 2D exfoliation, isostructural anion doping, aliovalent cationic doping, etc.), precise carbon network construction and anion-cation relay composite material strategies, and analyze the improvement mechanism involved. In addition, for the phosphate cathode-based spent lithium-ion batteries, new concepts such as simultaneous recycling of cathode and anode are proposed, realizing the green closed-loop recycling of "turning waste into treasure".



Figure

Keywords: sodium-ion batteries, cathode materials, phosphate

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2D Materials for High Energy-Density Lithium Metal Batteries

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ABSTRACT

To address the challenges of lithium dendrite growth and poor stability in lithium metal batteries, the presenter employed two-dimensional (2D) materials to enhance battery performance. Ultrathin 2D materials were used to regulate the thermal and kinetic behaviors of lithium metal anodes, enabling uniform lithium-ion flux distribution and elevated interfacial potential at the lithium metal/electrolyte interface. This dual mechanism effectively suppresses dendrite formation and parasitic reactions, resulting in a tenfold improvement in cycling performance. Furthermore, 3D ‘hard’ carbon is proposed to realize composite lithium metal anode to inhibit the volume swelling effects. At last, salt-template strategy combined with melt-assisted synthesis was developed to achieve precise control over particle size and layer thickness during large-scale production, enabling industrial-scale fabrication of 2D material/lithium metal composite electrodes. The resultant lithium metal pouch cells demonstrate an impressive energy density of 500 Wh/kg and long cycle stability.

Keywords: 2D materials, Li metal battery, Li dendrite, volume swelling, synthesis

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Organosulfide Molecules for Rechargeable Batteries

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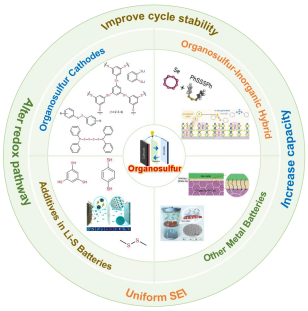
ABSTRACT

Organosulfide molecules such as dimethyl trisulfide (DMTS) containing sulfur-sulfur bonds are a class of potential high-capacity cathode materials for batteries. However, most of them are soluble in liquid electrolyte, which makes it difficult to keep them electrochemically reversible in rechargeable batteries. In 2016, our group reported the first study of DMTS as a cathode material in rechargeable lithium batteries by utilizing a carbon nanotube paper as current collector. Afterwards, we reported several organosulfide cathode materials such as diphenyl polysulfides and dipyridyl trisulfide etc. By using a series of characterization techniques, we are able to reveal their redox mechanisms in rechargeable batteries. In addition to being cathode materials, these organosulfide molecules can be used as functional materials as electrolyte additives, deep eutectic electrolyte, and key components in solid-electrolyte interphase in batteries. In this talk, I will introduce our approach to enable the electrochemical reversibility of these soluble molecules and reveal their redox mechanisms. The intriguing redox mechanisms associated with organosulfides provide a broad space to develop advanced cathode and batteries for the next-generation electrochemical energy storage devices.



Figure

Keywords: organosulfide, cathode, electrolyte, rechargeable battery

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Complex Hollow Structures for High-performance Li/Zn Metal Batteries

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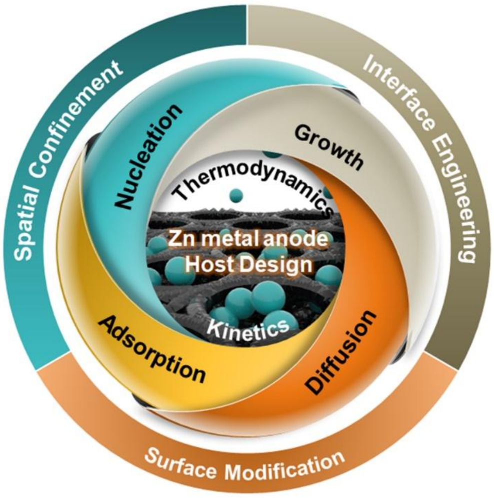
ABSTRACT

The energy crisis and greenhouse effect have aroused enormous research effort for developing effective electrochemical energy storage systems (EESs). Metallic Li/Zn is widely considered as the ultimate anode for the next-generation high-energy-density rechargeable batteries owing to its extremely high theoretical specific capacity and the low reduction potential. Despite these obvious superiorities, the practical application of the Li/Zn metal anode still faces great challenges associated with the repeated plating/stripping cycles. Particularly, inhomogeneous deposition leads to the formation and growth of dendrites, which could puncture the separator and cause internal short circuit. Among the available strategies, utilization of 3D porous/hollow carbonaceous scaffolds as both the Li/Zn host and current collector has been considered as an attractive strategy for dendrite-free Li/Zn metal batteries. Fabricating hollow nanostructures with high complexity by manipulating their geometric morphology, chemical composition, building block, and interior architecture has shown huge impact on the development of 3D porous/hollow hosts for Li/Zn metal batteries. This report summarizes our recent progress towards complex hollow nanostructure design as functional host for Li/Zn metal anode and take a prospect for its research future.



Keywords: hollow, porous, Zn ion batteries, Li ion batteries

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Theoretical study on controllable synthesis and property modulation of 2D materials

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ABSTRACT

The unique structure and quantum confinement effects of two-dimensional (2D) nanomaterials endow them with broad application prospects in fields such as information technology and energy. Designing 2D materials with superior physicochemical properties and achieving controllable synthesis of high-quality samples are prerequisites for studying their properties and applications. Multiscale approaches, including first-principles calculations and molecular dynamics simulations, provide atomic-level insights into material properties and synthesis mechanisms. This presentation will discuss the speaker's research progress in the theoretical design of 2D materials and the mechanisms of their controllable synthesis from the perspective of multiscale theoretical simulations, encompassing: (i) Development of multiscale simulation methodologies; (ii) Nucleation and growth mechanisms of 2D materials; (iii) Design and property modulation of 2D materials.

Keywords: 2D materials, multiscale calculations, crystal growth mechanisms, structure-property design and modulation

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Trajectory surface hopping molecular dynamics simulation with TDDFT for large complexed systems

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ABSTRACT

The time-dependent density function theory (TDDFT) provides accurate ab. initio potential energy surfaces for performing nonadiabatic molecular dynamic simulation for large photochemical systems, and global switching algorithm in which calculation for nonadiabatic coupling vectors are not necessary makes trajectory surface hopping molecular dynamics simulation even easier and faster. However, it is well-known that ordinary TDDFT has difficulty in describing the S0/S1 conical intersections. It was demonstrated that potential energy surfaces calculated by TDDFT with and without spin-flip can simulate quite similar answer for average quantities like quantum yields and lifetimes [1].

Furthermore, global switching trajectory surface hopping molecular dynamics simulation on ordinary TDDFT potential energy surfaces can correctly describe complicated conical intersection networks between the S0 and S1 for ultrafast photoisomerization of dMe-OMe-NAIP [2] as well as for retinal protonated Schiff-base photoisomerization [3]. Simulated quantum yields and lifetimes agree well with experimental measurements. It was confirmed that the ordinary TDDFT on-the-fly potential energy surfaces could be very reliable simulation method for large photochemical and photophysical systems associated with global nonadiabatic switching method in which quantum effect of nuclear motion is explicitly considered.

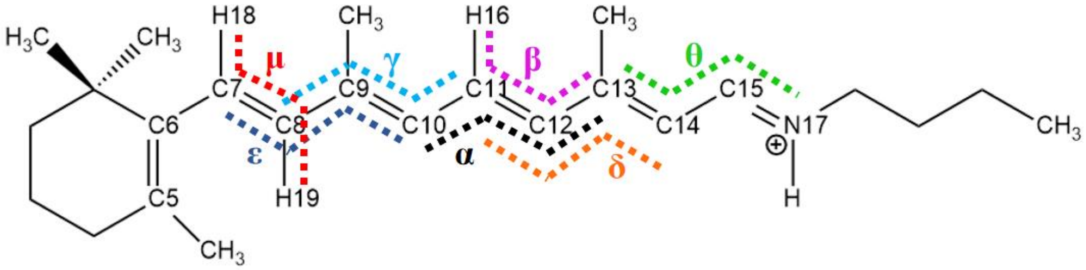

Figure. Seven dihedral angles form the complicated conical intersection networks for protonated Schiff-base photoisomerization

Keywords: Nonadiabatic molecular dynamics, TDDFT method, global switch, conical intersection, excited state potential energy surface.

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Artificial Intelligence-Driven Development of Nickel-Catalyzed Enantioselective Cross-Coupling Reactions

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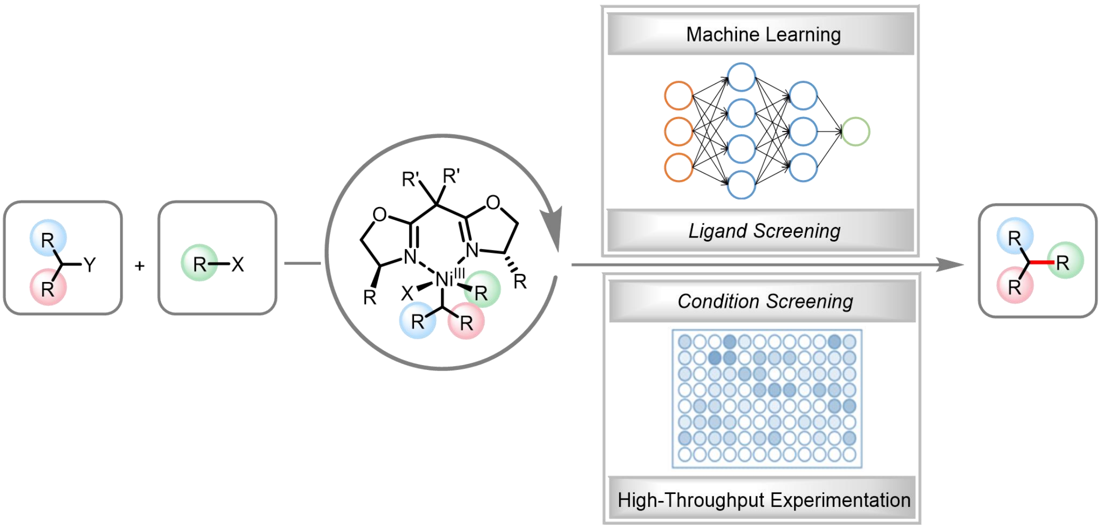
ABSTRACT

The conventional approach to developing asym metric synthetic methods relies heavily on empirical optimization. However, the integration of artificial intelligence (AI) and high throughput experimentation (HTE) technology presents a paradigm shift with immense potential to revolutionize the discovery and optimization of asymmetric reactions. In this study, we present an efficient workflow for the development of a series of nickel-catalyzed asymmetric cross-coupling reactions, leveraging AI and HTE technology. Many nickel-catalyzed enantioselective cross-coupling reactions share a common Ni(III) intermediate, which dictates the enantioselectivity. To harness this mechanistic insight, we embarked on developing a predictive model for nickel-catalyzed enantioselective coupling reactions, elucidating the general rules governing enantioselectivity. Through the application of data science tools and HTE technology, we curated a data set to construct an AI-based model. This model was subsequently utilized to facilitate the discovery of efficient nickel hydride-catalyzed enantioselective and regioselective cross-coupling reactions. Employing AI-assisted virtual ligand screening and HTE-enabled condition optimization, we successfully identified optimal ligands for eight coupling reactions. Consequently, a series of chiral sp3 C－C bonds were synthesized with high yield and enantioselectivity.



Keywords: artificial intelligence, high-throughput experimentation, nickel, cross-coupling, AutoGluon

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AI-Driven Closed-Loop Discovery and Development for Electrolyte of Lithium Batteries

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ABSTRACT

AI for Science provides an new opportunity to accelerate the research and development (R&D) of energy materials using AI. The discovery and development of new low-temperature electrolytes is crucial for lithium-ion batteries to maintain high energy density and stable cycle performance under subzero conditions, addressing critical challenges in cold-climate applications such as electric vehicles and energy storage systems [1]. Advanced electrolyte formulations enable lithium-ion batteries to overcome severe capacity fading and safety risks caused by sluggish ion transport and electrolyte solidification in extreme cold environments. Classical electrolyte R&D relies on manual, experience-based approaches with slow iterative cycles, while the current industry urgently demands AI-driven R&D paradigms to accelerate the discovery and optimization of advanced electrolyte formulations [2].

We established a closed-loop R&D framework involving AI-driven automated experiments, multi-dimensional characterization, and AI-accelerated calculation. The automated experimentation module combines electrolyte auto-formulation and automated cell assembly to eliminate human-induced errors, and the characterization module focuses on automated Raman spectroscopy analysis of electrolytes, where spectroscopic data enables in-depth investigation of lithium-ion solvation structures. Leveraging high-quality experimental electrochemistry and spectroscope data, the AI-accelerated calculation model, Uni-ELF, efficiently recommends optimal formulation ratios in collaboration with Prof. Weinan E and DP technology. In the first two rounds of formulation recommendations, the Uni-ELF algorithm prioritized coulombic efficiency and discharge specific capacity as optimization targets, generating two rounds of candidate formulations. The automated experimentation module subsequently conducted experimental replication of the recommended electrolyte compositions. The replicated results were then fed back into the algorithm for model refinement. During the third and fourth iterative cycles, we summarized and incorporated multiple chemical prior knowledge rules based on earlier experimental outcomes, which significantly enhanced the model's recommendation accuracy. After six closed-loop iterations, the AI model converges to an optimal formulation demonstrating a specific discharge capacity of 205 mAh g^{-1}—a 10% improvement over manual-experience-based formulations, validating the efficacy of the AI-driven closed-loop approach for electrolyte of lithium batteries.

As perspective, the development of AI for Science infrastructure will provide an open platform for scientists and industrial partners for collaboration on empowering R&D of energy materials using AI.

Keywords: Electrolyte design, Closed-loop iterative optimization, Fluorinated solvents, High-throughput experimentation, Synergistic electrochemical effects

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When Knots Break Chains: Harnessing Molecular Topology to Control Polymer Mechanics

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ABSTRACT

Long polymer chains inevitably form entanglements, including various molecular knots, which significantly impact their mechanical properties[1,2,3]. Using reactive molecular dynamics simulations[4], we systematically investigate how knot complexity influences the tensile deformation behavior of polyethylene chains. Our results reveal that knots essentially act as stress concentrators[5], drastically lowering the force required for chain scission and accelerating the bond rupture. Specifically, we discover that the elastic modulus exhibits a power-law dependence on the number of crossing points in these knotted chains. Moreover, the maximum force to induce chain failure is found to follow a stretched exponential relationship with knot complexity. In addition, we observe that the chain-breaking mechanism shifts with knot complexity: simpler knots rupture at entrance/exit crossing points, whereas highly complex knots also fracture at central crossings. Furthermore, our simulations reveal that higher pulling velocities suppress stress relaxation, resulting in increased tensile forces and more abrupt failure events, with fractures predominantly occurring at the knot entrance and exit points. These results provide fundamental insights into the mechanical behavior of knotted polymers and highlight the potential of topological control in polymer material design, particularly in applications requiring tailored mechanical responses.

Keywords: polymer, knots, reactive molecular dynamics, topology

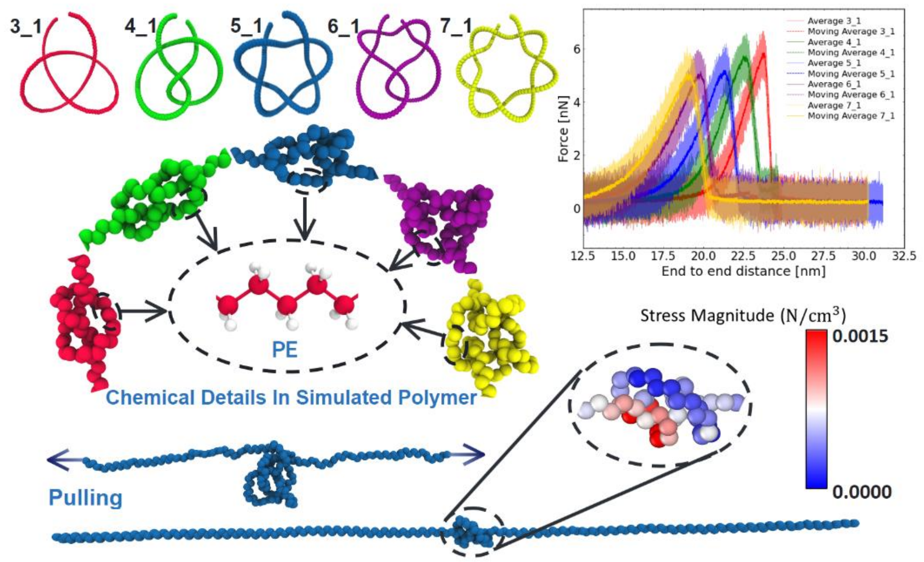

Figure: Graphic Abstract

Keywords: polymer, knots, molecular dynamics, ReaxFF, topology

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Efficient simulation of photo-induced dynamics processes and their spectroscopic characterization

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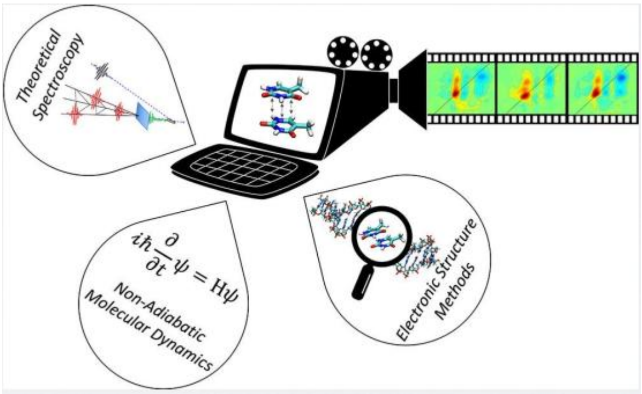
ABSTRACT

Modern techniques of ultrafast laser spectroscopy and ultrafast X-ray (electron diffraction), which are capable to achieve femtosecond and even attosecond time resolution and high spatial resolution, provide excellent probes of chemical reactions in various molecular systems. The constantly increasing body of experimental data on molecular and chemical reaction mechanisms necessitates the development of accurate theoretical methods, which enable us to explain spectroscopic signals of molecular systems as well as their associated structural changes in terms of the underlying nuclear and electronic dynamics. In the past years, I have developed various numerical methods based on variational wave function, quantum master equation, stochastic Schrödinger equation, mixed quantum-classical methods as well as machine learning techniques for the efficient simulation of quantum dynamics and nonlinear spectroscopic signals. My goal is to build a direct link between theory and experiment, to reveal the reaction mechanisms of photophysical and photochemical processes, and finally to provide important theoretical guidance for the design of efficient optoelectronic devices.



Figure

Keywords: variational wave function, quantum master equation, stochastic Schrödinger equation, mixed quantum-classical methods, ultrafast spectroscopy.

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AI4QD: Quantum dissipative dynamics in the age of machine learning

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ABSTRACT

Open quantum systems play a vital role in areas like quantum information, quantum memory, and energy transfer in photosynthesis. However, their complex nature makes exact characterization challenging. Traditional methods for investigating these systems are often limited by computational demands or an inability to fully capture quantum effects.

Recently, machine learning (ML) has shown promise in predicting quantum dynamics efficiently. Our research highlights ML's ability to speed up the propagation of quantum dynamics based on a short history.[1] In addition, we also demonstrate that we can bypass the need for historical data, enabling the prediction of future quantum states based solely on time and/or simulation parameters.[2,3] We've developed the open-source MLQD package[4] and the QD3SET-1[5] database to support these advancements, alongside a study comparing 22 ML models for simulating open quantum systems.[6] Moreover, we have proposed an approach to enforced physical constraints in ML-based quantum dissipative dynamics.[7, 8] In my talk, I will provide a detailed overview of these developments and their implications.

Keywords: Open quantum systems, Quantum dissipative dynamics, Machine learning

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Electronic polarization effects in organic optoelectronic materials

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Electronic polarization effects are commonly existing in organic optoelectronic materials, which have an important impact on the energetic levels of electronic states and organic optoelectronic mechanisms and properties. However, electronic polarization effects are a kind of long-range interaction, which need to include a large number of molecules and become a big challenge for theoretical calculations. Here, we developed accurate computational methods to evaluate the electronic polarization energies for organic optoelectronic materials. It was found that the polarization effects are beneficial to reduce the energy gap between the singlet and triplet excitons for donor-acceptor type organic thermally activated fluorescent molecules as well as the exciton binding energy and charge separation energy barrier for efficient organic photovoltaic materials, and thereby, new mechanisms were proposed for organic thermally activated fluorescence and free charge generation in efficient organic photovoltaics. In addition, we found that the doping efficiency of organic thermoelectrics is exponentially increased with the fluctuation of the polarization energy in organic semiconductors, which sheds light on improving organic thermoelectric doping efficiency.

Keywords: polarization effects, organic semiconductors, charge separation, thermally activated fluorescence

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Ab Initio Doorway-Window methods for simulation of nonlinear spectroscopic signals

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I will give a brief overview of a recently developed an *ab initio* theoretical framework and protocol for the on-the-fly simulation of femtosecond time-resolved transient-absorption pump-probe, electronic 2D, visible pump – X-ray probe, and strong-pump weak-probe spectra with quasi-classical trajectories [1]. The simulation protocol is based on the classical approximation to the doorway-window representation of third-order four-wave-mixing signals and accounts for the finite duration and spectral shape of the laser pulses involved.

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Unified Implementation of Relativistic Hamiltonians and Wavefunctions

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ABSTRACT

In this lecture, I will introduce a unified implementation of relativistic Hamiltonians based solely on physical arguments [1] as well as a unified implementation of relativistic wavefunctions via programming techniques [2,3]. The latter was made possible by first introducing a diagrammatical representation of four- or two-component relativistic Hamiltonians that is topologically the same as that used in the unitary group approach for evaluating the basic coupling coefficients between spin-free configuration state functions, and then by making full use of the metaprogramming furnished by C++. Once the module for the relativistic Hamiltonian matrix is made ready, no other modifications of the existing templates used for nonrelativistic wavefunction methods are necessary. In particular, there is no need to distinguish complex and real algebra.

Keywords: relativity, correlation, QED, iCI, metaprogramming

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The Defect Entropy

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ABSTRACT

Defects are intrinsic to soft matter systems. In this work, I will report the concept of the defect entropy. The applications of this new concept will be introduced in diverse fields.

Keywords: Entropy, defect, soft matter, polymer physics, Thomson problem

Reference

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Toward Fully Automated Scientific Research: Intelligent Agents for Simulation and Retrosynthesis Using Large Language Models

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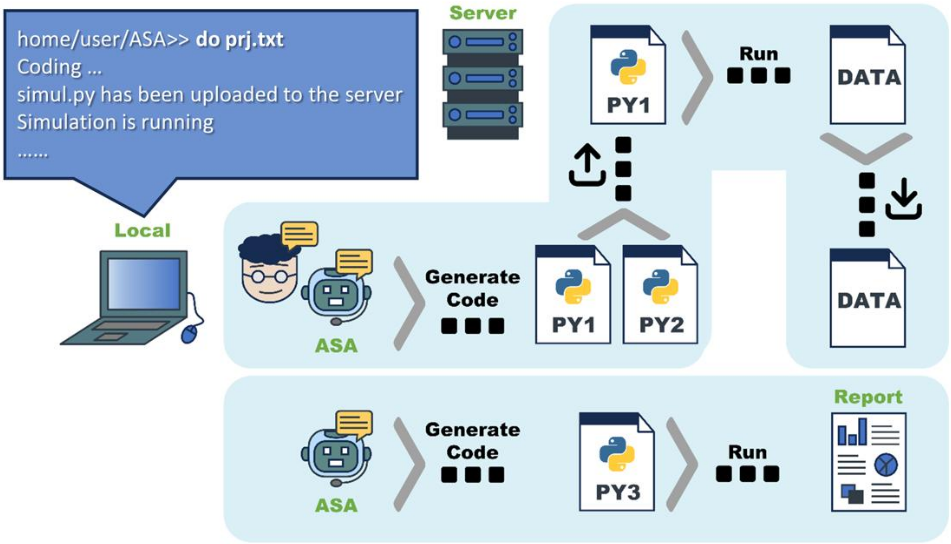
ABSTRACT

Large Language Models (LLMs) have opened new avenues for automating scientific research. This report presents an intelligent agent framework that enables end-to-end automation of simulation and synthesis workflows, requiring only a human-defined research plan. Two representative systems are highlighted.

The first is an Automated Simulation Agent (ASA) that automates the entire computational workflow—from program generation and remote execution to data analysis and report writing. Built using prompt engineering and dialogue history management, ASA demonstrates high reliability in tasks such as polymer chain conformation simulations. Notably, ASA can perform recursive tasks for up to 20 cycles without human input, illustrating its potential in long-duration automation.

The second system focuses on automated retrosynthesis planning for macromolecules, a domain traditionally hindered by ambiguous polymer nomenclature and sparse reaction databases. By integrating LLMs with a structured knowledge graph, the agent automatically retrieves literature, extracts reaction information, and constructs multi-branched retrosynthetic trees. A novel Multi-Branched Reaction Pathway Search (MBRPS) algorithm enables the discovery of complex synthesis routes. Applied to polyimide, the agent identified over 290 valid reaction pathways, including new alternatives.

Together, these systems represent the first reported attempts to realize fully autonomous research workflows in simulation and synthesis using LLMs. By combining text understanding, code generation, knowledge graph reasoning, and decision-making, the proposed framework significantly enhances research efficiency and points toward a new paradigm in AI-driven discovery.



```
home/user/ASA>> do prj.txt
Coding ...
simul.py has been uploaded to the server
Simulation is running
......
```

Figure Schematic of the automated simulation workflow

Keywords: Large Language Model, Automated Research Agent, Retrosynthesis Planning

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AI-Assisted Design of Polymer Structures

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ABSTRACT

Advanced polymer materials are playing an increasingly important role in aviation, aerospace, and civilian fields. However, traditional trial and error methods are difficult to solve some long-standing problems in material design and preparation and achieve disruptive changes. [1,2] Scientific research has shifted from experimental observation, theoretical deduction, and computational simulation to the fourth paradigm based on artificial intelligence (AI), and new research paradigms based on AI have made significant progress in fields such as life and pharmacy. [3] In recent years, a highly challenging topic has been the application of AI in the field of materials, transforming material research methods and achieving original innovation.

The reporter and team focused on polymer materials. They collected data, developed digital methods, and constructed a database. Moreover, through developing machine learning methods suitable for polymer characteristics, AI performance prediction models were established. Finally, they created a new method for structural design based on the concept of gene combination. A series of novel polymer materials have been designed and prepared using the new research paradigm. [4-7] For example, a database of epoxy matrix resins was established, descriptors describing cross-linking structures were developed, and a machine learning prediction model for the mechanical properties of epoxy resins was established based on Gaussian process regression. Based on this, resins with excellent mechanical properties were designed, and the mechanical properties of their composite materials were significantly improved. [6] In addition, this method has been applied to the design of organic photovoltaic materials. By establishing a photovoltaic material database, developing structural descriptors, and building a photovoltaic material performance prediction model based on deep learning, excellent photovoltaic materials with significantly improved performance have been designed. [7]

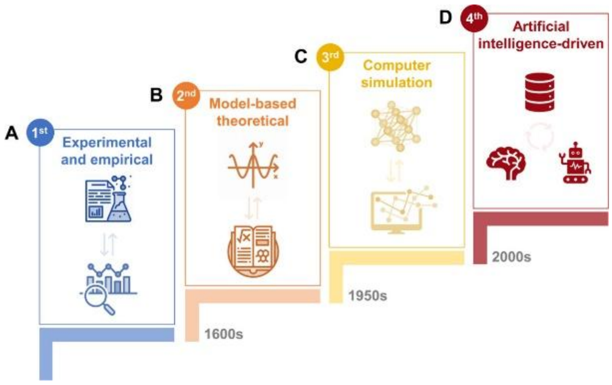

Figure1. Development of research paradigms: (A) experimental and empirical, (B) model-based theoretical, (C) computer simulation, and (D) artificial intelligence (AI)-driven paradigms.

Keywords: machine learning, polymer, structure design, high-performance resin

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Finite-Temperature Hole-Magnon Dynamics in an Antiferromagnet

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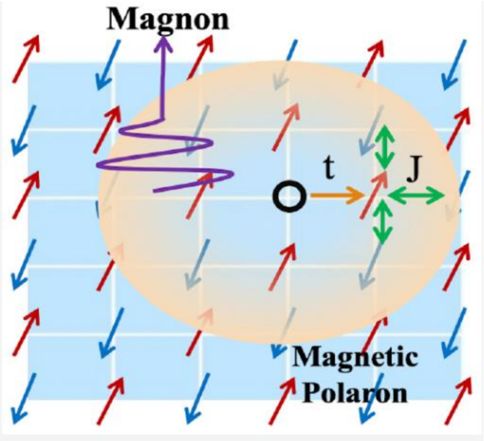
]

ABSTRACT

[Employing the numerically accurate multiple Davydov Ansatz in combination with the thermo-field dynamics approach, we delve into the interplay of the finite-temperature dynamics of holes and magnons in an antiferromagnet, which allows for scrutinizing previous predictions from the self-consistent Born approximation while offering, for the first time, accurate finite-temperature computation of detailed magnon dynamics as a response and a facilitator to the hole motion. The study also uncovers a pronounced temperature dependence of the magnon and hole populations, pointing to the feasibility of potential thermal manipulation and control of hole dynamics. Our methodology can be applied not only to the calculation of steady-state angular-resolved photoemission spectra but also to the simulation of femtosecond terahertz pump−probe and other nonlinear signals for the characterization of antiferromagnetic materials.]



Figure

Keywords: [*t*-*J* model, Thermo-field dynamics, Multiple Davydov D_2 Ansatz]

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Universal AI Models for Ground to Excited States

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ABSTRACT

Making universally transferable AI models for atomistic simulations promises to break through the cost/accuracy limitations of the traditional quantum mechanical (QM) methods. We have designed a series of such models for ground and excited state simulations. These models can be applied to almost all elements in the periodic table, molecules, and materials. Our AIQM-series models offer unprecedented robustness, accuracy, and computational efficiency across chemical compound space, particularly for organic and elemental-organic molecules, where the models are approaching accuracy beyond typical DFT for thermochemical properties, geometries, MD, IR spectra, and transition states.[1-5] We have also introduced the first-ever universal excited-state potential, OMNI-P2x.[6] In addition, we have created the foundational model for directly predicting MD trajectories, building on our previously proposed[7] novel concept.[8] All our implementations are available through MLatom (https://github.com/dralgroup/mlatom) and Aitomic (http://mlatom.com/aitomic/), and we provide online platforms for performing calculations via a web browser: Aitomistic Hub (https://www.aitomistic.xyz) and XACS cloud (https://XACScloud.com).

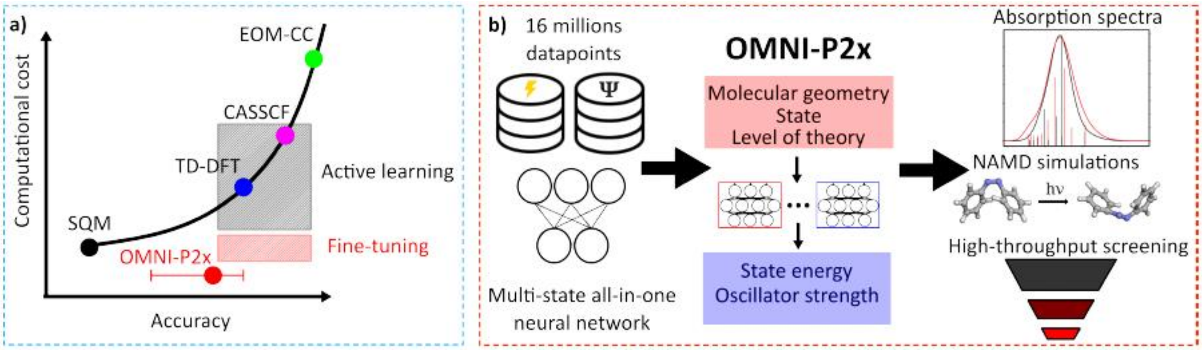

Figure. OMNI-P2x – the first-ever universal excited-state potential.[6]

Keywords: atomistic simulations, ML potentials, molecular dynamics, spectra, barriers.

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AB INITIO MODELLING OF PHOTOLUMINESCENCE

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In this contribution I present computational protocols to model photoluminescence in molecular systems which go beyond the nowadays routine modelling of emission energies. Our protocols merge state-of-the-art quantum chemical calculations, excited state decay rate theories (i.e., Fermi-golden rule based)[1] along with semi-classical nonadiabatic excited state dynamics to enable the quantitative determination of fluorescence lifetimes and quantum yields. In particular, I present an extensive analysis of the parameters influencing the excited state decay rate calculations.[2] Further, protocols to model anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states)[3] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical Non- Adiabatic Molecular Dynamics framework,[4] are presented. Finally, I present our recent efforts to expand our protocols from molecular systems to the solid state. In particular I present protocols allowing modeling the photophysical properties of organic molecular crystals. The objective is to evaluate the effect of various sources of disorder resulting in the broadening of UV-vis spectra.[5] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photophysics and photochemistry at the first principles level.

Keywords

Quantum chemical investigations, excited state decay rates, photoluminescence

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Importance of anharmonicities for describing vibronic coupling in excitation energy transfer dynamics of LH2

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ABSTRACT

The harmonic bath model has been adopted as an indispensable tool for simulating quantum dynamics of various complex systems such as photosynthetic pigment-protein complexes. However, molecular vibrations are intrinsically anharmonic and how important or unimportant the anharmonicities are is something that necessitates further discussion. For this discussion, we need very reliable vibrational potential energy surfaces but attaining enough reliability is often not so easy. The interpolation mechanics / molecular mechanics (IM/MM) has been proposed as a unique tool for combining physical reliability and computational efficiency toward simulating complex systems with their atomistic details [1]. In this presentation, we will discuss on my group's recent efforts on building the potential surface model for the light harvesting 2 (LH2) complex of purple bacteria. Through detailed comparison between the dynamics of a realistic molecular bath [2] with its harmonic representation [3], we will provide new details of the excitation energy transfer (EET) in LH2. We will see that the harmonic oscillator bath model can effectively reproduce the majority of the EET dynamics of those for anharmonic bath, confirming the validity of many spectroscopic data modelled by the harmonic oscillator bath. However, it falls short of representing the nonequilibrium nuclear dynamics even at qualitative level such as heat dissipation through anharmonic effects of pigment vibrations. Excitation-induced shape changes in the potential energy surface also influence the dynamics in a rather complex manner, suggesting that care is needed during the modelling stage for high fidelity simulations of vibronic dynamics. All in all, these results demonstrate the importance of accurately representing potential energy surfaces and correspondingly understanding dynamics for the elucidation of detailed molecular level features of light harvesting complexes.

Keywords: interpolation, anharmonicity, bath spectral density, semiclassical dynamics, pigment-protein complex

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Title: **Theory of adiabatic and non-adiabatic tunneling splitting**

Authors: Leonardo Raso, Michele Ceotto and Eli Pollak

Abstract:

The theory of tunneling splitting has challenged theory ever since Friedrich Hund discovered tunneling in double well potentials in 1927[i]. Estimating tunneling splittings is a long-standing quantum mechanical challenge for theoretical methods. Sometimes splittings are very small, i.e. within a fraction of a wavenumber, pushing the limits of experimental detection and computational precision.

Currently, most computational methods are able at best to obtain only ground state tunneling splittings, either for symmetric or asymmetric potentials. Obtaining tunneling splittings in excited states, apart from brute force numerical solution of the Schrödinger equation, remains a challenge. There is a difference between tunneling splitting as obtained on a single (adiabatic) electronic state to non-adiabatic induced coupling between two (or more) electronic states which then induces tunneling splitting. A third topic of interest is the difference between tunneling in symmetric and asymmetric systems. Typically, the tunneling probability in asymmetric systems is exponentially smaller than that of symmetric systems.

In this talk, I will present recent progress we have made[ii], by introducing a unified theoretical approach, based on a two-state approximation that can be equally applied to symmetric and asymmetric diabatic potential crossing and for excited states, providing reliable estimates even for states near the diabatic energy crossing. The method opens the door to analytic approximations for the tunneling splitting of model potential systems. It provides a framework for the introduction of vibrational perturbation theory to the estimation of nonadiabatic tunneling splittings. It also provides new insight into the semiclassical theory, leading to an instanton based steepest descent method applicable also to excited states. Numerical tests on model systems are promising, providing the groundwork for implementation to future multidimensional applications.

Energy near-degeneracy driven covalency analyzed by a two-electron two-orbital model

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ABSTRACT

A simple model based on the two-electron two-orbital textbook problem is presented and used to analyze pairwise interatomic interactions in metal-ligand bonding [1,2]. The covalency described by the model relies on the ratio $|v|/\Delta$ of two parameters, familiar from simple molecular orbital theory/diagrams, the interaction matrix element $|v|$ between two orbitals on different centers and the energy difference Δ between these orbitals. In particular the two types of covalency discussed during the last decade for actinide-ligand interactions, overlap/interaction driven and energy-near-degeneracy driven covalency [3,4], as well as their influence on the bond strengths and interatomic charge build-up are discussed (Figure 1). Special types of covalency, e.g., energy (near-)degeneracy driven covalency ('non-classical covalency'), cannot be clearly separated from the usual covalency discussed in chemistry. At best changes of covalency can be termed as overlap/interaction driven or energy (near-)degeneracy driven. Both the experimentally observed strengthening and weakening of bonding upon increasing the covalency can be explained. Hydration complexes $M(H_2O)_n^{4+}$ of selected tetravalent lanthanide and actinide ions are used to probe the performance of the model for an analysis of calculations as well as for predictions.

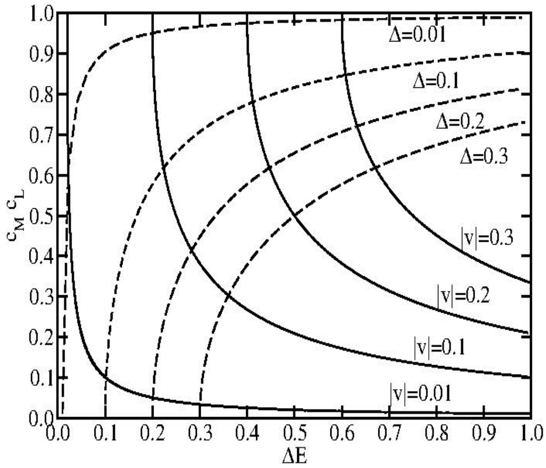

Figure 1: Measure for interatomic charge buildup vs. energy gain for two-center covalent bonding. Isolines for constant interaction |v| and constant energy gap Δ denote energy (near-)degeneracy driven and interaction driven changes of covalency.

Keywords: covalency, actinide compounds,

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Modeling Classical and Quantum Charge Transport in Advanced Electronic Materials

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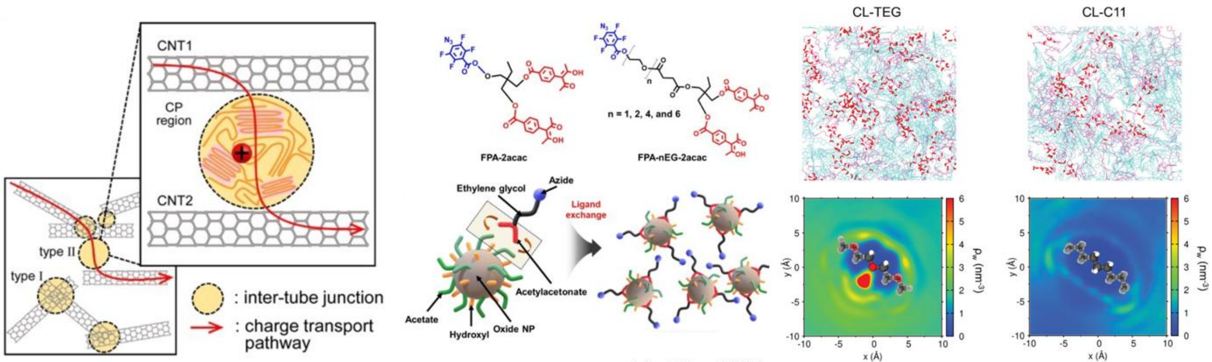
ABSTRACT

Charge transport plays a fundamental role in a wide range of advanced electronic materials, governing their efficiency and functionality. From energy storage and conversion to biological processes, charge carriers—ions, protons, and electrons—move through complex environments where their transport properties are dictated by molecular interactions, structural heterogeneity, and quantum effects. In this talk, I will present our efforts to model charge transport across diverse systems using advanced computational techniques, bridging classical and quantum descriptions to capture the underlying mechanisms.

Particularly, three ongoing development stories will be discussed: (1) developing first-principles based predictive polarizable force fields to model ion transport in highly charged liquid electrolytes and polymer electrolytes, where strong polarization and heterogeneous solvation environment produces complex correlated ion motion such as negative cationic transference number, (2) a novel hybrid Monte Carlo/molecular dynamics (MD) simulation approach to efficiently model proton transfer event in large scale condensed phase systems applicable to membrane fuel cell and biophysical channel proteins. (3) multi-scale simulation approach to the conjugate polymer interfaces at molecular level, including a CP-carbon nanotube (CNT) interface for thermoelectric application, and a CP-water interface for photocatalytic application. Through this, we offer novel insights for designing functional electronic materials in highly charged environments through advanced simulation techniques.



Adv. Electron. Mater. (2023)

Adv. Mater. (2024)

Adv. Sci. (2024)

Figure

Keywords: First-principles force-fields, Conjugated polymer, Proton transport, Charged interface, Polymer electrolyte

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Beating the viscosity-conductivity inverse relation barrier to create a breakthrough electrolyte for emerging battery applications: Quantum mechanics holds the key

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Candidate systems for next-generation battery electrolyte materials, such as deep eutectic solvents and ionic liquids, often suffer from the limitation of an inverse relation that exists between viscosity and conductivity, known as Walden's rule, which can suppress rates of charge transport and limit their performance characteristics. A strategy for circumventing this problem draws its inspiration from the world of fuel-cell based ion exchange membranes and the types of charge transport processes operative in these systems. In this talk, I will describe a project aimed at leveraging machine learning and Feynman path-integral based quantum simulation strategies, in combination with experimental synthesis and characterization, to develop a novel class of battery electrolytes that demonstrates an ability to escape the limitations of Walden's rule. In particular, I will describe how the charge transport processes in this new class electrolytes achieve breakthrough performance by harnessing their unusual quantum character to drive the structural diffusion or Grotthuss diffusion mechanism, a phenomenon discoverable due to the power of machine learning. I will discuss the selection of candidate chemical species for each of the component processes, protocols for combining these components into a high-performance electrolyte, current results, and next steps in the evolution of the project. This work will serve to illustrate both the power of modern computational and machine learning approaches in the design of electrochemical systems but also to broaden the perspective on what constitutes a "breakthrough" electrolyte.

Benchmarking Study of Deep Generative Models for Inverse Polymer Design

Molecular generative models based on deep learning have increasingly gained attention for their ability in de novo polymer design. However, there remains a knowledge gap in the thorough evaluation of these models. This benchmark study explores de novo polymer design using six popular deep generative models: Variational Autoencoder (VAE), Adversarial Autoencoder (AAE), Objective-Reinforced Generative Adversarial Networks (ORGAN), Character-level Recurrent Neural Network (CharRNN), REINVENT, and GraphINVENT. Various metrics highlighted the excellent performance of CharRNN, REINVENT, and GraphINVENT, particularly when applied to the real polymer dataset, while VAE and AAE show more advantages in generating hypothetical polymers. The CharRNN, REINVENT, and GraphINVENT models were further trained on real polymers utilizing reinforcement learning methods, targeting the generation of hypothetical polymers with high glass transition temperatures. The findings of this study provide critical insights into the capabilities and limitations of each generative model, offering valuable guidance for future endeavors in polymer design and discovery.

HETEROTRISPIN MOLCULAR MAGNETIC MATERIALS SYNTHETIC STRATEGIES

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The combination of different spin carriers is a valuable synthetic strategy to obtain molecular magnetic materials. Indeed, most of the 3-D molecule-based magnets and Single Chain Magnets (SCMs), as well as numerous Single Molecule Magnets (SMMs) are 3d-nd, nd-4f, 2p-nd, and 2p-4f heterobispin complexes. As far as the heterotrispin systems are concerned, they are less numerous. Such compounds contain either three different paramagnetic ions,[1] or two different paramagnetic ions and an organic radical (2p).[2] We currently develop new synthetic strategies leading to SMMs and SCMs, which are based on the combination of three different spin carriers (nd and 4f transition metal ions, as well as 2p or 3p radicals). The synthetic approach consists of self-assembly processes involving high spin anisotropic oligonuclear complexes (nodes) and various paramagnetic metalloligands (spacers).

In this lecture I will present our recent and most representative examples of heterotrimetallic complexes with relevance in molecular magnetism (3d-3d'-3d'', 3d-3d'-4f, 3d-4d-4f, 3d-5d-4f, 2p-3d-4f). They show a rich structural variety (discrete polymetallic entities, as well as coordination polymers) and interesting magnetic properties (Single Molecule Magnets and Single Chains Magnets).

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Explicitly Correlated Effective Hamiltonian From Projective Transcorrelation

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ABSTRACT

The construction of effective Hamiltonian that implicitly includes dynamic correlation is crucial for accurate electronic structure calculations within a limited configuration space. This is especially important when employing approximate full configuration interaction (FCI) solvers or aiming to reduce the number of qubits in quantum simulations. Recently, there has been renewed interest in the transcorrelated (TC) method of Boys and Handy [1] primarily driven by these objectives. Although TC Hamiltonian is universal and terminating at three-body interactions, the local nature of the Jastrow factor prevents the satisfaction of different cusp conditions for singlet and triplet pairs [2]. To address this limitation, we recently introduced an alternative framework, nonunitary projective transcorrelation (pTC), inspired by the explicitly correlated F12 ansatz [3]. The pTC Hamiltonian features spin-free with simultaneous satisfaction of the cusp conditions, albeit with terms up to four-body operators. We demonstrate that perturbative analysis enables efficient pruning of pTC Hamiltonian. Applications of pTC are presented in conjunction with selected coupled-cluster (the so-called full coupled-cluster reduction (FCCR) [4-6]), and quantum emulations.

Keywords: electron correlation, cusp conditions, downfolding

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基于预训练的蛋白质工程通用人工智能(Venus 模型)

洪亮

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关键词：通用人工智能，蛋白质工程

摘要：AlphaFod 解决得是蛋白质及其复合物三维结构的预测，即使有正确的三维结构也不意味着蛋白有特定的功能，一个蛋白的序列改动 1%，其结构并没有明显变化，但新获得的蛋白 95% 功能变差，因此结构是功能的必要非充分条件，设计优秀的蛋白核心是解决功能预测。我们团队在过去 3 年开发了一套基于预训练的蛋白质工程的通用人工智能 Venus 系列。与 AlphaFold 预测结构不同，Venus 系列实现了从序列直达功能的精准蛋白质设计。通过预训练方法，让大模型学习自然界已知蛋白质序列和结构特征，并探索序列与功能的映射规律，利用极少量（数十个）的湿实验样本微调使得大模型能很好的预测特定蛋白的稳定性、活性等功能指标，从而实现优秀功能的蛋白质设计。利用这种方法在短短 2 年时间，我们已经成功设计和改造 30 余款蛋白质并被湿实验验证（包括核酸聚合酶，基因剪辑酶, IVD 酶，生物农药合成酶等），其中近 10 款实现放大生产并产业化应用。

个人简介

2004 年本科毕业于中国科学技术大学物理专业，2006 年硕士毕业于香港中文大学物理专业，2010 年博士毕业于美国阿克伦大学高分子科学专业。2010 年在美国橡树岭国家实验室进行计算生物学的博士后研究，2014 年 12 月份加入上海交通大学。目前就职于上海交通大学自然科学研究院/物理天文院/药学院 特聘教授，上海交通大学张江高研院人工智能生物医药中心主任。从事计算，人工智能和实验相结合的方式进行分子生物物理和蛋白质设计研究。2016 年入选国家高层次人才青年专家，2021 年入选教育部长江学者。在 nature，PNAS，PRL 等期刊上发表 80 余篇 SCI 论文。参与并主导开发了多个创新算法来提升小分子药物，和功能蛋白质的研发效率。

研究方向： 分子生物物理，AI 蛋白质工程

理实迭代学习的机器化学家探索

量子力学等微观理论已建立百年，应用于真实体系却过于复杂难以求解。实测数据往往珍贵稀疏，理论大数据缺失了现实复杂度，导致理实脱节，科研创新过程常常受限于相对低效的实验试错研究模式。

我们研制了数据智能驱动的机器化学家平台，开发并集成了移动机器人、智能化学工作站、高通量计算系统与智能化学大脑，驱动机器人展开高质量科研实践，以高精度实验数据迁移学习并校准理论大数据预训练模型，实现理实迭代学习的科研全流程覆盖：大胆假设（阅读文献并提出方案）、小心求证（执行计算-合成-表征-测试）、揭示规律（构建理实交融智能模型）、解决问题（指导化学品全局优化）。在光/电催化、功能分子、能源材料等领域提升效率>3 个数量级，突破了传统试错研究范式的瓶颈，例如将试错开发高熵催化剂所需的 1400 年缩短为 5 周，展现了理实迭代学习的优势，推动化学前沿向“知识数字化、操作指令化、创制智能化”转变。

报告人简介：

江俊 中国科学技术大学讲席教授，中科院上海技术物理所与瑞典皇家工学院联合培养博士。获批自然科学基金委杰出青年基金、中科院机器科学家青年团队负责人。发展融合人工智能与大数据技术的量子化学模拟方法，研制“理实交融”的机器科学家平台，探索物理化学应用领域中的实际问题（光电转化、功能材料、光化学等）。担任 Elsevier 智能领域旗舰期刊 AI Chemistry 创刊主编。获中国化学会唐敖庆青年理论化学家奖、日本化学会亚洲杰出讲座奖。

Core-valance separated multi-reference correlation methods based on hole-particle symmetry graphical unitary group approach

Qi Song, Bingbing Suo*

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X-ray spectra has attracted a lot of experimental and theoretical studies due to the development of advanced synchrotron light sources and X-ray free electron lasers. In this talk, we will demonstrate how to use the Graphical Unitary Group Approach (GUGA)-based MRCISD with Core–Valence Separation (CVS) approximation to compute the core-excited states. Thanks to application of the hole-particle symmetry in GUGA, the core-valance separation approximation could be utilized easily in the internally contracted MRCISD (CVS-icMRCISD) by modifying the Distinct Row Tabular (DRT) of the active orbital space. Eliminating the valence-excited configurations from the CVS-icMRCISD expansion space can prevent variational collapse in the Davidson iteration diagonalization. Benchmark calculations indicate that CVS-icMRCISD could reproduce well-matched vertical core excitation energies that are consistent with experiments by combining large basis sets and a rational reference space. Furthermore,the CVS approximation is implemented in multi-state n-electron valance second order perturbation theory (MS-NEVPT2) and static-dynamic-static second order perturbation theory (SDSPT2), giving rise to CVS-MS-NEVPT2 and CVS-SDSPT2. Although the errors of CVS-MS-NEVPT2 and CVS-SDSPT2 methods were slightly larger, both methods maintained acceptable accuracy, making them suitable for medium-sized molecules by significantly reducing computational costs.

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A Quantum Schrödinger-Langevin Equation Approach for Nonadiabatic Quantum Dynamics in Molecular Systems

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Quantum dissipative dynamics govern critical processes in complex physical and chemical systems, including quantum devices, conjugated polymers, and photosynthetic complexes. However, accurately modeling these open quantum systems—particularly those involving strong electronic–vibrational coupling—remains a long-standing challenge. To address this, we have developed the quantum Schrödinger–Langevin equation (QSLE) approach, which treats condensed-phase electronic and nuclear dynamics on equal footing, enabling the simulation of a wide range of non-trivial quantum behaviors in molecular systems. Moreover, by directly simulating dissipative nonadiabatic wave-packet dynamics with QSLE—including exact system–field interactions—we can calculate a variety of two-dimensional spectra. In this talk, I will highlight applications of the QSLE framework to elucidate complex, coupled electronic–vibrational quantum dynamics in molecular systems and to uncover spectral signatures of subtle quantum phenomena such as Berry phase effects and Fermi resonances. These results demonstrate the power of the QSLE approach in capturing coherent quantum phenomena and open new avenues for investigating nonadiabatic electronic–vibrational dynamics in complex molecular environments.

Water Trimer: Rigorous Twelve-Dimensional Quantum Calculations of Intermolecular Vibrational States, Tunneling Splittings, and Low-Frequency Spectrum

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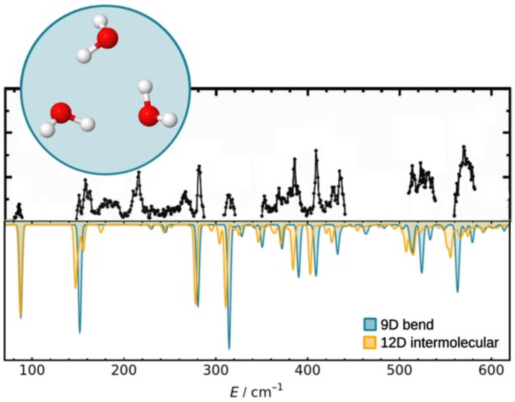
ABSTRACT

Water trimer is of fundamental importance as the smallest water cluster in which the nonadditive three-body interactions arise. They play a key role in shaping the structural, dynamical, and spectroscopic properties of liquid and solid phases of water and aqueous solutions. The trimer has 12 coupled large-amplitude intermolecular vibrational degrees of freedom (DOFs), and 9 intramolecular DOFs. The complexity of their quantum dynamics is greatly increased by the presence of two low-barrier tunneling pathways, which give rise to elaborate patterns of tunneling splittings. I will present our newly developed methodology which for the first time allows rigorous 12D quantum calculations of the coupled intermolecular vibration-tunneling states of $(H_2O)_3$, with the monomers treated as rigid [1]. The absorption spectrum of the low-frequency vibrations of water trimer simulated using these 12D eigenstates agrees remarkably well with the experimental far-infrared spectrum of the trimer in helium nanodroplets measured by Havenith, Bowman, and co-workers, over the entire frequency range of the measurements from 70 to 620 cm^{-1}, as evident from the figure. Moreover, the calculated 12D ground-state torsional tunneling splittings are in excellent agreement with the spectroscopic data. The peaks in the 12D spectrum are often split by the intermolecular stretch-bend Fermi resonances.



Keywords: clusters, vibrational states, spectroscopy, quantum calculations.

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Water Trimer: Rigorous Twelve-Dimensional Quantum Calculations of Intermolecular Vibrational States, Tunneling Splittings, and Low-Frequency Spectrum

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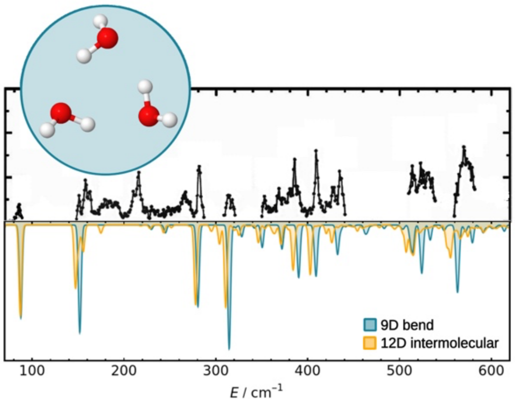

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Universal AI Models for Ground to Excited States

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ABSTRACT

Making universally transferable AI models for atomistic simulations promises to break through the cost/accuracy limitations of the traditional quantum mechanical (QM) methods. We have designed a series of such models for ground and excited state simulations. These models can be applied to almost all elements in the periodic table, molecules, and materials. Our AIQM-series models offer unprecedented robustness, accuracy, and computational efficiency across chemical compound space, particularly for organic and elemental-organic molecules, where the models are approaching accuracy beyond typical DFT for thermochemical properties, geometries, MD, IR spectra, and transition states.[1-5] We have also introduced the first-ever universal excited-state potential, OMNI-P2x.[6] In addition, we have created the foundational model for directly predicting MD trajectories, building on our previously proposed[7] novel concept.[8] All our implementations are available through MLatom (https://github.com/dralgroup/mlatom) and Aitomic (http://mlatom.com/aitomic/), and we provide online platforms for performing calculations via a web browser: Aitomistic Hub (https://www.aitomistic.xyz) and XACS cloud (https://XACScloud.com).

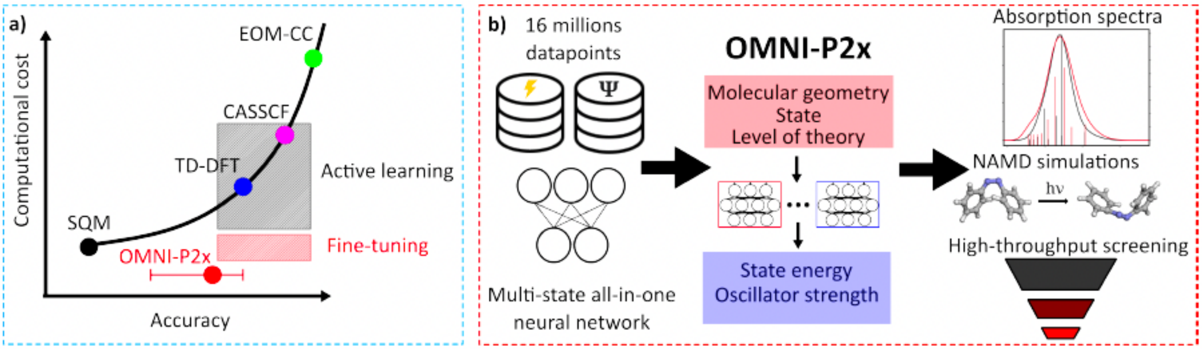

Figure. OMNI-P2x – the first-ever universal excited-state potential.[6]

Keywords: atomistic simulations, ML potentials, molecular dynamics, spectra, barriers.

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AB INITIO MODELLING OF PHOTOLUMINESCENCE

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In this contribution I present computational protocols to model photoluminescence in molecular systems which go beyond the nowadays routine modelling of emission energies. Our protocols merge state-of-the-art quantum chemical calculations, excited state decay rate theories (i.e., Fermi-golden rule based)[1] along with semi-classical nonadiabatic excited state dynamics to enable the quantitative determination of fluorescence lifetimes and quantum yields. In particular, I present an extensive analysis of the parameters influencing the excited state decay rate calculations.[2] Further, protocols to model anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states)[3] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical Non- Adiabatic Molecular Dynamics framework,[4] are presented. Finally, I present our recent efforts to expand our protocols from molecular systems to the solid state. In particular I present protocols allowing modeling the photophysical properties of organic molecular crystals. The objective is to evaluate the effect of various sources of disorder resulting in the broadening of UV-vis spectra.[5] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photophysics and photochemistry at the first principles level.

Keywords

Quantum chemical investigations, excited state decay rates, photoluminescence

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Polariton Chemistry: Quantum Control with Cavity Photons

Jianshu Cao (MIT)

The first part of the talk, I will introduce the emerging topic of ‘polariton chemistry’ and discuss recent work on vibrational strong coupling (VSC). Our quantum transition state theory calculation [1] attributes the modification of reaction rates in the VSC regime to the vibrational frequency shifts in the reactive well and reactive barriers, thus explaining the thermodynamic origin of cavity-catalyzed reactions. Application of the generalized resonance energy transfer (gRET) theory [2] explains the resonant and cooperative effects in vibrational energy relaxation in cavities. Though the two theories reveal complementary perspectives of VSC polariton dynamics, new mechanisms [3] are needed to explore the intriguing phenomena reported in the VSC regime.

In the second part of the talk, I will discuss recent results on quantum dynamics of exciton-polaritons. In optical cavities, disordered molecules are coupled to cavity photons collectively, such that the cooperativity in the light-matter interaction can overcome the Anderson disorder and lead to a turnover in transport at an optimal level of static disorder.[4] Further, cavity photons can drastically enhance the coherent time-scale of wave-packet motion and lead to noise-enhanced wave-packet spreading in the ballistic regime. [5]

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New Methods for Spatial Proteome Analysis

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ABSTRACT

Spatially resolved proteome mapping of tissues is essential to understand physiological and pathology status. Laser capture microdissection (LCM) coupled to nanoLC-MS/MS is a powerful tool to correlate the proteome information with spatial distribution. However, it is of great challenge to balance the throughput and the spatial resolution, limited by the time-consuming nanoLC-MS/MS analysis of hundreds LCM slices. To solve this problem, herein ordered colloidal crystal (800 nm) packed columns were prepared to shorten the separation time. Contributed by the column efficiency over 1 million theoretic plates/m, more than 4000 proteins were identified from protein digests equivalent to those from one 100-μm human liver FFPE slide within 2-min gradient by Orbitrap Astral MS, which demonstrated the great promising of ordered colloidal crystal columns for spatially resolved proteomics with high resolution and high throughput.

Furthermore, spatially resolved characterization of proteoforms has great potential to significantly advance our understanding of physiological and disease mechanisms. However, it faces challenges regarding throughput and coverage. Herein, we developed a robust method for high-throughput proteoform imaging (HTPi) by combining matrix-assisted laser desorption ionization mass spectrometry imaging (MALDI MSI) and region-specific top-down proteomic analysis. MALDI MSI enabled imaging proteoforms on tissue sections at a rate of 7 h/cm^2 (100-μm spatial resolution), and the identification sensitivity of proteoforms was improved by narrow-bore monolithic columns with low adsorption, yielding 366 annotated proteoform images from the mouse brain. The obtained proteoform images revealed differential expression of individual proteoforms across the brain regions, and distinct spatial distribution patterns of various proteoforms generated from a single gene. Given its ability for proteoform visualization, HTPi was further applied to explore spatial pathological changes in 5×FAD mice associated with Alzheimer's disease (AD). We obtained more than 100 annotated proteoform images in hippocampus regions at 50-μm spatial resolution, illuminating 14 differential proteoforms in the subiculum region and foregrounding their significant associations to Aβ pathology in AD. Our results highlight the power of HTPi in unraveling the intricate molecular landscape of brain tissues and its potential in elucidating disease mechanisms.

Keywords: Spatial proteome analysis, bottom up strategy, top-down strategy, ordered colloidal crystal packed columns, MALDI-MS imaging

Development of novel carbene cascade for late-stage modification

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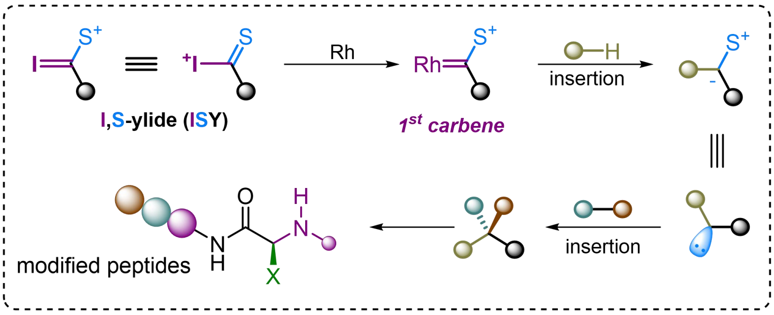
ABSTRACT

Our research group focuses on developing highly selective catalytic processes for late-stage functionalization, particularly those involving well-defined transient intermediates. Among these, carbenes, as unique reactive species, offer significant opportunities for innovation in medicinal chemistry. To better understand and regulate the diverse reactivity of these divalent carbon species, we have developed a novel carbene relay catalysis strategy. This involves introducing heteroatoms to the carbene center to tune its reactivity and selectivity. At this symposium, I will present our latest research on a new reagent class—iodonium and sulfoxonium ylides (ISY). As dual carbene precursors, ISY can sequentially generate two transient carbenes in a single reaction and perform modifications of peptides and drug molecules.



Figure

Keywords: carbene, enantioselectivity, cascade, late-stage modification, unnatural amino acid

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Bioorthogonal chemistry based on o-diones

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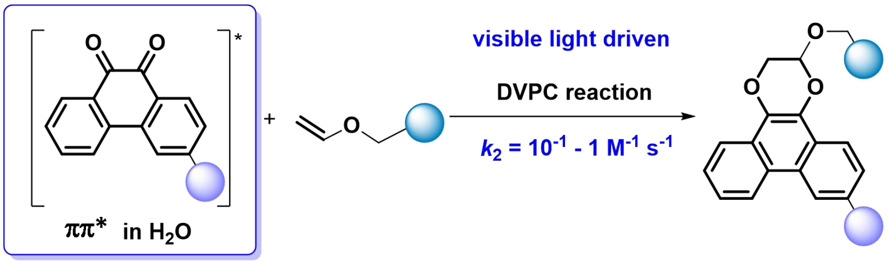
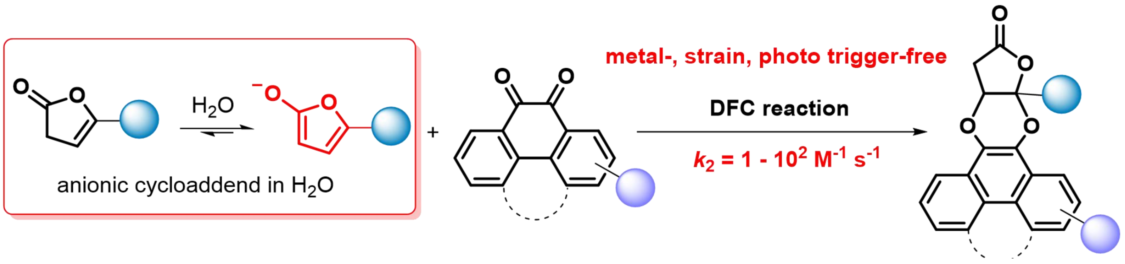
The establishment of bioorthogonal reaction made it possible for in situ labeling of biomolecules in living systems, which was considered as a milestone in the field of chemical biology. Photo-controllable bioorthogonal reactions add spatial-temporal resolution to bioorthogonal reactions and provide photo-controllable molecular tools in chemical biological studies. To realize photo-control on bioorthogonal reactions, we proposed and realized bioorthogonal bond-formation approach based on the photo-excited states of *o*-diones with special properties in polar solvents such as water. Using this unique strategy, we established the visible-light driven bioorthogonal DVPC reaction, which allowed satial-temporal labeling of antibodies on live cells. [1] DVPC was also orthogonal to the strain-promoted azide alkyne click reaction (SPAAC), which enabled orthogonal labeling of two proteins in one batch. Further exploration on the cycloaddition reactions between o-diones and other electron-rich C=C bonds led to the discovery of the bioorthgonal DFC reaction[2], which was the first anionic cycloaddend-promoted bioorthogonal cycloaddition reaction. With the water-mediated formation of the highly electron-rich anionic cycloaddend from furan-2(3H)-one derivatives, which is stabilized in water with high polarity, DFC reaction with ground state o-diones proceeds rapidly in aqueous solution and on live cells. The combined utilization of this reaction together with the two other widely used bioorthogonal reactions SPAAC and IEDDA allows for mutually orthogonal labelling of three types of proteins or three groups of living cells in one batch without cross-talking. Using bioorthogonal reactions, we were able to build various bio-active molecules to visualize or regulate biological systems with spatial and temporal resolution.[3-5]





Keywords: bioorthogonal reaction, photo-driven, DVPC, DFC

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Spatiotemporal Delivery of Protein Therapeutics and Genome Editing Tools Using Supramolecular Nanoparticles

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ABSTRACT

Proteins are central regulators of cellular function and disease progression, making them promising for developing biotherapeutics and genome editing. However, the inability of native proteins to spontaneously cross cell membranes or to target specific tissues remains a critical barrier to their chemical biology study and clinical translation. To address these challenges, we develop spatiotemporally resolved protein delivery platforms through integrating synthetic/supramolecular chemistry and protein engineering. In this presentation, I will describe our recent study on designing supramolecular protein assemblies for therapeutic protein delivery. By leveraging non-covalent interactions, such as hydrogen bonding interaction between surface-exposed amino acids and supramolecular nanoparticles, we design protein-encapsulated nanoparticles with tunable physicochemical properties that enables efficient intracellular delivery. Notably, we demonstrate that modulating the surface chemistry of these nanoparticles (e.g., size, charge) enables tissue-selective delivery to the lungs, achieving spatiotemporally-controlled genome editing in vivo. This approach not only facilitates the study of protein function in complex biological settings but also establishes a versatile framework for developing precise protein therapies.

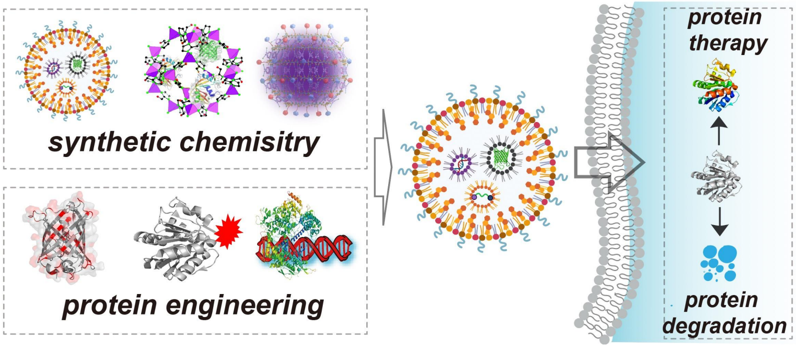

Figure Integrating supramolecular chemistry and protein self-assembly for protein therapy

Keywords: Protein Delivery; Genome Editing; Supramolecular Chemistry; Nanomedicine; Protein Therapy

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Chemical Approaches to Decode Histone Epigenetics

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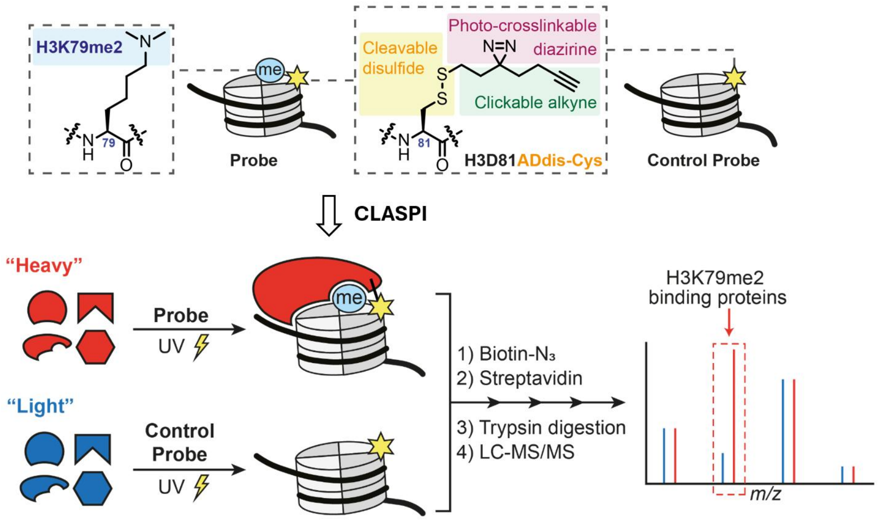
ABSTRACT

Histone posttranslational modifications (PTMs), such as phosphorylation, methylation and acetylation, play crucial roles in regulating many fundamental cellular processes, such as gene transcription, DNA replication, DNA damage repair, chromosome segregation and cell differentiation. Increasing evidences have indicated that PTMs of histones can serve as a heritable ‘code’ (so-called ‘histone code’), which provides epigenetic information that a mother cell can pass to its daughters. Histone code is ‘written’ or ‘erased’ by enzymes that generate or remove the modifications of histones. Meanwhile, ‘readers’ of histone code recognize specific histone modifications and ‘translate’ the code by executing distinct cellular programs necessary to establish the diverse cell phenotypes.

While a large number of PTMs have been identified on histones, the biological significance of vast majority of them remains poorly understood. This is particularly the case for those newly discovered histone modifications such as lysine crotonylation, succinylation, fatty-acid acylation, and the modifications present at histone cores such as methylation at H3 lysine 79. Studies of these new PTMs are hindered by the lack of knowledge about their regulating enzymes (i.e., ‘writers’ and ‘erasers’) and functional binding proteins (i.e., ‘readers’). To fill this knowledge gap, here I present the development of novel chemical tools and approaches, in combination with the state-of-the-art biochemistry, proteomics and cell biology methods, to comprehensively identify ‘writers’, ‘erasers’ and ‘readers’ of histone PTMs and examine their regulatory mechanisms and cellular functions."



Keywords: Chemical epigenetics, Histone posttranslational modifications, Histone PTM readers, Nucleosome photoaffinity probes, Chemical proteomics

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Single-Cell Analysis of Glycans

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All cells are coated with a dense layer of glycocalyx consisting of various glycans. Cell-surface glycans play essential roles for many important biological processes. Analysis of glycans has been mostly performed in bulk samples, which misses the information on heterogeneity of glycosylation at the single-cell level. For example, overexpressed cell-surface sialoglycans on cancer cells suppress the activation of tumor-infiltrating leukocytes (TILs) via binding to inhibitory receptors, and thus have emerged as a promising target for cancer immunotherapy. On the other hand, the functional significance of siaologlycans on TILs remains incompletely understood, owing to their great heterogeneity at the cellular level. In this talk, I will present the development of single-cell correlative analysis of sialoglycans and transcriptomes, a method that correlates the cell-surface sialylation status in a sialoside linkage-specific manner with gene expression by single-cell sequencing. Applying this method in TILs, we uncovered that sialylation regulates anti-tumor immunity of TILs.

Chemical strategies to modulate RNA epigenetic modifications

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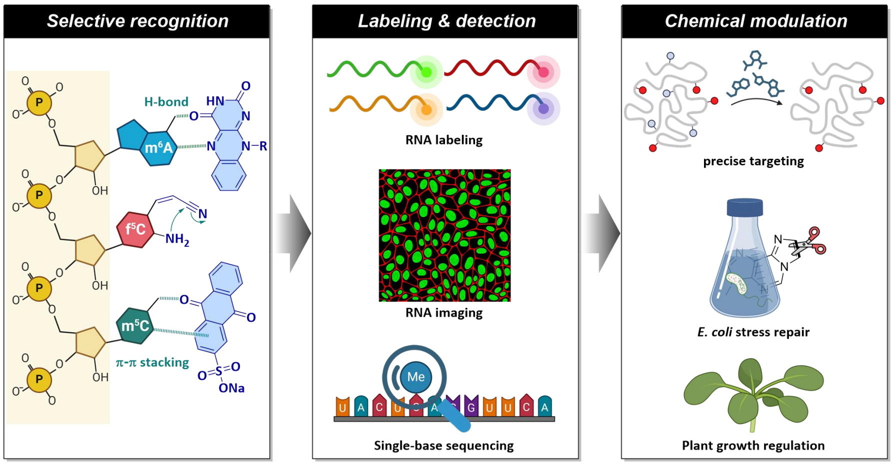
ABSTRACT

The study of RNA epigenetic modifications has rapidly grown over the past decade, revealing a previously underappreciated layer of regulation in gene expression and cellular function. Modifications such as N^6-methyladenosine (m^6A) and 5-methylcytidine (m^5C) can dictate RNA stability, localization, translation, and interactions with key cellular factors. Understanding these modifications is not just a fundamental pursuit but also holds therapeutic promise, given their links to diseases including cancers, metabolic disorders, and neurological conditions. Conventional methods have largely relied on manipulating endogenous enzymes -- “writers,” “erasers,” and “readers” -- or using genetic interventions to alter RNA modifications. While effective in some contexts, these approaches encounter limitations, such as reliance on the availability of functional enzymes, potential off-target effects, and challenges with specificity.

In this talk, we will showcase how chemistry-focused approaches -- encompassing small molecules and bioorthogonal reactions -- can offer alternative, highly controlled means of modulating RNA epigenetic marks without depending solely on cellular enzymes. The primary aim is to elucidate in detail how these chemical strategies were conceived, optimized, and translated to living systems, offering unprecedented precision and flexibility. We also explore the broader implications of these tools, including the promise they hold for deciphering mechanistic underpinnings of RNA modifications, enabling novel forms of in-cell labeling, and repairing damage arising from internal or environmental insults. Our vision is that these methodologies will help bridge gaps in our understanding of RNA’s role in health and disease, spurring advances in high-throughput sequencing, targeted therapeutic design, and plant biotechnology.



Keywords: RNA modification, Chemical modulation, Bioorthogonal chemistry

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Regulating the cell surface receptors with immunoglobulin-directed phase separation systems (IgPS)

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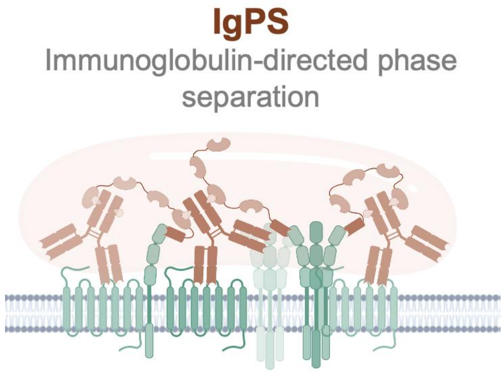
ABSTRACT

Cell surface receptors serve as crucial gateways for cellular interaction with the external environment. Recent high-throughput protein interaction studies have unveiled widespread instances of unknown functional co-clustering of cell surface receptors on the cell membrane[1,2]. To delve deeper into the biological roles and mechanisms of these co-clustering phenomena, there is a pressing need for versatile and highly adaptable co-clustering modulation strategies. Our lab has long been dedicated to developing novel antibody-based molecules for modulating the functionality of membrane proteins and has previously created a phase-separation scaffold for receptor clustering based on natural proteins[3]. In order to establish a stable and structurally engineerable receptor co-clustering modulation strategy, we have utilized the fundamental principles of protein phase separation. Through the interaction of mutated antibodies and specific peptides, we have developed an immunoglobulin-directed phase separation system (IgPS), enabling precise control over the aggregation and spatial segregation of cell surface receptors. By constructing IgPS targeting the cell surface receptors CXCR4 and DR5, we have been able to selectively activate DR5 signaling in CXCR4+ cells, achieving cell-specific receptor activation. Importantly, the CXCR4/DR5-targeting IgPS system effectively induced apoptosis in tumor cells and suppressed tumor growth in xenograft models, demonstrating the potential of this system for in vivo receptor function modulation.



Figure

Keywords: protein condensate, receptor clustering, antibody engineering, cell-specific agonist

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AI-driven, Multidimensional, and High-Content Fluorescence Imaging and Analysis for Tumor Immunotherapy

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Abstract:

Recent breakthroughs in tumor immunotherapy have been achieved, yet challenges such as low response rates and difficulties in efficacy prediction persist. The lack of precise quantitative imaging tools has limited our understanding of key factors influencing therapeutic outcomes, including the molecular dynamics of immune cells, cellular composition, and spatial organization of the tumor immune microenvironment. Here, we present a novel cross-scale light-sheet three-dimensional imaging technology and high-dimensional dynamic fluorescence image reconstruction algorithms. Combined with fluorescent probe labeling and microfluidic cell manipulation techniques, our approach enables precise characterization of subcellular structures and molecular dynamics at the single immune-cell level, while also resolving the cellular composition and spatial relationships within the tumor microenvironment. Through clinical trials, we aim to establish correlations between imaging-derived metrics and therapeutic efficacy. This work advances a new computational light-sheet microscopy framework for accurately mapping the dynamic 3D landscape of tumor immunity, uncovering the mechanistic basis of heterogeneous immunotherapy responses, and driving innovation in life and health sciences.

面向肿瘤免疫治疗的智能、多维、高内涵荧光成像和分析

费鹏[1]

[1]华中科技大学光学与电子信息学院

摘要：肿瘤免疫治疗近年来取得突破，但仍面临响应率低、疗效预测难等问题。由于缺乏精准的定量成像工具，目前对免疫细胞的分子动态、肿瘤免疫微环境的细胞成分和空间排布等影响疗效的因素了解有限。本报告介绍我们开发的跨尺度光片三维成像新技术和高维动态荧光图像重建算法，结合荧光探针标记和微流控细胞操控技术，精确刻画单免疫细胞尺度的亚细胞结构/分子动态，并解析肿瘤微环境细胞组成和空间关系。通过临床试验，我们可建立分析与疗效的关联映射，推动以新型计算光片显微成像技术为基础精准绘制肿瘤免疫的动态三维全景图，揭示免疫治疗差异化的本质，推动生命健康科学的前沿发展。

Protein Electrostatics in Catalysis and Evolution

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ABSTRACT

Life is sustained by a symphony of chemical reactions carried out by enzymes in extraordinarily high rates. How do enzymes achieve catalytic proficiency and is there a unifying physical basis? Recently a number of enzymes have been found to use protein architecture to organize charges and dipoles that impose strong electric fields onto reactive chemical bonds and stabilize their transition states. This talk will present the key electrostatics employed by beta-lactamases to break up beta-lactam antibiotics, as studied by vibrational spectroscopies, isotope labeling, and amber suppression. We found that the catalytic electrostatics were acquired from an ancient evolution dating back billions of years and are continuously improving against modern antibiotics.[1] During our studies of the covalent inhibition of beta-lactamases, protein electrostatics emerged to us as a new handle for modulating reactivities of covalent drugs.[2] We have further optimized the electrostatics in the active site of alcohol dehydrogenase by rationally designed mutations and achieved activities surpassing nature.[3]

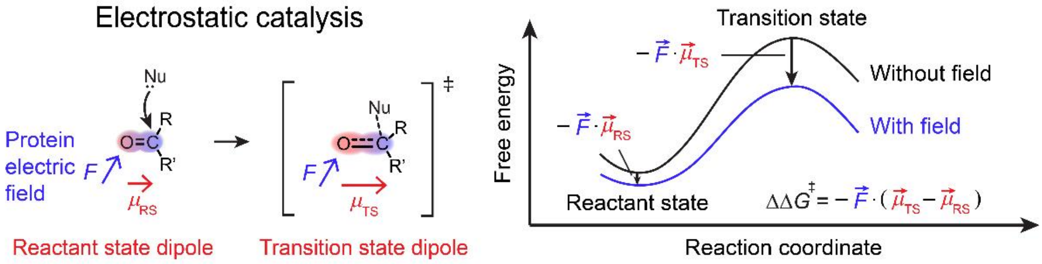

Figure Concept of electrostatic catalysis.

Keywords: Enzyme Catalysis, Electrostatics, Protein Rational Design, Directed Evolution, Covalent Inhibitor

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Chiral Nanomaterial Fabrication for Life Regulation

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Chirality is typical character of biomacromolecules. The spatial morphology and size are very important during biological recognition and interaction. We have found unique chiral nanoparticles recognize specific protein or DNA, and then intervene life process. Recently, we studied the interaction between chiral nanoparticles and the gut microbiota, it showed that left-handed nanoparticles promote special gut metabolite production, which could reduce neuroinflammation in vivo through the blood-brain barrier (BBB), offering a promising therapeutic target for the amelioration of neuroinflammation and treatment of neurodegenerative diseases. The field of chiral inorganic nanostructures is rapidly expanding. In particular, we can generate a wealth of chiral nanoparticles by rational control of different scale and constituents. In this talk, I will highlight recent advances in the broad utility of chiral nanocrystals for virus recognition and immune response regulation.

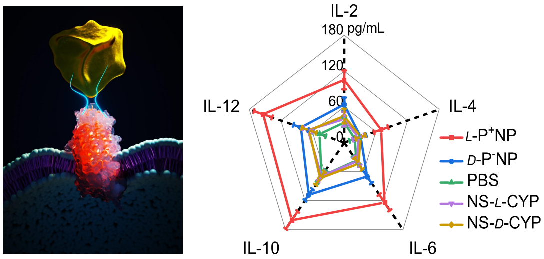

Figure1. Enantiomer-dependent immunological response to chiral nanoparticles

Keywords: Chiral nanoparticles, Specific recognition, Optical activity

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Sulfhydrylation of the Chlorobenzene-based Pesticides in Sulfur-Rich Vegetables from Cultivation to Sample Analysis and Risk Assessment

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ABSTRACT

[Abstract, Times New Roman, 10.5pt, Justified, line spacing single]

Chlorobenzene-based pesticides (chlorothalonil, fluazinam, etc.) are widely used in vegetables and fruits. However, over the past few decades, chlorothalonil has seldom been detected in some vegetables. This anomalous phenomenon inspires us to investigate the degradation of chlorobenzene in agro-products.

Recently, we discovered for the first time that chlorothalonil (CHT) and fluazinam rapidly transformed to sulfhydrylated-products in sulfur-rich vegetables, such as cabbage, pak choi, and garlic chives. Pesticide sulfhydrylation has been comprehensively studied using the pak choi as sulfur-rich vegetable model. Additionally, field experiments were carried out with actual application dosage of CHT.

The important research progress was as follows [1-3]: (1) CHT sulfhydrylation mechanism. 4-sulfhydyrlated chlorothalonil (4-SH-CHT) is produced by CHT sulfhydrylation with H_2S and H_2S donors. In intact raw pak choi, 4-SH-CHT exhibited low concentrations. Along with the tissue destruction of pak choi, CHT sulfhydrylation rates increased owing to the release of H_2S and various H_2S donors. Over half of the CHT in pak choi was transformed during homogenization at room temperature. (2) Analytical method. An efficient strategy based on liquid nitrogen homogenization and solvent acidification was proposed to inhibit CHT transformation during the entire analytical procedure. Thereby, an efficient analytical method for the simultaneous determination of CHT, 4-OH-CHT, and 4-SH-CHT in pak choi was developed. (3) Exposure risk assessment. CHT concentrations in pak choi homogenates were mistaken for those in intact pak choi, resulting in an underestimation of CHT concentration levels and exposure risk. We demonstrated that several pak choi samples collected after safety intervals (7 d and 10 d) at the maximum recommended dosage exhibited chronic exposure risk. 4-SH-CHT in some pak choi homogenates (7 d and 10 d) exhibited P97.5 daily intakes over its TTC threshold level.

This study provided a foundation for comprehensive exposure risk assessment of CHT and 4-SH-CHT in pak choi and pak choi-related products. In addition, this study provides an important reference for further studies on the degradation of H_2S-sensitive pollutants in sulfur-rich vegetables.

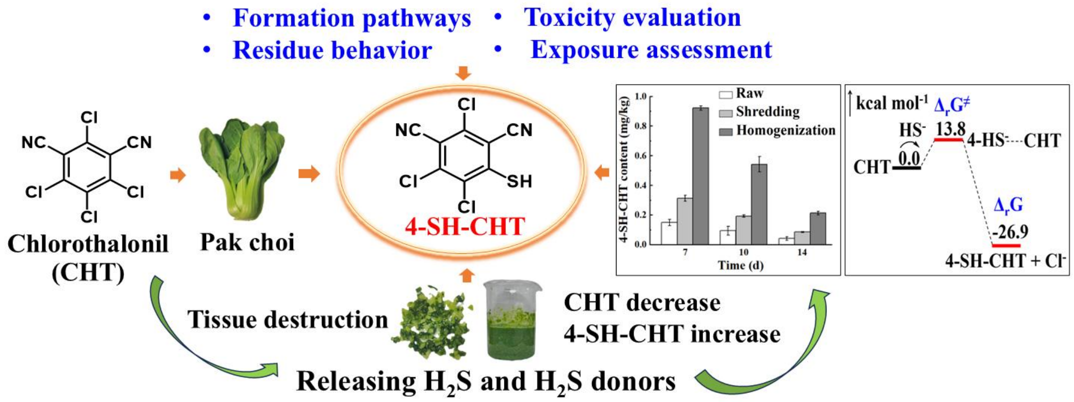

Figure 1. The Graphic Abstract

Keywords: Pesticide transformation, sulfhydrylated degradation products, sulfur-rich vegetable, residue behavior, risk assessment

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Electrochemical Analysis of Single Nerve Vesicles

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ABSTRACT

Neuronal vesicles are the main subcellular organelles responsible for exocytosis, and the development of single vesicle analytical chemistry methods can provide powerful tools for neuroscience research. By effectively designing and constructing a nano tip carbon fiber cone electrode, we have developed a single vesicle in situ electrochemical counting method and achieved quantitative detection of dopamine, a neurotransmitter encapsulated within a single vesicle, in PC12 cells. By comparing the amount of neurotransmitters released by vesicles during exocytosis with the single-cell current method, we found that most vesicles did not release all the neurotransmitters they contained during exocytosis, revealing that exocytosis is not an "All or None" quantum process. By combining these two methods, we further investigated the regulation or effects of cisplatin, zinc ions, DJ-1 protein, and other chemicals on neural signal transduction. We found that these chemicals have a significant impact on the proportion of neurotransmitters released from vesicles during exocytosis.

Recently, our team developed a fresh brain tissue single vesicle electrochemical analysis method and pioneered the construction of an IVIEC analysis method designed for fresh brain tissue slices to detect the storage of neurotransmitters within individual vesicles in fresh brain slices (Figure 1). Combining it with SCA reveals the complexity of neurochemical signal transduction mechanisms. For the first time at the single vesicle level, a significant decrease in the storage of neurotransmitters in dopamine neuronal vesicles was discovered in an animal model of Parkinson's disease, while the process of exocytosis and release was inhibited, providing insights into the potential pathogenesis of Parkinson's disease. In addition, the study also delved into the heterogeneity of single vesicle storage and exocytosis release of other neurotransmitters (norepinephrine, serotonin) in different brain regions (dorsal striatum, ventral tegmental area, locus coeruleus, and raphe nucleus). This study provides a new strategy for investigating the biological processes of chemical signal transmission and exploring the disruption mechanisms of neurological diseases at the level of single vesicles in fresh brain tissue.

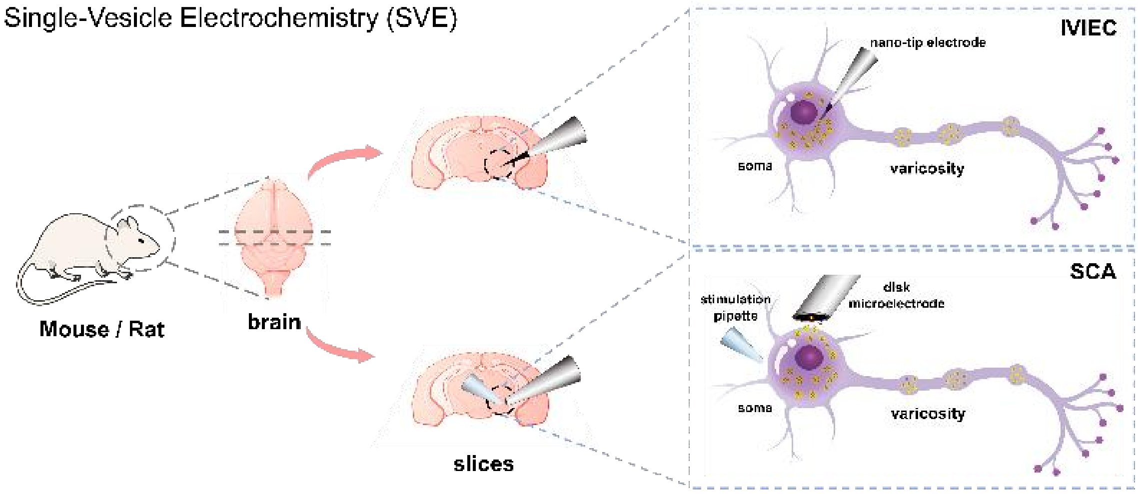

Fig. 1 Schematic of single-vesicle electrochemical (SVE) platform for fresh brain tissue.

Keywords: neural vesicle; electrochemical analysis; neurotransmitters; exocytosis; synapse

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Novel PROTAC Development Platrom: The Split-and-Mix Approach

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ABSTRACT

The development of proteolysis-targeting chimeras (PROTACs) typically involves a time-consuming process with extensive optimization requirements. In this study, we introduce a split-and-mix nanoplatform, a self-adjustable system that simplifies screening procedures, allows for programmable ligand ratios, and enables multifunctional applications. We have demonstrated the potential of split-and-mix PROTACs (SM-PROTACs) in targeting therapeutic targets through either the proteasome or lysosome systems. Our results have confirmed the effectiveness and versatility of SM-PROTACs across nine tumor-related targets. We further explored a liposome-based variant, LipoSM-PROTAC. This variant not only showed improved biocompatibility but also required lower effective concentrations. In addition, it exhibited excellent anti-tumor activity in vivo. By implementing the "split-and-mix" approach, we have streamlined the design of multifunctional PROTACs. These include multi-target degraders, tumor-selective degraders, dual E3 ligase degraders, long-acting SM-PROTACs, and facilitated anchoring-strategy screening. Overall, this platform exhibits broad applicability and flexibility, offering a powerful solution to the challenges encountered in PROTAC technology.

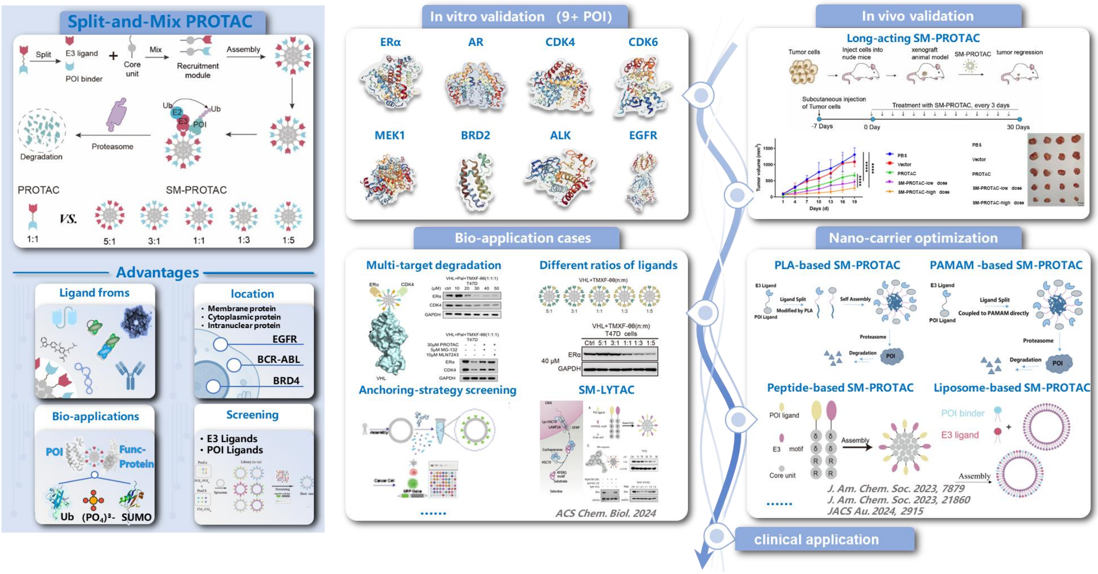

Figure 1. The Split-and-Mix Approach for PROTAC Ddevelopment

Keywords: Targeted protein degradation, Split-and-Mix PROTAC, Multifunctional Degrader, Tumor-selective Degrader.

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Computational design and genetic incorporation of lipidation mimics in living cells

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ABSTRACT

Protein lipidation, which regulates numerous biological pathways and plays crucial roles in the pharmaceutical industry, is not encoded by the genetic code but synthesized post-translationally. In this talk, I will share a computational approach for designing lipidation mimics that fully recapitulate the biochemical properties of natural lipidation in membrane association and albumin binding. Furthermore, we establish an engineered system for co-translational incorporation of these lipidation mimics into virtually any desired position of proteins in Escherichia coli and mammalian cells. We demonstrate the utility of these length-tunable lipidation mimics in diverse applications, including improving the half-life and activity of therapeutic proteins in living mice, anchoring functional proteins to membrane by substituting natural lipidation, functionally characterizing proteins carrying different lengths of lipidation and determining the plasma membrane-binding capacity of a given compound. Our strategy enables gain-of-function studies of lipidation in hundreds of proteins and facilitates the creation of superior therapeutic candidates.

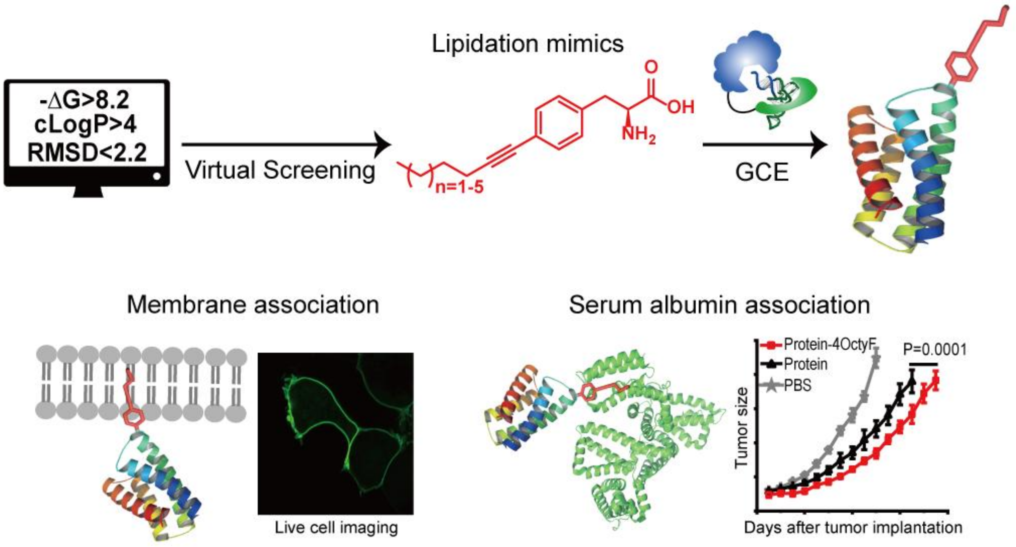

Figure. Genetic incorporation of lipidation mimics in living cells

Keywords: protein lipidation, genetic code expansion, computational design, protein drugs

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Development of β-Branched Aromatic α-Amino Acids Modified PSMA Radioligand for Radiometric Imaging

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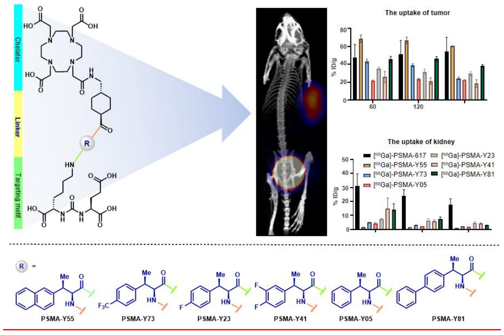
ABSTRACT

Prostate cancer, the second most common malignancy among males, is imposing an increasingly heavy global burden due to its dual characteristics of high incidence and difficulty in treatment once metastasized. Despite the clinical success of prostate-specific membrane antigen (PSMA)-targeted radionuclide therapy (e.g., [^{177}Lu]-PSMA-617), off-tumour toxicity remains critical challenges. Therefore, the development of new and improved PSMA ligands for radiotheranostics remains highly significant. Given the crucial role of the linker moiety in the structure of PSMA-617 for drug targeting and pharmacokinetic properties, the development of PSMA ligands featuring novel linker architectures is anticipated to enhance their targeting capabilities and pharmacokinetic profiles. In this study, we designed and synthesized a novel PSMA radioligand incorporating (*2S, 3R*) β-branched aromatic α-amino acids within the linker segment of its structure. This innovative approach aims to optimize the ligand for positron emission tomography (PET) imaging of prostate cancer, thereby potentially improving diagnostic accuracy and therapeutic outcomes. **Methods:** (*2S, 3R*) β-branched aromatic α-amino acids were synthesized by chemoenzymatic synthesis, precursor peptides were assembled by solid-phase peptide synthesis and labeled with ^{68}Ga. Small animal PET/CT imaging was performed on RM-1 tumor-bearing mice at 1h, 2h and 4h after injection. **Result:** All aforementioned radioligands were notably accumulated at tumors. [^{68}Ga]-PSMA-Y55, [^{68}Ga]-PSMA-Y73, and [^{68}Ga]-PSMA-Y81 showed comparable or even better tumor uptake than [^{68}Ga]-PSMA-617. Notably, [^{68}Ga]-PSMA-Y55 demonstrated an exceptionally high uptake at the tumor site, reaching 71.7% ID/g, with a sustained level of 60% ID/g even after 240 minutes, markedly surpassing that of [^{68}Ga]-PSMA-617. Furthermore, all the (*2S, 3R*) β-branched aromatic α-amino acids modified PSMA radioligand exhibited a more rapid renal clearance rate than [^{68}Ga]-PSMA-617, with an average renal uptake of less than 10% ID/g, as opposed to 25% ID/g for [^{68}Ga]-PSMA-617, significantly reducing kidney damage. **Conclusion:** This confirms our hypothesis about increasing the targeting of ligands and metabolic stability in vivo by increasing the structural rigidity of the linking subparts. We anticipate that the introduction of alternative configurations of β-branched aromatic α-amino acids, or the further modification of the aromatic ring within these amino acids, holds significant potential for improving the targeting and pharmacokinetic properties of the ligand.



Figure

Keywords: Prostate cancer, PSMA radioligand, β-branched aromatic α-amino acids, PET/CT imaging

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Molecular measurement at the cell membrane interface

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ABSTRACT

The cell membrane interface is a critical site for cells to exchange information and substances with the outside world. Molecules at this interface play essential roles in regulating vital cellular processes such as signal transduction, metabolism, and immune responses. Thus, accurate measurement of these molecules is of great significance for exploring life mechanisms, understanding disease etiology, and promoting precision medicine, presenting a frontier topic in life-analytical chemistry. However, the high spatiotemporal heterogeneity of membrane-interface molecules, particularly within the nanoscale, poses challenges to traditional analytical methods. To address this, we focused on chemical probe design. The main innovative results include: constructing an amphiphilic three-dimensional functional nucleic acid probe for efficient and stable membrane modification, enhancing the acquisition of dynamic molecular information; devising a probe-positioning strategy based on the plasma membrane's topological structure to overcome signal crosstalk and enable in-situ analysis of transmembrane signal transduction; and creating a size-programmable probe for spatiotemporal measurement at cell-interaction interfaces, providing new insights into immune-cell signaling mechanisms.

Keywords: DNA nanotechnology, Cell analysis, Biosensing, Fluorescent probe, Cellular immunity

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NIR-II fluorophores and their application for in vivo imaging

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ABSTRACT

Fluorescence bioimaging in the near-infrared II window is a promising area due to its deep tissue penetration and high contrast. Efficient design strategies for near-infrared II fluorophores are scarce. Here, we develop certain near-infrared II fluorophores with outstanding spectroscopic properties by modulate the conjugation of fluorophore with p-aminostyryl group. Time dependent density functional theory calculation and transient absorption spectra were used to depict the usual excitation and emission process, which lead to the large Stokes shifts and long wavelength. We demonstrate the applications of these fluorophores in multicolor imaging, dynamic imaging in various scenarios. This work provides insights into the excited-state photophysical processes in near-infrared II window, offering inspiration for designing fluorophores with extended emission and large Stokes shifts.

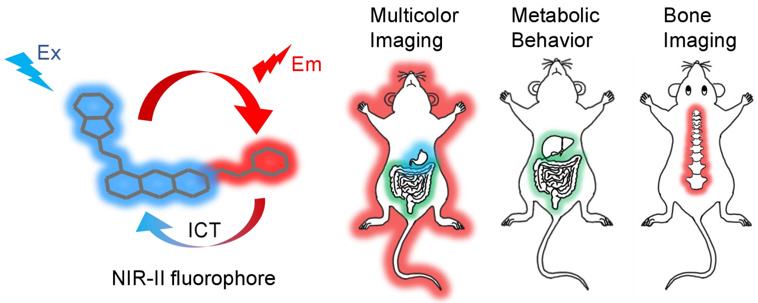

Figure 1 NIR-II fluorophores and in vivo imaging

Keywords: NIR-II, fluorophore, fluorescent imaging, in vivo

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Microfluidics-Driven Molecular Profiling of Extracellular Vesicles

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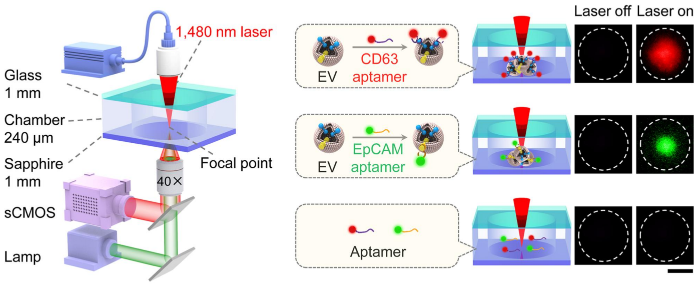
ABSTRACT

Noninvasive, rapid, and low-cost methods for screening and classification of early stage cancers are of great significance. Despite the promise of liquid biopsy in early cancer diagnostics, significant efforts are required to overcome the technological challenges in isolation, detection, and interpretation of heterogeneous circulating biomarkers. Here we develop a one-step thermophoretic aptasensor (TAS) for early stage cancer detection and classification, as well as monitoring of cancer recurrence through profiling the surface proteins of extracellular vesicles (EVs) in less than 1 μL serum samples. In a pilot study (n = 172), this EV assay achieves 95 % sensitivity and 100 % specificity for detection of Stage I cancers, with an overall accuracy of 68 % for discriminating six cancer types (Stage I to IV). For prostate cancer (n = 60), EV signature is superior in its ability to discriminate prostate cancer and benign disease than serum PSA, and acts as a promising biomarker to monitor biochemical recurrence after radical prostatectomy. This TAS method demonstrates a huge translational potential for EVs-based cancer diagnostics.



Figure

Keywords: Microfluidics, Extracellular vesicles, Biosensing, Liquid Biopsy

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Unraveling Proteins and their Transient Interactions with nucleic acids with AI-driven Automated Liquid-phase TEM Analysis

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In the post-AlphaFold era, the problem of folded structures of proteins is well resolved, and the challenge of observing their dynamics while they are in action in liquid remains. The interaction dynamics that critically define the energy landscape are usually obtained by ensemble methods (nuclear magnetic resonance spectroscopy and scattering methods) and single molecule methods (fluorescence and tweezer experiments). These experiments with high-resolution structures resolved by cryogenic electron microscopy or X-ray crystallography have provided evidence for the classic "lock and key" model for describing interactions between proteins that have defined three-dimensional structures. However, discrepancy remains, especially for proteins interacting with nucleic acids that are equally ill-defined in structures or when they contain flexible regimes. Here, using liquid phase transmission electron microscopy (LP-TEM) and deep learning-assisted instrument automation and image segmentation and classification, with molecular ergodicity of protein molecules and nucleic acids in a graphene liquid cell confirmed via direct imaging, our finding assures that LP-EM can be used for probing the intrinsic dynamic properties of these systems. The first example investigates conformational changes and interaction pathways of Calcineurin, a calcium- and calmodulin-binding protein containing IDR. Activation of Calcineurin by Calmodulin was directly imaged by LP-TEM. Intermediate states and conformational dynamics during binding are quantified by correlative analysis of LP-TEM images and computer simulation using customized template-matching methods. In particular, we identified critical intermediate states and intermediate dependent pathways that are unique to IDP. In the second example, we observe RNA structural diversity via direct imaging and their conformation-dependent interaction with protein. These studies may shed light on protein and nucleic acids' interaction dynamics, transition, and assembly pathways, revealing key processes underpinning many fundamental biological functions.

Functional Nucleic Acid-enabled Precise Detection of MicroRNAs

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ABSTRACT

MicroRNAs (miRNAs) play essential regulatory roles in biology, which carry important pathological information that may serve as emerging biomarkers for many diseases including cancer. There is an increasing need to develop new methods to enable sentitive, specific, and high throughput detection of miRNAs. Towards this end, herein, we developed a series of functional nucleic acid-based biosensing systems for miRNA detection by harvesting the programmability and codability of nucleic acids.[1-5] For instance, we coupled rolling circle amplification with CRISPR-Cas13a to realize highly sensitive and specific detecton of miRNAs for the diagnosis of prostate cancers.[1] To avoid the preamplification process, an ultrasensitive, unified, modular, allostetic DNAzyme sensor was designed to achieve sensitive and specific detection of miRNAs with femtomolar/attomolar sensitivity and single-base discrimination specificity.[2] Lastly, we developed Direct-miR-seq, a nanopore-based sequencing method to sequence and analyze a large number of miRNA species in parallel (~2000).[3] Direct sequencing of miRNAs can offer quantitative information on their sequences, modifications, and relative abundance, which, however, has remained challenging due to their short length (~23 nt). Here, by elongating short miRNAs at both ends, Direct-miR-seq ensures full-length sequencing of miRNAs with high accuracy and coverage. In comparison to standard direct RNA sequencing (DRS) methods, Direct-miR-seq exhibited a 26-fold sequencing yield, reduced bias across different miRNA species, high miRNA coverage (~100%), and a much-simplified protocol. Taken together, these methods may serve as good tools to offer precise and quantitative analysis of miRNAs for many biological and medical applications.

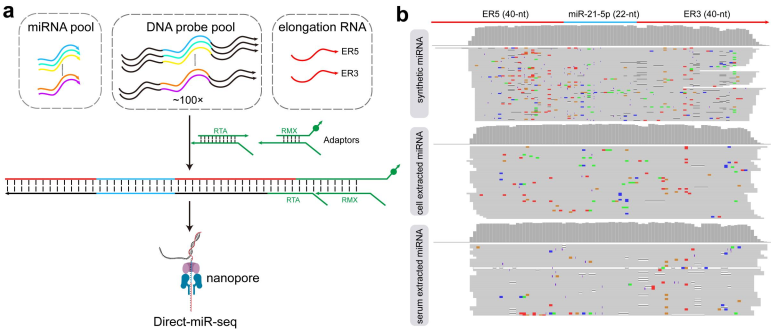

Figure 1. Quantitative detection of miRNAs by nanopore sequencing. **a,** Schematic illustration of Direct-miR-seq for enabling direct sequencing of miRNA molecules in a quantitative and multiplexing manner. **b,** IGV snapshots of Direct-miR-seq mapped reads from synthetic miRNA (upper panel), miRNA from AGS cell line (middle panel) and miRNA from human serum (lower panel). Positions

with a mismatch frequency greater than 0.2 are colored, whereas those showing mismatch frequencies lower than 0.2 are shown in gray.

Keywords: functional nucleic acids, miRNA, cancer diagnosis

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精神活性物质化学生物学

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摘要

虽然当前脑科学基础研究取得了很大的进展，但治疗神经精神系统疾病的药物发现严重滞后。报告人利用精神活性物质作为化学工具，致力于典型毒品与致幻剂等精神活性物质的作用机制及其作为化学探针的脑科学研究，包括精神活性物质神经免疫作用机制、创新戒毒策略发现及精神活性物质的转化应用等研究，探索化学在解决神经脑科学领域核心科学问题的可能性。

Construction of Photofunctional Composites Based on Conjugated Polymers and Their Biological Applications

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ABSTRACT

Conjugated polymer-based photofunctional composites with excellent optical functionality and good biocompatibility have been widely used in biological and medical fields such as sensing, imaging, disease diagnosis and therapy. By rationally designing the structure of conjugated polymers and selecting the conjugated components, a variety of photofunctional composites with excellent properties can be prepared. [1-4] We have covalently linked conjugated oligomers with gold nanoclusters to construct a novel nano-heterojunction.[5] This artificial material can be rapidly internalized into cyanobacteria cells and coupled with intracellular electron transfer processes, forming an efficient bio-electronic interface (Figure 1). It directly introduced exogenous photogenerated electrons into the photosynthetic electron transport chain, successfully achieving direct interaction between artificial semiconductors and microbial internal electron transfer processes. This significantly enhances the photoelectric conversion efficiency and biomass yield, demonstrating great application potential in the field of bioenergy.

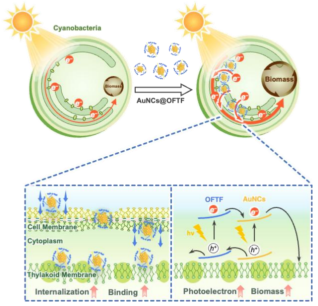

Figure 1. Conjugated molecule/gold cluster heterojunctions regulate electron transport processes in cyanobacterial cells

Keywords: Self-assembly, Conjugated polymers, Photofunction, Interfacial interaction, Biological application

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Visual Point-of-Care Diagnostics Based on Microfluidic Chips

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ABSTRACT

In an aging society, the prevention, monitoring, and diagnosis of various diseases are closely related to everyone's well-being. How to achieve disease detection in an effective, rapid, and convenient manner poses a significant scientific challenge to sustaining human health. Visual point-of-care diagnostics based on microfluidic chips offer a promising solution, characterized by low detection costs, simple operation, and rapid result generation.[1-3] These technologies enable end-users to instantly obtain disease-related metrics and clarify their health status. Highly integrated and miniaturized microfluidic chips serve as reliable and versatile platforms for point-of-care diagnostics. Extensive immune and aptamer recognition mechanisms[4,5] provide a rich library of target identification for integrated biochemical sensing applications, establishing a universal analytical platform for various clinical biomarkers. Additionally, visual signal transduction mechanisms enable simple signal readout and quantification for general populations, eliminating the need for bulky instruments, offering high cost-effectiveness, and ensuring ease of use. Consequently, microfluidic chip-based point-of-care diagnostics can meet the demands of high-frequency, large-scale, and long-term disease screening, as well as the control of sudden biochemical crises. This technology holds significant research value and potential for clinical applications.

Keywords: Microfluidics, Biochemical Sensor, Point-of-Care Diagnostics, Immune Recognition, Nucleic Acid Amplification.

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Polymer-based platinum(IV) prodrugs and their future development directions

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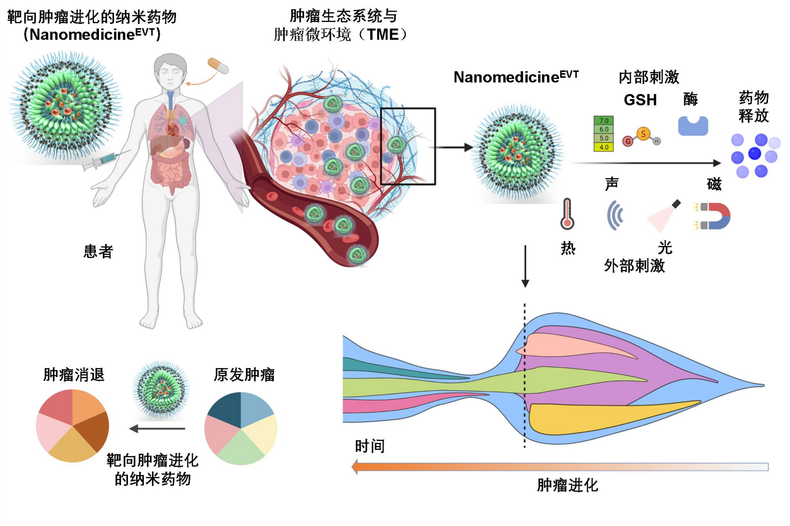
ABSTRACT

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 system systems have been developed. It is generally believed that these delivery systems can deliver platinum(IV) prodrugs 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 [1].

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 [2].



Keywords: Polymer, platinum (IV), Drug delivery, Tumor evolution, Targeted therapy.

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From sugar transporters to glycoconjugated ion channels

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Carbohydrates are the most abundant biomolecules on Earth. Despite their physiological importance, the structural biology of glycans has significantly lagged behind that of proteins and nucleic acids. The crystal structure of the human glucose transporter GLUT3 bound to D-glucose at 1.5 Å resolution clearly demonstrates that the transporter can recognize both α- and β-anomers. This finding underscores the power of high-resolution structures in elucidating the stereochemistry of sugars. While cryo-EM has enabled the structural resolution of glycan chains that modify the extracellular surface of membrane proteins, it has largely been limited to a small number of sugar residues near the modification site and at moderate resolutions. We have been striving to solve high-resolution structures of full glycan chains with little success until recently. By employing a strategy called CryoSeek, we have successfully resolved the high-resolution structures of numerous glycans with higher-order structural assemblies. In this presentation, I will focus on the serendipitous discovery of an 8,000-residue glycoprotein, which we named Mstax. This protein serves as the central shaft for the lateral hairs, known as mastigonemes, that line the cilia of *Chlamydomonas*. Mstax alone extends over 600 nm from the cilia surface. Notably, it contains a PDK2-like transmembrane domain, which provides an immediate explanation for the previously reported association between mastigonemes and PKD2 subunits. Whether Mstax and PKD2 proteins, along with a third component SIP, form a functional channel remains to be investigated.

Chemical Targeting RNA Epigenetic Proteins

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ABSTRACT

Epigenetics comes to RNA, introducing a new dimension to gene expression regulation. The N^6-methyladenosine (m^6A) is an abundant internal modification on eukaryote mRNA, while the significance of m^6A in mRNA had been long neglected until the fat mass and obesity-associated (FTO) enzyme was identified as the first m^6A demethylase. m^6A dynamically regulates nearly every aspect of RNA metabolism, thereby influencing gene expression at multiple levels and playing pivotal roles in cancer progression, metastasis, and immune evasion. To deepen our understanding of m^6A biology and accelerate anticancer drug discovery, the development of selective chemical probes and drug-like molecules targeting m6A-modifying enzymes is essential. Here, we highlight recent advances in small-molecule inhibitors of FTO and ALKBH5, with a focus on their mechanisms of action [1]. We also discuss our recent development of the first FTO-targeting PROTAC degrader, which demonstrates potent antileukemic activity *in vivo* [2]. In addition, we emphasize progress in designing dual inhibitors of FTO and ALKBH5 for targeting glioblastoma. These RNA epigenetic modulators not only provide powerful tools for elucidating gene regulation mechanisms but also offer promising therapeutic avenues for cancer treatment.

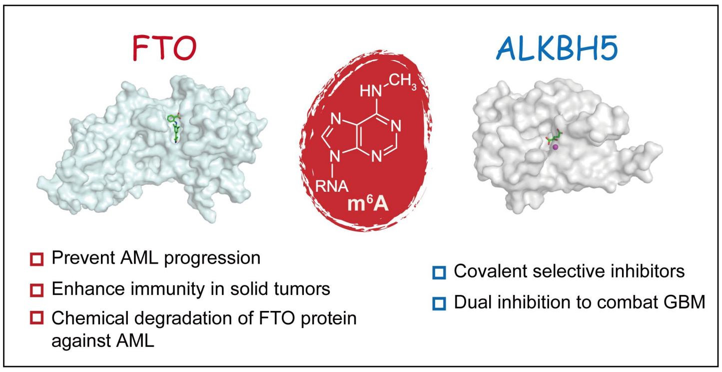

Figure 1. Targeting the RNA demethylases for cancer therapy

Keywords: RNA methylation, m^{6}A demethylase, Chemical interventions, Anti-tumors Reference

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Synthetic fluorescent proteins and RNAs for live cell imaging

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ABSTRACT

Fluorescent proteins (FPs) are the most widely used tools for tracking cellular proteins and sensing cellular events, whereavs fluorescent RNAs (FRs), aptamers that bind and activate small fluorogenic dyes, are emerging tools .have provided a particularly attractive approach to visualizing RNAs in live cells. However, limitations such as low brightness and limited availability of dye/aptamer combinations with different spectral characteristics have limited utility of these tools in live mammalian cells and in vivo. We develop Peppers and Clivias, two series of monomeric, bright, and stable FRs with a broad range of emission maxima spanning from cyan to red. These FRs allow simple and robust imaging of diverse RNA species in live cells with minimal perturbation of the target RNA's transcription, localization, and translation. In combination, Pepper and Clivia allow single-excitation two-emission dual-color imaging of cellular RNAs in both single-photon and two-photon microscopy, as well as the simultaneous visualization of multiple genomic loci by CRISPR display. We also chemically evolved the self-labeling SNAP-tag into a palette of semisynthetic fluorescent proteins (SFPs) that possess bright, rapidly inducible fluorescence ranging from cyan to infrared. As with FPs, SFPs are integral chemical-genetic entities based on the same fluorogenic principle as FPs, i.e., induction of fluorescence of non-emitting molecular rotors by conformational locking. We demonstrate the usefulness of these SFPs in real-time tracking of protein expression, degradation, binding interactions, trafficking, and assembly, and show that these optimally designed SFPs outperform FPs like GFP in many important ways. We believe these synthetic FRs and FPs will be useful tools for live imaging of cellular RNAs and proteins.

Keywords: fluorescent, label, protein, RNA, genetically encoded

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Second Near-Infrared Window Fluorescent Probes for in vivo Dynamic Multiplexed Bioimaging

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ABSTRACT

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.

Keywords: Rare earth luminescent nanomaterials, NIR, Biomedical analysis

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Biomedical applications of platinum coordination complexes

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ABSTRACT

Despite the broad clinical applications of platinum-based anticancer drugs including cisplatin, their side effects and resistance issues have encouraged researchers to look for novel metal-based anticancer complexes. Non-traditional platinum compounds, especially Pt(IV) complexes, have been extensively studied, and they hold great promise to be further developed as the next-generation platinum drugs.[1,2] Selective activation of prodrugs within a tumor is particularly attractive because of their low damage to normal tissue. In this presentation, I will introduce the design, activation mechanism, and antitumor activity of photo- and sono-activatable Pt(IV) prodrugs.[3-7] These small-molecule prodrugs have controllable activation properties: they are shown to be inert in the dark but under short-period irradiation with low intensity of visible light or ultrasound, and without the need for any external catalyst, the prodrugs are efficiently reduced. The prodrugs display superior antitumor activity both in vitro and in vivo in human carcinoma models. Our recent progress in revealing components responsible for activating Pt(IV) prodrugs in live cells will be briefly discussed. I will also introduce our recent progress in the applications of Pt(IV) complexes as photoinitiators and photocrosslinkers for hydrogels and protein labeling.

Keywords: platinum drugs; platinum(IV) prodrugs; photoactivation; sono-activation

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Aptamer-based Targeted degradation technology

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ABSTRACT

Targeted protein degradation (TPD) is a technology that uses eukaryotic cells' own protein clearance system to complete the precise removal of disease-causing proteins, which provides a new and effective strategy for the treatment of undruggable proteins, and shows great application prospects in the field of tumor treatment. At present, the most studied TPD methods mainly include proteolysis-targeted chimeras (PROTACs), lysosome-targeted chimeras (LYTACs), autophagy-targeted chimeras (AUTACs), and molecular glues, etc. However, different TPD methods also have their own limitations, and the development of new targeted protein degradation strategies is of great significance for expanding degradable protein targets and supplementing protein degradation methods. To this end, based on the high affinity, high specificity and programmability of aptamers, we have developed a series of novel targeted protein degradation technologies, such as Apt-LYTACs and MembTACs, using membrane proteins as targets. In addition, RNA, as the upstream of proteins, is also one of the important research directions and means to solve undruggable targets for the direct degradation of RNA, among which ribonuclease-targeting chimeras (RIBOTACs) have attracted much attention. However, the design process of small molecule-based RIBOTACs is complex, the cell uptake efficiency is low, and the tumor specificity is lacking. To this end, we have developed Aptamer-RIBOTACs, a simple and versatile tumor-specific miRNA degradation strategy, for targeted degradation of oncogenic miRNAs (onco-miRs) based on the tumor targeting and cellular internalization capabilities of aptamers.

Keywords: aptamer, targeted degradation, cancer therapy, molecular probe

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DNA Frameworks-based Biosensors

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ABSTRACT

Self-assembled DNA frameworks with precise sizes allow a programmable “soft lithography” approach to engineer the interface of electrochemical DNA sensors. By using millimeter-sized gold electrodes modified with several types of tetrahedral DNA frameworks (TDFs) of different sizes, both the kinetics and thermodynamics of DNA hybridization were profoundly affected. Because each DNA probe is anchored on an individual TDF, its lateral spacing and interactions are finely tuned by the TDF size. By simply varying the size of the TDFs, the hybridization time was decreased and the hybridization efficiency was increased. More significantly, the detection limit for DNA detection was tuned over four orders of magnitude with differentially nanostructured electrodes, and achieved attomolar sensitivity with polymeric enzyme amplification. Our programmable biosensing interface can be easily generalized to the sensitive detection of proteins, small molecules and even cells by conjugating antibody or aptamer on the top vertex of our DNA framework probe.

Keywords: framework nucleic acids, biosensor, analytical

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The amorphous phase and the microstructure effect on the titania-based nanocomposites photocatalytic activity

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ABSTRACT

Much attention is usually paid to the study of the dependence of the oxide materials properties on their phase composition, and the identification of such patterns is the subject of study in a large number of research papers. Nevertheless, the estimation of the amorphous phases effect on the materials properties is a difficult problem, the solution of which requires both the use of various analytical methods and subsequent comparison of the obtained results from the same samples. Such studies cannot be carried out for all known systems and materials. In practice, such correlations can only be reliably established for well-characterized materials with comprehensively studied physicochemical properties. Another problem is to determine the characteristics of contacts in metal/semiconductor composites. The properties associated with the charge transfer processes between the metal and the semiconductor will depend significantly on such contact properties. In the case of contact between nanoparticles, direct electrophysical measurements are not possible, however, the contact characteristics can be evaluated using results of indirect studies. In this work the structural features and their effect on the photocatalytic properties of the commercial titania samples (P25 Evonik (formerly Degussa), Hombikat UV100), pre-synthesized titania, Au/TiO_2 and Ag/TiO_2 nanocomposites were systematically studied. The amorphous phase content in titania was determined using X-ray diffraction pattern analysis of titania mixtures with a crystalline silicon standard. The reference intensity ratios (RIR) of crystalline phases were used for the calculation. The reproducibility of the proposed method was confirmed by measuring the amorphous content in mixtures of the samples and amorphous titania. The contributions of amorphous titanium oxohydroxides $TiO_{2-0.5n}(OH)_n \cdot xH_2O$ and physically adsorbed water on the amorphous phases were distinguished by thermogravimetric analysis. The obtained results show that the photocatalytic activity of the titania samples decreases with an increase in the weight percentage of the amorphous phase [1]. Analyzed P25 Evonik (formerly Degussa) and pre-synthesized crystalline titania [2] were taken as photocatalytic matrices for composite synthesis. Composites were obtained using different wet chemistry techniques such as impregnation by previously prepared nanoparticles (NPs) sols, *in situ* reduction by sodium borohydride, sodium citrate, and UV irradiation. Varying the synthesis method, due to the reduction rate differences results in different interaction between metal NPs and titanium dioxide, and hence different metal/TiO_2 contacts were observed. All the obtained metal/TiO_2 samples were

analyzed by XRD, SEM, TEM and EDX. Using the statistical analysis of the TEM images, the correlation between the formation rate of metal NPs and their anisotropy was evaluated. Combining the obtained results with the optical spectroscopy data the correlation between observable anisotropy and contact quality was confirmed. Finally, the effect of the synthesis method on the photocatalytic activity (PCA) of nanocomposites was demonstrated [3].

Keywords: titania, crystallinity, nanocomposites, nanoparticles anisotropy, photocatalysis

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Molecular design and characterization of one and 2D materials

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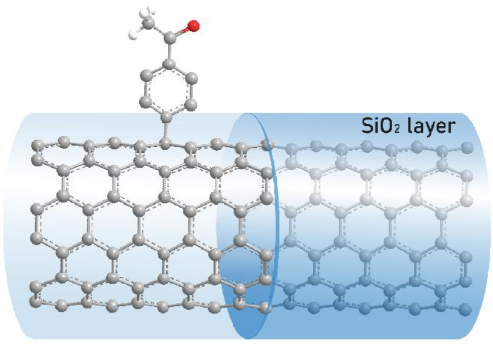
ABSTRACT

We demonstrate two different strategies for molecular design of low-dimensional materials. In the case of 1D materials - single-walled carbon nanotubes (SWCNTs), we developed a novel approach to efficiently increase a photoluminescence (PL) signal from individual SWCNTs by their surface protection with SiO_2 nanolayer synthesised by a modified Stöber method. The aryl functionalized (6,5)-SWCNTs covered with silicon dioxide layer demonstrate emission peaks from individual defect sites in the spectral range of 1100 – 1300 nm. Since the PL signal strongly depends on the local dielectric environment, the silicon dioxide shell and its formation condition creates favorable conditions for the configurations with red-shifted emission (E11**, ortho+) at ~1260 nm [1]. This approach offers strong potential for sp^3 defects on larger diameter nanotubes in the development of room temperature quantum light sources capable of operating at telecommunication wavelengths.

Van der Waals (vdW) 2D magnetic materials (MM) have emerged as an exciting field to explore novel physical phenomena, such as strain- and doping-induced magnetic quantum phase transitions and layer-dependent magnetic ordering. Large-scale growth of 2D-MM is critical for hetero-integration with other 2D materials and for scaling towards real-world applications. In the study we developed a systematic approach for centimeter-scale growth of semiconducting 2D-MM CrCl3 films (on mica substrate), via Physical Vapour Transport Deposition [2]. Light-management during synthesis, very-high carrier gas flow, precursor flux, and oxygen/water removal, are collectively responsible for wafer-scale growth. Optical, stoichiometric, structural, and magnetic characterization identify crystalline, phase-pure 2D-MM $CrCl_3$. This scalable vapour deposition approach can be applied for growth of several 2D-MM.

The work was supported by the Ministry of Education and Science of Russia, Agreement 075-15-2024-680



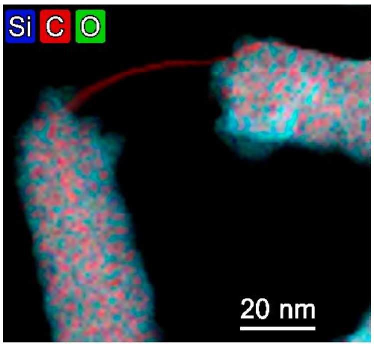


Figure 1. Sp^3-modified SWCNT protected by SiO_2 layer (left) and color-coded STEM-EELS elemental map demonstrating a uniform coating by amorphous silica.

Keywords: single-walled carbon nanotubes, functionalization, 2D magnetic materials

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Mineral-like complex iron-copper sulfides for thermoelectric application: a Mössbauer study

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ABSTRACT

In recent years, the development and application of new environmentally friendly materials for energy production have gained significant attention. These materials could help address the critical issue of low efficiency in heat engines. The lost energy is primarily released into the environment as waste heat. Thermoelectric materials (TEMs), which enable the conversion between thermal and electrical energy, can reduce heat waste and improve the efficiency of energy devices. Moreover, thermoelectric materials offer advantages such as environmental friendliness, high stability, long service life, compactness, and silent, vibration-free operation. Thus, thermoelectric materials are functional materials with broad application prospects, playing a crucial role in enhancing energy efficiency in various processes.

Currently used TEMs are based on bismuth and lead tellurides, making them expensive and environmentally unfriendly. As a result, new thermoelectric materials based on synthetic copper-sulfide minerals are being actively studied, as they exhibit comparable efficiency to traditional materials.

This study presents the results of microscopic-level investigations of several classes of mineral-like complex solid solutions based on iron-copper sulfides [1 - 5]: tetrahedrites, colusites, and owensites. The primary research method employed was Mössbauer spectroscopy at ^{57}Fe nuclei. The study examined the local crystallographic structure, and the charge state of transition metals. The research not only identified the stability ranges of the solid solutions but also established correlations between composition, local and extended crystal structure, and the thermoelectric properties of these phases.

It was shown that for all minerals, an increase in iron content initially leads to the formal reduction of Cu^{2+} cations to Cu^{1+}, followed by the oxidation of iron atoms to Fe^{3+}. For a series of tetrahedrite compositions, dynamic behavior of the $Fe^{3+} \rightleftarrows Fe^{2+}$ equilibrium was demonstrated, exhibiting an activation-dependent nature. In contrast, colusites displayed similar dynamic behavior directly in "iron-copper" pairs: $Fe^{3+} + Cu^{+} \rightleftarrows Fe^{2+} + Cu^{2+}$. The study of owensites using Mössbauer

spectroscopy enabled crystallochemical identification of iron ions and revealed the existence of the $Fe^{3+} + Cu^{+} \rightleftarrows Fe^{2+} + Cu^{2+}$ equilibrium, which was significantly shifted to the left.

Keywords: Mössbauer spectroscopy, Thermoelectric materials, Copper sulfides

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His research spans inorganic chemistry, materials science, solid-state physics and chemistry, radiochemistry, quantum chemistry, and nuclear physics. He has extensive expertise in physical methods of compound analysis, including diffraction techniques, Mössbauer spectroscopy, and high-pressure/high-temperature inorganic synthesis.

With a strong publication record, he has authored over 140 academic papers (including more than 45 as first or corresponding author) in prestigious journals such as: Journal of the American Chemical Society, Inorganic Chemistry, Chemistry of Materials, Journal of Physical Chemistry C, Physical Review B, etc.

Additionally, he has delivered more than 175 conference presentations, including over 20 invited or keynote talks, at international and national chemistry and physics conferences.

Structural regularities and thermal stability in the series of actinide double sulfates $Cs[An(SO_4)_2(H_2O)_3]\cdot H_2O$ (An = U, Np, Pu or Am)

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The actinides (An) constitute a unique group of elements with filled 5f-orbitals. However, the extent of actinide contraction and the involvement of valence orbitals in covalent bonding across actinide compounds remain topics of ongoing debate. While the 5f-orbitals of lighter actinides (up to americium) exhibit significant chemical activity, those of the heavier actinides become highly localized and core-like, resembling the 4f-orbitals of the lanthanides. Studying isostructural compounds containing actinides in the same oxidation state is of both fundamental and practical importance.

Double sulfate hydrates are the most stable form for lanthanides, which predominantly adopt the +3 oxidation state. In contrast, stabilizing light actinides in the +3 state demands stringent conditions—such as inert gloveboxes, anhydrous solvents, and controlled temperatures. For over five decades, double sulfates containing group IA metals or ammonium have been used to isolate light actinides in this less common oxidation state.

In this work [1], we synthesized and characterized the An^{3+} double sulfates $Cs[An(SO_4)_2(H_2O)_3]\cdot H_2O$ (An = U, Np, Pu, or Am) using complementary analytical techniques. Single-crystal X-ray diffraction reveals that all studied compounds feature identical actinide coordination polyhedra, consisting of distorted tricapped trigonal prisms. The Voronoi-Dirichlet polyhedron volumes for the actinide (An) atoms in $Cs[An(SO_4)_2(H_2O)_3]\cdot H_2O$ decrease sequentially from U to Pu. XANES spectroscopy and solid-state absorption spectroscopy in the visible region confirm the +3 oxidation state of the actinides in these double sulfates. Over a timespan of ~1 year, self-irradiation alters the local environment of Am^{3+}, as evidenced by spectral distortions in its absorption features, while the sulfate (SO_4^{2-}) ions remain largely unaffected. The compounds exhibit notable thermal stability in both inert and air atmospheres. Dehydration occurs between 100–300 °C without side reactions, yielding anhydrous An^{3+} sulfates that could be valuable for preparative chemistry. Upon further heating, sulfate decomposition occurs, culminating above 900 °C in the formation of cesium uranates (for the U compound) and NpO_2/PuO_2 mixed with Cs_2SO_4 (for the Np/Pu compounds).

Keywords: *actinide double sulphates, XANES-spectroscopy, Raman spectroscopy*

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Fuel-cladding chemical interaction and constituent redistribution in U-10Zr fuel

ABSTRACT

With the global pursuit of low-carbon energy, advanced nuclear energy systems have emerged as a key direction for future clean energy development due to their high efficiency and low emissions. Different types of nuclear systems vary in coolants, operating temperatures, and fuel cycle strategies, leading to diverse performance requirements for nuclear fuels. In addressing the material challenges of Generation IV nuclear energy systems, the speaker has conducted systematic studies on the key failure mechanisms of metallic fuels. Focusing on the issue of fuel–cladding chemical interactions, the speaker introduced specific elements to stabilize reactive fission products, and have demonstrated their effectiveness in suppressing interfacial reactions and enhancing the in-service stability of fuels. This work provides a practical pathway for the material design of metallic fuels. Looking ahead, the core of fuel research lies in achieving multiscale modeling and accurate prediction of material behavior, which fundamentally depends on obtaining experimental parameters at the micro- and atomic scales to support model development and validation. Given the current scarcity of experimental and characterization data, a key scientific challenge is how to leverage advanced in situ and ex situ techniques to obtain insights into cross-scale coupling mechanisms.

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Highly stable BATA chelator for binding Ac-225 and REE radionuclides for targeted radiopharmaceuticals

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ABSTRACT

A number of radiopharmaceutical companies are making significant progress in developing new radiopharmaceuticals for cancer therapy and diagnostics. The most promising area today is targeted alpha therapy (TAT), which uses alpha emitters with high linear energy transfer (LET), such as Ac-225, and application of ^{44,47}Sc, ^{90}Y as well as Ln(III) such as ^{132,133}La, ^{153}Sm, ^{149,152,155,161}Tb, ^{177}Lu and others. Currently, radioimmunotherapy methods using monoclonal antibodies, which are heat-sensitive molecules, are actively being developed. Radionuclides of metals bind to biomolecules through the formation of coordination complexes with chelator, which is covalently linked to the biomolecule.

The benzoazacrown ether with carboxylate coordinating groups, BATA, is capable of forming stable complexes with Ac^{3+} immediately at room temperature [1]. The stability constants of Ac^{3+} complexes with BATA and well-known chelator DOTA were determined. That is particularly valuable given the extremely limited thermodynamic data available for actinium complexes. The values $\lg K([AcBATA]^{-}) = 25.74 \pm 0.01$ and $\lg K([AcDOTA]^{-}) = 20.32 \pm 0.03$ were obtained indicating the exceptional thermodynamic stability of the $[AcBATA]^{-}$ complex. The stability constant of $[ScBATA]^{-}$ was also obtained using a radioactive label ^{44}Sc. The obtained value is again higher than for the complex with DOTA ($\lg K([ScBATA]^{-}) = 30.7 \pm 0.1$). The standard method of potentiometric titration was used to determine stability constants for complexes with Ln(III). $\lg K([LaBATA]^{-}) = 27.05 \pm 0.01$ and the remaining constants in the lanthanide series did not differ significantly from each other. DFT calculations showed a decrease in bond lengths with decreasing cation size, which correlates with an increase in the stability constant with decreasing ionic radius.

Labeling of BATA with all studied cations was performed under the room temperature and the complex was formed immediately. The stability of the obtained complexes was then studied *in vitro*.

The complex of $[^{225}Ac]AcBATA^{-}$ was stable in 10-fold excess of fetal bovine serum for at least 5 days. The stability of REE complexes with BATA was also studied. A decrease in stability was observed with a decrease in the radius of REE(III): the complex with Sc^{3+} dissociated in the first hour of the experiment, whereas starting with Gd^{3+} and larger cations in the lanthanide series, no dissociation of the complexes was observed for at least 7 days. The stability of $[^{225}Ac]AcBATA^{-}$

was also studied *in vivo*, and fast clearance and stability was discovered within 6 h. Thus, high thermodynamic stability cannot serve as an unambiguous criterion for the stability of the complex *in vitro*.

In summary, BATA forms complexes at room temperature, and forms stable complexes with large cations. Taken together, BATA is a superior candidate for further conjugation with targeted molecules.

Keywords: radiopharmaceuticals, chelator, macrocycle, Ac-225.

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Solvent extraction systems for the separation of trivalent *f*-elements

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Nuclear power is an important energy resource with minimal carbon dioxide emissions. However, for further sustainable development of nuclear energy, it is necessary to implement the concept of a closed nuclear fuel cycle, which involves the extraction and reuse of valuable components from spent nuclear fuel. The diverse composition of spent nuclear fuel requires the development of new highly selective extraction systems for the extraction of *f*-elements. One of the key challenges is the separation of Am(III) and lanthanides(III).

"N,O-donor ligands represent a promising class of compounds for the extraction and separation of trivalent f-elements. Among them, diamides based on 1,10-phenanthroline are particularly notable (Figure). A significant advantage of this class of compounds is the ability to modify the extraction and coordination properties of the ligand, both by introducing substituents at the 4,7-positions of the phenanthroline core and by altering the substituents on the amide nitrogen atoms. Understanding the relationship between 'ligand structure - complex structure - extraction properties' is crucial for the further development of molecules with desired coordination and extraction properties.

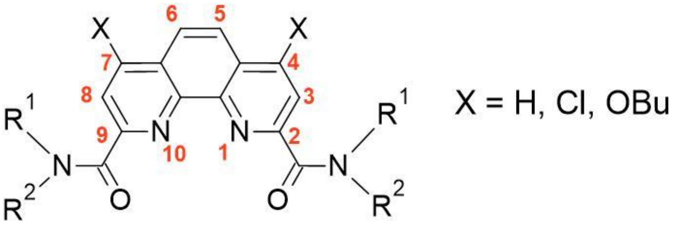

Figure. The general formula of 1,10-phenanthroline-2,9-dicarboxylic acid diamides.

This study summarizes the extraction and coordination properties of a broad range of 1,10-phenanthroline-2,9-dicarboxamides. The structure of the complex compounds in solution was determined using the equilibrium shift method and UV-Vis titration for lanthanide nitrates. To elucidate the structure of the complexes in the solid state, single crystals of the ligand complexes with lanthanide(III) nitrates were obtained and analyzed via X-ray crystallography.

It was shown that diamides with a combination of alkyl and aryl substituents at the amide nitrogen atoms have higher extraction efficiency and selectivity compared to tetraalkyl diamides. Furthermore, the additional introduction of an alkyl group at the ortho-position of the aryl fragment significantly increases the separation factors for Am(III) and light lanthanides(III), making these ligand-based extraction systems suitable for the isolation of Am(III) from high-level waste.

The influence of electron-withdrawing (-Cl) and electron-donating (-OBu) substituents at the 4,7-positions of the phenanthroline core on the Brønsted and Lewis basicity of the ligand was also shown, which, in turn, affects the solvent extraction process.

Keywords: solvent extraction, americium, lanthanides, N,O-donor ligands

Solvent extraction systems for the separation of trivalent *f*-elements

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Mariia is a specialist in solvent extraction, especially for the extraction and separation of actinides and lanthanides for the processing of high-level waste. In particular, her area of scientific interest is the study of extraction systems based on N,O-donor heterocyclic ligands for the separation of trivalent americium and lanthanides. Also, the study of the mechanisms of extraction and complexation of polydentate N,O-donor ligands.

^{225}Ac/^{213}Bi medical generators for rapid synthesis of radioimmunoconjugates

ABSTRACT

Among alpha emitters suitable for targeted alpha-therapy, ^{225}Ac ($T_{1/2}$ = 9.9 days) and the product of its decay ^{213}Bi (46 min.) are the most promising. Clinical trials are confirming higher efficacy and less toxicity of the radiopharmaceuticals labeled with these radionuclides in comparison with similar beta-emitting ones. A prospective method of producing ^{225}Ac (more than 1 Ci for a 10-day run) by irradiation of natural thorium with medium-energy protons followed by chemical isolation has been developed at the Institute for Nuclear Research of the Russian Academy of Sciences (INR RAS) [1]. A long-lived ^{227}Ac (21.7 years) is also formed (~0.1% of ^{225}Ac activity at the end of irradiation), and direct medical application of the product seems questionable. However, ^{225}Ac with small impurity of ^{227}Ac is appropriate as a mother radionuclide for ^{225}Ac/^{213}Bi generator.

^{225}Ac/^{213}Bi generators based on ion exchange (AG MP-50, AG 1, BioRad) and extraction chromatography resins (Actinide Resin, UTEVA Resin, Triskem Int.) are well described. However, all the generators have been developed for isotopically pure ^{225}Ac, while the presence of ^{227}Ac and its decay products in ^{213}Bi eluate may be important. Moreover, the reported generators produce a ^{213}Bi eluate assuming further labeling and purification. Since the half-life of ^{213}Bi is short, the total process from a generator elution to a labeled compound is rather long resulting in undesirable decay losses. Generators developed at INR RAS provide rapid and effective synthesis ^{213}Bi-labeled compounds with high radiochemical and radionuclidic purity [2-3].

The generator «Afrabis» consists of two chromatographic columns connected together in a closed loop. The formation and concentration of ^{213}Bi in the second column was realized by continuous separation of intermediate ^{221}Fr (4.9 min) from ^{225}Ac fixed in the first column filled with Actinide Resin sorbent arranged in circulation mode. The two-column construction allows us to vary the size of the first column and distribute ^{225}Ac uniformly without compromising the characteristics of the generator. It was demonstrated that ^{213}Bi can be extracted from the second column filled with cross-linked dextran gel Sephadex G-25 using a bioconjugate solution. In this case, the labeling of the bioconjugate takes place directly inside the generator, and the user receives a solution that is already purified and ready for injection into the patient. As a result, the proposed synthesis route is three to four times faster than a traditional one including the generator elution, labeling and purification and taking more than 20 min. DTPA-Nimotuzumab for radioimmunotherapy of EGFR-overexpressing carcinomas and DOTA-Substance P for glioma treatment were successfully tested for this purpose and the corresponding ^{213}Bi- radioimmunoconjugates were obtained.

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Molecular clusters of f-elements: from synthesis to deep learning insights

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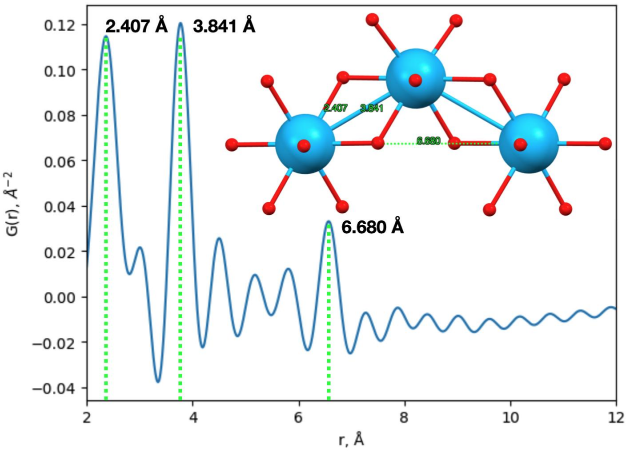
ABSTRACT

Lanthanide-based coordination polymers and polynuclear clusters have been extensively studied for their unique magnetic and luminescent properties, making them attractive candidates for applications in fields such as optoelectronics, molecular magnetism, and quantum materials. Actinide chemistry plays an important role in the areas of nuclear materials and nuclear waste management. The structural investigation of polynuclear f-block clusters is an intriguing area of study, with early research on thorium clusters in solution laying the foundation for the field [1]. However, despite significant advancements, many challenges persist, including low crystallinity, structural disorder, and the absence of well-defined initial models for structural refinement.

This report will cover a combination of synthetic, crystallographic, and computational techniques that has been employed to address these challenges. Conventional single-crystal X-ray diffraction remains the gold standard for structure determination, but its applicability is often limited for disordered or poorly crystalline materials. Total scattering techniques combined with pair distribution function (PDF) analysis provide a complementary approach, enabling the study of local atomic structure in systems where long-range order is insufficient for traditional crystallographic methods.

In parallel, machine learning is emerging as a powerful tool for structural chemistry, offering new strategies for data analysis and pattern recognition. The integration of PDF analysis with convolutional neural networks presents a promising avenue for significant improvements in the efficiency and accuracy of structural characterizations. Recent studies demonstrate how such computational techniques can extract meaningful structural information from complex datasets [2]. As machine learning continues to evolve, its synergy with experimental methods holds the potential to transform the way structural problems in lanthanide chemistry are approached, bridging the gap between experimental observation and predictive modeling.



Pair distribution function G(r) as a representation of a trinuclear metal-oxygen cluster

Keywords: lanthanides, synthesis, crystallography, total scattering, machine learning

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Protein Conjugation with Synthetic Polypeptides: Chemistry and Biomedical Applications

ABSTRACT

Synthetic polypeptides, also known as poly(α-amino acid)s (PαAAs), are biomimetic polymers holding great potential for a variety of biomedical applications. Possessing the same peptide bonds as natural proteins, polypeptides can also adopt typical well-defined secondary structures including α-helix and polyproline II (PP-II) helix, which have been shown to significantly impact the physicochemical properties and biological outcomes of materials. In this talk, I will present progresses on the manipulation of helical conformation-associated anti-biofouling coatings, cellular uptake regulation, immunomodulatory hydrogel for tissue engineering, and reducing immunogenicity of polypeptide-protein conjugates.

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Sensing Platforms on the basis of Plasmon Nanomaterials with Controlled Spectral and Recognition Properties for Biological and Ecological Monitoring

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ABSTRACT

The creation of highly sensitive, selective sensor systems based on plasmonic nanocomposites with controlled spectral and recognition properties for multiplex determination of biologically active substances and ecotoxicants is an important task of modern biological and environmental monitoring.

A nanocomposite is a multicomponent material with new improved properties (sensitivity, selectivity, stability and reproducibility), consisting of a optically transparent polymer base (matrix), nanoparticles of noble metals of various sizes and shapes, additional reagents that help reduce background signals from analytes and/or the matrix of the analyzed samples, prevent oxidation of the surface or analytes, as well as recognizing indicator substances that, when interacting with the analyzed substance or their group (in multiplex determination), provide the appearance of characteristic - sensitive and selective signals in the Raman spectrum. The report will focus on obtaining nanostructured polymeric materials with conductive properties for their use in the electrochemical (EC) version of surface-enhanced Raman spectroscopy (SERS) analysis (EC-SERS), and the creation of photocatalytic materials. Approaches to control the hydrophilicity/hydrophobicity of the sensor surface and its surface charge will also be discussed. This will not only expand the range of analyzed samples, but also regulate the orientation of analyte molecules (specific functional groups) on the plasmonic surface. The latter will increase the selectivity of the SERS method due to the possibility of multiplex determination of molecules similar in structure and properties. The development of such new multifunctional approaches in the creation of plasmonic sensors will significantly expand the analytical capabilities of surface-enhanced Raman spectroscopy, move from high-resolution devices to portable equipment, thereby making the method available for use in clinical diagnostic laboratories, biological and environmental monitoring, in quality control of pharmaceutical and food products at various industry enterprises, etc.

Keywords: SERS, Plasmon Nanomaterials, Controlled Spectral and Recognition Properties, Chemical Analysis

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Suppression Strategies of Lithium Filaments formation in ceramic electrolytes for all solid state batteries

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ABSTRACT

The 2019 Nobel Prize in Chemistry for the creation of lithium-ion batteries was undoubtedly recognition of the great importance of electrochemical energy and solid-state chemistry as the most important areas of modern scientific and technological progress. At the same time, there is an increasing demand to improve the energy density and safety of conventional Li-ion batteries. The use of ceramic solid-state electrolytes is promising to address these issues. The complex and not fully understood mechanism of formation of lithium filaments in the solid electrolyte is a key point that determines the choice of chemical composition, structure and properties of the electrolyte. The work presents important insights for achieving the desired key parameters of ceramic solid state electrolyte to suppress the propagation of Li filaments in solid state electrolytes, the formation of which prevents the industrialization of solid state batteries.

Keywords: ceramic solid state electrolyte, lithium filament, electro-chemo-mechanics, solid state batteries

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New generation of bioceramics with complex structure and chemical composition for personalized bone tissue engineering.

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ABSTRACT

The rapid development of modern medicine requires the creation of new types of materials with improved performance characteristics, including bioceramics with enhanced mechanical properties. Ceramics are unique materials in the here and now due to their range of amazing properties. The main scientific problem is the development of physicochemical and engineering principles for bone tissue reconstruction using tissue-engineered structures based on resorbable highly porous phosphate ceramics with a given complex architecture as a carrier for cells and drugs. Modern approaches to bone defect repair practically do not consider the moments of complex bone tissue structure and multimodal conjugation with the complex of adjacent tissues. The complex nature and functionality of each organ results in different rates and mechanisms of their regeneration, which can ultimately lead to the dominance of recovery of one type of tissue over the others. In this context, the scaffold design should take into account the complexity of the structure and environment of the reconstructed bone and therefore be a combination of different materials with individual macrostructures, chemical compositions and a range of mechanical properties.

This work was supported by the RSF [projects #22-19-00219, 23-79-10103, 24-29-00396]. The authors acknowledge the partial support from the Lomonosov Moscow State University Development Program.

Keywords: bioceramics, 3D printing, calcium phosphates, complex structure

Site-Specific Assessment of the Structure and Dynamics of Amyloid Fibrils

ABSTRACT

Many spectroscopic techniques, such as infrared (IR) spectroscopy and fluorescence spectroscopy, are widely used in biological sciences. However, most biological systems lack an intrinsic and suitable molecular signal that can be used to extract site-specific chemical or physical information of interest via spectroscopic measurement and hence require labeling of an external reporter that bears desired spectroscopic property. In this regard, unnatural amino acid-based (UAA-based) spectroscopic probes have recently gained popularity in the study of the structure, dynamics, hydration, and electrostatics of proteins in a site-specific manner. In this talk, we will focus on discussing the application of UAA-based IR probes to site-specifically interrogate the local structure and hydrogen-bonding (H-bonding) dynamics of amyloid fibrils, as well as the effect of dehydration on the kinetics and mechanism of amyloid fibril formation.

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Feng Gai is a Chair Professor at Peking University (PKU). Before moving to PKU in 2021, he was the Edmund J. and Louise W. Kahn Term Professor of Chemistry at the University of Pennsylvania. He was elected fellow of the American Association for the Advancement of Science in 2012 and fellow of the American Physical Society in 2011. He has won several awards, including the NFS CAREER Award and the ACS Philadelphia Section Award. His research mainly focuses on the development and application of novel spectroscopic probes and methods, such as multidimensional spectroscopy, to study the structure, dynamics, and function of proteins under both in vitro and in vivo conditions.

Main challenges for the FAB integration of 2D electronics from the reliability point of view

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ABSTRACT

Recent research advances at fabricating FETs with 2D semiconductors have inspired the industry to begin with integration of these new technologies into FAB process flows, thereby potentially making them interesting for advanced manufacturing areas. For instance, Intel already has 300mm FAB process for MoS_2, WS_2, WSe_2 and $MoSe_2$ at CMOS compatible temperatures and recently reported complementary integration of MoS_2 n-type FETs and WSe_2 p-type FETs. Imec has also demonstrated functional MoS_2 and WS_2 FETs produced using their 300mm FAB lines. However, the transition of new 2D technologies from research labs to FAB process lines is still very challenging due to a number of open questions, such as the need to satisfy CMOS thermal budget below 450^{o}C, top-gate integration by growing 3D oxides on 2D channels and, most importantly, reliability limitations due to possible presence of mobile ions in gate insulators or charge trapping near the channel/insulator or top gate/insulator interfaces.

In this talk I will summarize recent progress made by the industry at integrating 2D FETs into FAB lines, discuss the main challenges which arise on this way, and try to benchmark reliability limitations of first FAB 2D FETs based on our recent experimental results. I will also touch the related problems for 2D photodetectors which are still behind FETs on their way to advanced manufacturing applications, even though an enormous progress has been recently made at the prototype level.

Keywords: 2D materials, FAB integration, reliability, charge trapping