8-10th June, 2026

International Conference on

Fundamental and Advanced Research in Chemistry (FARC-2026)

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International Conference on Fundamental and Advanced Research in Chemistry 2026

FARC 2026 : 8-10 June 2026 (Auditorium, North Campus, IIT Mandi)		
Time	**Day 1: 8 June, 2026**	
8:00-9:00	**Registration**	
9:00- 9:30	**Inauguration (Lamp Lighting, Welcome Address (FARC Chair; School Chair & Director IITM)** **(Moderators: Garima Agrawal & Narayan Sinha)**	
Session1	**Talk**	**Session Chair: Chayan Kanti Nandi**
9:30-9:55	**Talk 1** Jim Thomas	**Title**: Metal complexes as super-resolution microscopy cell probes, phototherapeutics and antimicrobials
9:55-10:20	**Talk 2** Anunay Samanta	**Title**: Charge Carrier Dynamics in Perovskite Nanocrystals
10:20 – 10:45	**Talk 3** Amitava Das	**Title**: Supramolecular Integration of N-Capped Peptides for Multivalent Recognition and Precision Therapeutics
10:45-11:10	**Talk 4** Swapan K Pati	Title: Computational Modeling of Molecules and Materials for Applications in Energy Conversion and Storage
11:10- 11:30	**High Tea (Foyer)**	
Session2	**Talk**	**Session Chair: Venkata Krishnan**
11:30-11:55	**Talk 5** Hitesh Handa	**Title**: From Bench Innovation to Clinical Impact: Nitric Oxide–Releasing Device Coatings
11:55-12:20	**Talk 6** PC Ravikumar	**Title**: Synthetic Strategies using C-C and C-H bond Functionalization
12:20-12:45	**Talk 7** Prabal Banerjee	**Title**: Electrochemical Generation of Ketyl Radical Anions: Synthetic Utilization in the Construction of Diverse Cyclic and Acyclic Scaffolds
12:45-13:05	**Sponsor 1**	ATOS
13:05-14:30	**Lunch; (Fountain Area)**	
Session3	**Talk**	**Session Chair: Pradeep C Parameswaran**
14:30-14:55	**Talk 8** Sanjit Koner	**Title:** New Insight into Bistable Hofmann-Type frameworks: Kinetic Trapping and THz response
14:55-15:20	**Talk 9** Tomohiro Ogawa	**Title:** New insights into photoactive earth-abundant Fe(II) complexes
15:20-15:45	**Talk 10** Saptarshi Mukherjee	**Title:** Intracellular Subdegree Temperature Sensing and Dynamics by Thermoresponsive Silver Nanoclusters as Molecular Probes
15:45- 16:10	**Talk 11** Sudip Malik	**Title:** Aryl-Substituted Buta-1,3-Diene as Luminescent Core for Monomers and Copolymers: Design, Synthesis and Applications
16:10-16:30	**High Tea (Foyer)**	
Session4	**Talk**	**Session Chair: Garima Agrawal**
16:30-16:55	**Talk 12** Debashis Adhikari	**Title**: Redox Active Ligands in Homogeneous Catalysis
16:55-17:20	**Talk 13** Laura Zanetti	**Title**: Probes and Tracers – An Advanced Microscopy Perspective
17:20-17:45	**Talk 14** Debapratim Das	**Title**: Breaking the equilibrium to secure information
17:45-19:30		**Poster Presentation (Chair: Narayan Sinha & Garima Agrawal)**
19:30-22:00		**Dinner**

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Time	**Day 2: 9 June, 2026**	
Session5	**Talk**	**Session Chair: Moupriya Das**
9:00 -9:25	**Talk 15** Stanley Botchway	**Title:** Time resolved imaging of DNA labelling probe towards chromosome structural characterisation
9:25 -9:50	**Talk 16** Anindya Datta	**Title:** Exciton dynamics in semiconductor nanocrystals: from curiosity to applications
9:50-10:15	**Talk 17** Sanjay Puri	Title: Phase Separation in Active Mixtures
10:15-10:40	**Talk 18** Biswarup Pathak	**Title:** Graph Neural Network for High-Throughput Screening of Nanocluster Electrocatalysis
10:40-11:00	**High Tea (Foyer)**	
Session6	**Talk**	**Session Chair: Abhishek Dewanji**
11:00-11:25	**Talk 19** Ralf Eichhorn	**Title:** An artificial motor protein that walks along a DNA track
11:25-11:50	**Talk 20** Santanu Pal	**Title:** Discotic Liquid Crystals as Self-assembled Molecular Semiconductors for Nanoscale Organic Electronics
11:50-12:15	**Talk 21** Prasun Mandal	**Title:** Single Particle Spectroscopic and Ultrafast Dynamical Exploration of Quantum Dots and Perovskite Nanocrystals
12:15-12:40	**Talk 22** Asish Pal	**Title:** Photoswitch tethered Peptide to Dictate the Fate of Supramolecular Polymerization
12:40-12:50	Sponsor 2	Sci Finder
12:50-13:00	Sponsor 3	RSC
13:00-14:30	**Lunch (Fountain Area)**	
Session7	**Talk**	**Session Chair: Narayan Sinha**
14:30-14:55	**Talk 23** Artur Stefankiewicz	**Title:** Toward Adaptive Systems: Amino Acid-Based Self-Assembled Nanostructures
14:55-15:20	**Talk 24** Srabanti Ghosh	**Title:** Powering Solar Fuels with Next-Generation Semiconductor Heterostructures: Trends, Breakthroughs, and Mechanisms
15:20-15:45	**Talk 25** Aasheesh Srivastava	**Title:** Enzyme-Assisted Preparation of Organic Nanoparticles for Bioanalyte Detection and Photothermal Therapy
15:45- 16:10	**Talk 26** Bijay Tripathi	**Title:** Stimuli-Responsive Microgels and Hydrogels: From Switchable Microreactors to Tunable Permeation and Atmospheric Water Harvesting
16:10-16:30	**High Tea (Foyer)**	
Session8	**Talk**	**Session Chair: Indu Bala**
16:30-16:55	**Talk 27** Elena V. Ushakova	**Title**: Chiral Carbon Dots and Their Bioconjugates: Synthesis and Optical Properties
16:55-17:20	**Talk 28** Debabrata Mukherjee	**Title:** σ-Bond Activation by Stable Azomethine Ylides
17:20-17:45	**Talk 29** Yashveer Singh	**Title:** Hydrogels/ gels and nanomaterials for biomedical applications
17:45-19:30		**Poster Presentation (Chair: Narayan Sinha & Garima Agrawal)**
19:30-22:00		**Gala Dinner**

International Conference on Fundamental and Advanced Research in Chemistry 2026

FARC 2026 : 8-10 June 2026 (Auditorium, North Campus, IIT Mandi)		
Time	**Day 3: 10 June, 2026**	
Session 9	**Talk**	**Session Chair: Prem Felix Siril**
9:00 -9:25	**Talk 30** Mostofa Ataur Rohman	**Title:** Expanding self-healing dyes towards the blue-green spectral region via modular linkers
9:25 -9:50	**Talk 31** Kuljeet Kaur	**Title:** Swelling-activated phenomenon: From thin polymer films to bulk polymer materials
9:50-10:15	**Talk 32** Md. LH Choudhury	**Title:** Designing Sustainable Methods for the Synthesis and Functionalization of Small Molecules
10:15-10:40	**Talk 33** Vandana Bhalla	**Title:** Chiral/Achiral Assemblies: Understanding the Regulation of Self-Assembly
10:40-11:00	**High Tea (Foyer)**	
Session`10	**Talk**	**Session Chair: Subrata Ghosh**
11:00-11:25	**Talk 34** Subi George	**Title:** Bio-inspired, Non-Covalent Synthesis of Precision Supramolecular Polymers
11:25-11:50	**Talk 35** Akkattu T. Biju	**Title:** N-Heterocyclic Carbene-Catalyzed Synthesis of C-N, C-O and N-N Axially Chiral Molecules
11:50-12:15	**Talk 36** Pratik Sen	**Title:** Protein Stability and Activity in Alternate Media: An Unified explanation through Associated Water Stabilization Mechanism (AWSM)
12:15-12:40	**Talk 37** Virendra V. Singh	**Title:** Metal Organic Frameworks and their hybrid for Advanced Chemical Defence Applications
12:40-12:50	**Sponsor 4**	Merck
12:50-13:00	**Sponsor 5**	Bruker
13:00-14:30	**Lunch; (Fountain Area)**	
Session 11	**Talk**	**Session Chair: Abhimanew Dhir**
14:30-14:55	**Talk 38** Ramananda Maity	**Title:** Iridium (III) NHC Complexes: Selective C–H Bond Activation and Asymmetric Catalysis
14:55-15:20	**Talk 39** Tasneem Parvin	**Title:** Green and Step-Economic Synthesis of Bioactive Hybrid Heterocycles
15:20-15:45	**Talk 40** Hema K.	**Title:** Balancing Molecular Freedom: Confinement and Constraints in Supramolecular Materials Design
15:45-15:55	**Award Distribution**	
15:55-16:00	**Closing Remarks &Vote of Thanks (FARC Chair)**	

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Abstracts

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3	Abhilekha Borah	P3
4	Abhipsa Ghosh	P4
5	Abul Hasnat	P5
6	Ajay	P6
7	Ajeeba PS	P7
8	Akhilesh Sharma	P8
9	Akriti Gautam	P9
10	Akshata Umesh Rathod	P10
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Abstract

Speakers

Enzyme-Assisted Preparation of Organic Nanoparticles for Bioanalyte Detection and Photothermal Therapy

Aasheesh Srivastava,[1] *Manas K. Pradhan,*[1] *Surya S. P.,*[1] *Prinyanka Payal,*[2] *Sharad Gupta*[2]

[1]Dept. of Chemistry, IISER Bhopal, Bhopal 462066. Email: asrivastava@iiserb.ac.in

[2]Dept. of Biosciences and Biomedical Engineering, IIsT Indore, Indore 453552.

Abstract: Designing benign protocols for preparing uniform organic nanoparticles for biomedical applications with batch-to-batch consistency is much needed to realize the translational potential laboratory outcomes. We achieved enzyme-assisted synthesis of uniform nanoparticles from suitably designed amino acid-derivatives. For this, phenylalanine and alanine derivatives containing horseradish peroxidase (HRP)-responsive tyramine residues were prepared. Treatment of their aqueous solutions with HRP and H_2O_2 yielded uniform nanoparticles. By co-entrapping Glucose oxidase and HRP in these nanoparticles, we achieved fluorimetric sensing of salivary glucose. Subsequently, we embarked on creating photothermal nanoparticles from these nanoparticles by coating them with a layer each of polydopamine (PDA) and gold nanoparticles (AuNPs). The resulting composite nanoparticles provided strong temperature enhancement of >19 °C upon NIR illumination at 1 W/cm^2 for 4 minutes. Entrapping Doxorubicin within these particles allowed a combination chemo-/photothermal-therapy producing strong in vitro cancer cell death.

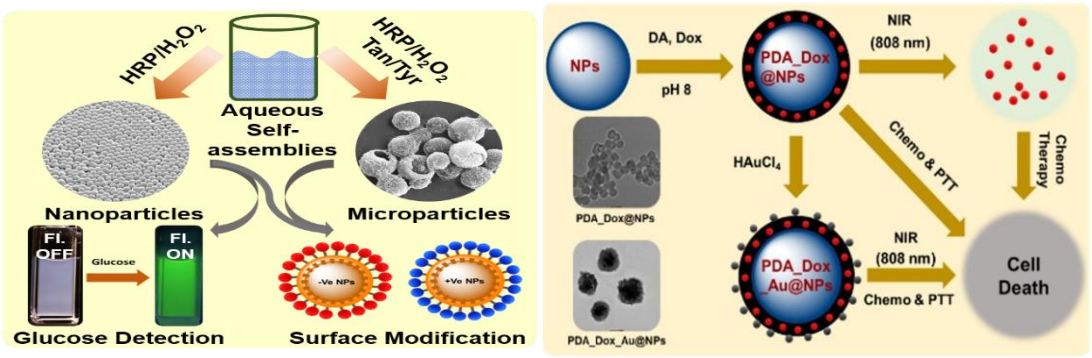

Figure 1. Left: Creating uniform hollow nanoparticles and microparticles through enzyme-assisted dimerization of alanine-tyramine conjugates. Right: Employing these nanoparticles for chemotherapy + photothermal by entrapping Doxorubicin (Dox) within them and coating with polydopamine (PDA) and gold nanoparticles (AuNPs).

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1) Kumar Pradhan, M.; Suresh Puthenpurackal, S.; Srivastava, A. Enzymatic Dimerization-Induced Self-Assembly of Alanine-Tyramine Conjugates into Versatile, Uniform, Enzyme-Loaded Organic Nanoparticles. *Angewandte Chemie Int. Ed.* **2024**, *63* (2), e202314960. https://doi.org/10.1002/ange.202314960

2) Kumar Pradhan, M.; Payal, P.; Sharma, R.; Ubnare, K.; Gupta S.; Srivastava, A. Polydopamine-Coated Polyphenol-Based Nanoparticles for Synergistic Chemotherapy and Photothermal Therapy. ACS Applied Nano Materials, 2026, 9, 2885-2896. https://doi.org/10.1021/acsanm.5c05215

N-Heterocyclic Carbene-Catalyzed Synthesis of C-N, C-O and N-N Axially Chiral Molecules

Akkattu T. Biju

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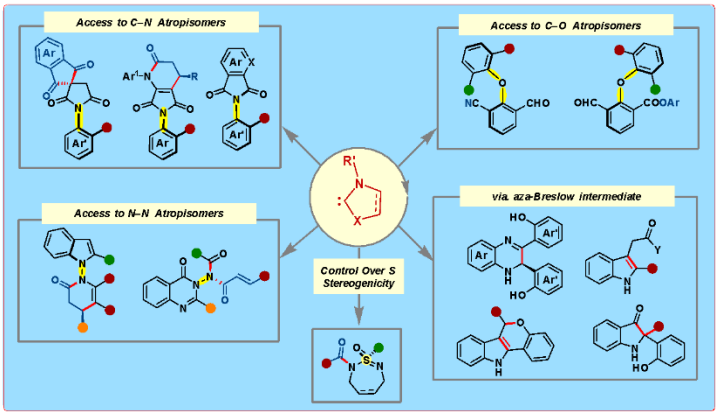
Abstract: Organocatalysis using N-heterocyclic carbene (NHCs) has been widely utilized for the polarity reversal of aldehydes (*umpolung*).[1] Although NHC catalysis is well demonstrated for the enantioselective synthesis of target molecules, related application to the synthesis of axially chiral molecules is limited (especially the heteroatom-containing axis). We have recently reported the NHC-catalyzed atroposelective synthesis of C-N axially chiral N-aryl succinimides,[2] phthalimides/maleimides,[3] N-N axially chiral 3-amino quinazolinones,[4] indoles and pyrroles as well as C-O axially chiral diarylethers.[5] In addition, precise control over S(VI)-stereogenic center has recently be achieved by the enantioselective synthesis of N-acyl cyclic sulfonimidamides.[6] The details of these works will be discussed.



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3) Barik, S.; Ranganathappa, S. S.; Biju, A. T. *Nat. Commun*. **2024,** *15*, 5755.
4) Balanna, K.; Barik, S.; Barik, S.; Shee, S.; Manoj, N.; Gonnade, R. G.; Biju, A. T. *ACS Catal.* **2023**, *13*, 8752. (b) Ranganathappa, S. S.; Dehury, B, S.; Singh, G. K.; Shee, S.; Biju, A. T. *ACS Catal.* **2024**, *14*, 6965.
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Supramolecular Integration of N-Capped Peptides for Multivalent Recognition and Precision Therapeutics

Amitava Das

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Abstract: Recent advances in therapeutic design increasingly emphasise the precise delivery and activation of functional agents at disease sites to maximise efficacy while minimising systemic toxicity.[1] Stimuli-responsive systems, guided by molecular recognition, offer powerful strategies to achieve this balance. In this lecture, I will discuss our efforts toward the rational design of short, purpose-built peptides as versatile scaffolds for programmable therapeutics.[1,2] By integrating supramolecular recognition elements with targeting sequences, we develop constructs capable of selective activation and multivalent engagement with disease-relevant biomolecules.[3] A key example involves a chemically engineered composite targeting amyloid-β_{42}, where cooperative interactions enable both inhibition of aggregation and active disassembly of pathogenic assemblies through a distinct mechanistic pathway.[4] These systems not only modulate aggregation but also restore cellular homeostasis and function in disease models. I will try to convince the hypothesis of developing a generalizable design paradigm that integrates precision molecular recognition, adaptive responsiveness, and functional outcomes, bridging fundamental chemistry with translational relevance in next-generation therapeutics.

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1) Dutta, S.; Tripathy, S.; Bej, S.; Parvin, S.; Jana, B.; Patra, C.R.; Das, A.; Chem. Sci. (2025) 16, 16573 - 16583; Pramanik, S. K., Sreedharan, S., Kandoth, N.; Das, A.; Thomas, J. A. Nature Chem. Rev. 2025, 9, 733–748;.
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Exciton dynamics in semiconductor nanocrystals: from curiosity to applications

Anindya Datta

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Abstract: Semiconductor nanocrsytals (NCs) have held centre stage for the last couple of decades because of their immense promise in diverse fields of application. Using ultrafast transient absorption spectroscopy (TAS), fluorescence correlation spectroscopy (FCS) and FLIM, we have explored the intricacies of carrier dynamics in several nanocrystals. Of particular interest to us is the phenomenon of photoinduced electron transfer from the NCs to electron acceptors, which is a key process for photosensitization of molecular catalysts for applications like CO2 reduction. Proper analysis of data is of utmost importance in this kind of research, as will be discussed with a couple of examples from our group.

Charge Carrier Dynamics in Perovskite Nanocrystals

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Abstract: The lead halide-based hybrid and all-inorganic perovskites are currently the focus of intense investigation because of their potential in solar photovoltaic and light-emitting applications.[1] Considering the fact that our understanding of the fundamental photo-processes in these systems like the deactivation pathways and dynamics of the photo-generated charge carriers, which is essential for proper utilization of these substances in different applications, is still very limited, we have been looking into these substances addressing a variety of issues including those mentioned above. This talk will focus on how a combination of femtosecond pump-probe and single-particle fluorescence techniques can provide valuable information on the nature and energy states of the photogenerated species, pathways and dynamics of relaxation of the charge carriers, location and nature of the trap states and their role in fluctuation of the photoluminescence of different caesium lead halide ($CsPbX_3$) perovskite nanocrystals.[2-5]

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Toward Adaptive Systems: Amino Acid-Based Self-Assembled Nanostructures

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Abstract: The self-assembly of molecular building blocks through non-covalent interactions offers a powerful strategy for creating functional materials. Moving beyond purely synthetic or natural systems, current research focuses on hybrid platforms that combine rational design with biologically inspired motifs. Amino acid-based components are particularly attractive, as they enable the formation of precisely organized nanostructures that exhibit adaptive behavior reminiscent of biological systems. Inspired by the dynamic and responsive nature of biopolymers, we explore how amino acid-derived building blocks can generate self-assembled nanostructures functioning as adaptive systems.[1-4] Through reversible interactions and structural programmability, these architectures can respond to environmental stimuli and modulate their properties at the nanoscale. This presentation will highlight selected examples illustrating the design of adaptive amino acid-based nanostructures with potential applications in biotechnology, medicine, and advanced materials engineering (more information at www.arsgroup.amu.edu.pl).

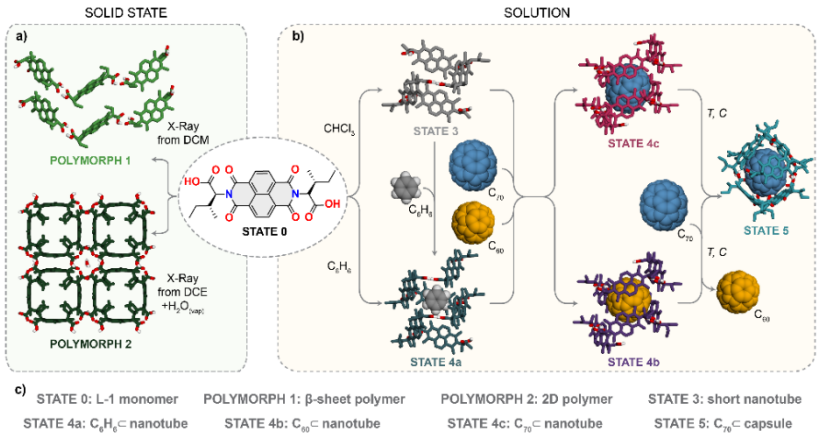

Figure 1. A structural reorganization of this artificial system into five distinct supramolecular states was accomplished, through modulation of solvent, temperature, concentration, and guest molecules.

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Strategies for Modulating Electronic Structures and Photochemistry of Ruthenium Polypyridyls for Phototherapeutic Applications

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Abstract: Ruthenium coordination chemistry provides a combination of structural diversity, tunable geometries, accessible redox and electronic states, and adaptable ligand-substitution kinetics for reactions with biotargets etc.[1] Ru(II)-polypyridyl photosensitizers exhibit exciting and diverse photophysical properties through multiple deactivation pathways of excited states, including photo-substitution reactions (Figure 1). By employing a rational design that leverages the varying stereo-electronic properties of ligands, we can achieve spatiotemporal control over the selective release of bioactive ligands to precisely target specific biological processes that enhance their therapeutic effectiveness.[2] Here, we will discuss the intricate photophysics and photochemistry of light-induced Ru(II)-polypyridyls, including modulating their excited electronic states by incorporating electronically diverse ligands. Our focus is on establishing an optimized relationship between electronic structure and photoreactivity for their potential use in Photoactivated Chemotherapy (PACT).[3-6] Selected rational design principles will be highlighted by strategically conjugating bioactive ligands and varying polypyridyl or ancillary ligands to modify their excited electronic states, biocompatibility, and ROS generation ability for targeted applications. Stereo-electronic variables over ligand-photosubstitutions for spatiotemporal control of photoactivated chemotherapy (PACT) will be emphasized.

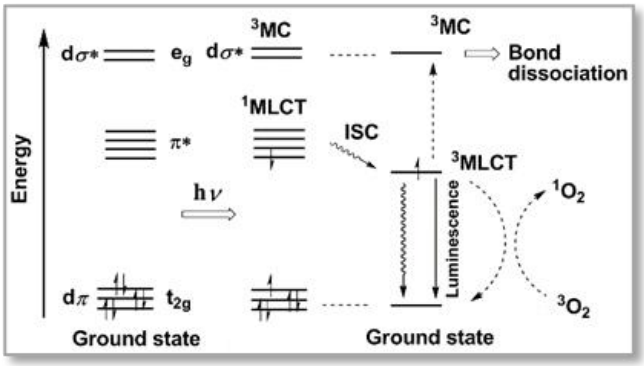

Figure 1. Schematic energy-transfer diagram showing the possible routes in ruthenium(II) polypyridyl complexes (d^6) that can adopt upon absorption of a photon.

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Photoswitch tethered Peptide to Dictate the Fate of Supramolecular Polymerization

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Abstract: Supramolecular polymerization enables the construction of functional architectures via reversible non-covalent interactions. The self-assembly process navigates complex energy landscapes, influenced by molecular symmetry, solvent composition, temperature, and external stimuli. Assembly follows mechanisms like isodesmic or cooperative pathways, with on- and off-pathways competing based on energy barriers. Photoswitches like azobenzene enable precise control over material organization. In this regard, peptide amphiphiles (PAs) serve as versatile scaffolds for supramolecular assemblies, with π–π stacking and H-bonding interactions guiding variable nanostructure formation in response to variations in the local microenvironment. We designed a series of symmetric azobenzene-functionalized peptide amphiphiles, wherein the peptide sequence has been modified from amyloidogenic to non-amyloidogenic. This strategic point mutation was investigated for its influence on self-assembly dynamics and photoisomerization behavior. Kinetic analyses revealed that the amyloidogenic peptide fragment preferentially facilitated the formation of a kinetically trapped nanofibrous state. A systematic evaluation of solvent composition, temperature was conducted to elucidate their roles in modulating self-assembly pathways and photoisomerization kinetics upon varying molecular structures from amyloidogenic to non-amyloidogenic peptide sequence.

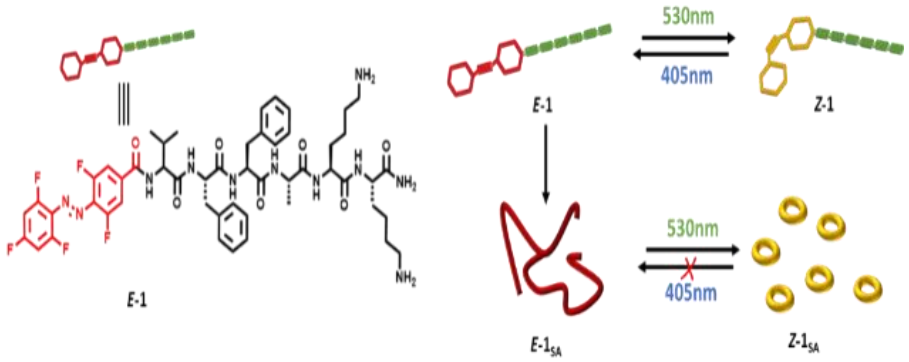

Figure 1. Visible-light driven *E*□*Z* isomerization programs pathway selection in peptide self-assembly, switching nanofibers into kinetically trapped nanotoroids.

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Stimuli-Responsive Microgels and Hydrogels: From Switchable Microreactors to Tunable Permeation and Atmospheric Water Harvesting

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Abstract: Responsive microgels and hydrogels have emerged as highly versatile soft materials, owing to their tunable porosity, stimuli-responsiveness, and readily customizable surface functionality. This talk presents research spanning synthetic biology, atmospheric water harvesting, and membrane-based water purification, unified by the rational design of these adaptive polymer networks for real-world applications. Temperature-responsive microgels based on N-isopropylacrylamide, polyethyleneimine, and serine were engineered as interfacially active building blocks for constructing Pickering emulsion-stabilized colloidosomes, which is termed "microgelsomes".[1, 2] These biomimetic vesicles exhibit high encapsulation efficiency, selectively permeable membranes, and programmable biocatalytic activity, making them promising microreactors for enzyme cascade reactions. The same design principles were extended to nanostructured membranes, where zwitterionically functionalized and enzyme-immobilized core-shell microgels were assembled into antifouling, self-cleaning filtration layers with thermo-regulated water flux, high solute rejection, and biocatalytic degradation of organic foulants.[3] Addressing freshwater scarcity from a complementary direction, amino acid-based thermoresponsive hydrogels were integrated with metal-organic frameworks and hygroscopic salts to yield composite sorbents with exceptional atmospheric moisture uptake capacities of up to 4.9 $g.g^{-1}$ at 90% relative humidity.[4, 5] The synergistic photothermal activity of the MOF components and the reversible hydrophilic-hydrophobic phase transition of PNIPAM-based hydrogels enable efficient, solar-driven water release and cyclable freshwater generation even under low-humidity conditions, with additional demonstrated performance in desalination and oil-water separation. Together, these findings establish functional microgels and hydrogels as a unified, adaptable materials platform that bridges biomimetic design principles and pressing environmental challenges.

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Graph Neural Network for High-Throughput Screening of Nanocluster Electrocatalysis

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Abstract: Nanoclusters represent an emerging class of heterogeneous electrocatalysts with properties tunable at the atomic scale, enabling reactivity beyond traditional structure–activity relationships. However, their catalytic behavior is highly complex due to diverse morphologies and structural fluxionality, leading to multiple coexisting isomers. In this work, we employ advanced graph neural network (GNN) models trained on a density functional theory (DFT)-curated dataset of bimetallic nanocluster alloys for the oxygen reduction reaction (ORR). A systematic benchmarking of state-of-the-art GNN architectures reveals that attention-based models provide superior predictive accuracy for catalytic activity. The proposed framework is scalable, interpretable, and capable of capturing morphology-dependent reactivity in nanoclusters. This approach significantly accelerates the discovery of high-performance nanocluster catalysts and can be extended to a broad range of catalytic processes beyond.[1-4]

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σ-Bond Activation by Stable Azomethine Ylides

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Abstract: Azomethine ylides are 1,3-dipolar zwitterions, mostly transient in nature and mainly used in constructing N-heterocycles by 3+2-cycloadditions with various dipolarophiles. We report here pyridyl/quinolyl-tethered isolable azomethine ylides (**AY-1** and **AY-2**, Figure 1) that activates a series of H–E (E = B, Si, Al, O) and E-E (E = B, S) s-bonds.[1] All the reactions are probed mechanistically by DFT calculations and each case appears to be markedly distinct from others. The stereoelectronic divergence between **AY-1** and **AY-2** also makes a major impact towards their reactivity in this context.

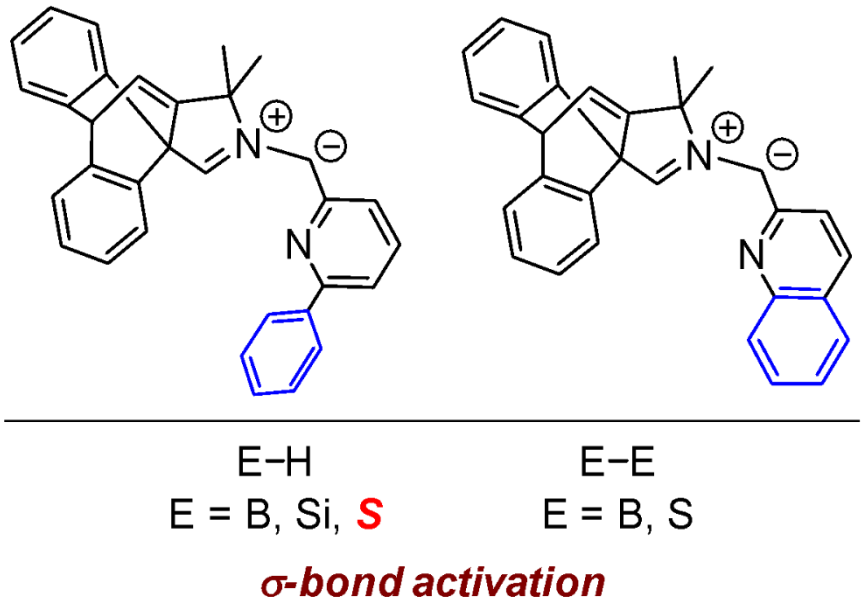

Figure 1. Stable azomethine ylides towards σ-bond activation.

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Breaking the equilibrium to secure information

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Abstract: Information theft and data counterfeiting are rising at an alarming rate. This global concern demands acute scientific attention as the present world is thriving on information exchange and data transmission. Securing messages and protecting information requires sophisticated, advanced and convenient anti-counterfeiting techniques that ensure safe storage alongside smart data access at the right time. Right information at the wrong time can also pose severe threats. A modern solution to this age-old problem is offered by the time-regulated transitory colours arising from stimuli-adaptive molecules and dynamic supramolecular assemblies. Chemically triggered life-like dynamic systems and phosphorescent afterglow materials are often accompanied by broad-spectrum transitions in visible colours with temporal tunability. These works showcase that time-resolved cryptic colours can be implemented in state-of-the-art security strategies to construct a stimuli-specific multi-dimensional platform for advanced time-encoded anti-counterfeiting data encryption. They demonstrate how the enhanced security from the additional time-dimension can be achieved in a hierarchical method addressing increasing complexities at each level - conveniently starting with solutions that offer higher dynamicity through non-equilibrium chemical clocks (molecular colours and emissive assemblies) and extending to rigid and restricted solid matrices through phosphorescent afterglows.

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Redox Active Ligands in Homogeneous Catalysis

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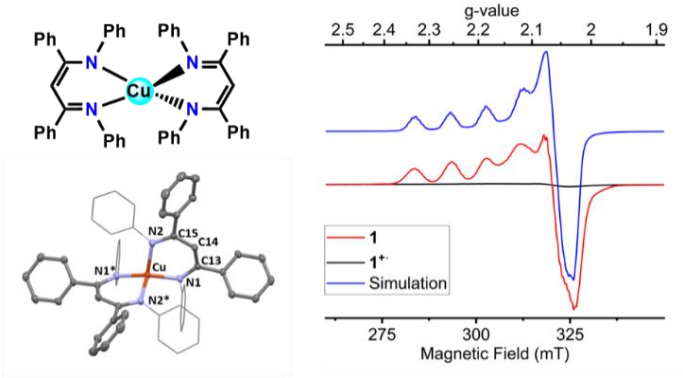
Abstract: A large class of ligands possessing a delocalized π-electron cloud has been behaving as noninnocent when they are coordinated to transition metal centers, given the site of the redox process is not precise anymore. Typically, such ligand classes prohibit the unambiguous determination of the oxidation state of the metal and themselves take participation in redox reactions. We have been exploring the capability of such ligands to behave as a redox reservoir and utilizing them for efficient chemical transformations. Our efforts spanned to formazanate class of ligands,[1] azophenolates[2] and very recently even beta-diketiminates.[3] In this lecture we will showcase the noninnocent behavior of a CuL_2 (L = β-diketiminate) complex, where the oxidation event largely takes place at the ligand backbone keeping the copper's oxidation state (+2) intact. The ligand-based redox process has been investigated by a series of techniques including cyclic voltammetry, EPR, solid-state magnetometry and UV-vis spectroscopy. Utilizing the capacity to hold electron, an electron transfer catalysis has been designed that breaks a substrate C-Br bond via reductive cleavage. The nature of M-L covalency plays a preponderant role in such electron transfer where the metal center behaves as a template. Onto the metal, the substrate binding takes place to find tune its redox demand. Utilizing this noninnocence behavior of the β-diketiminate, we perform 2-alkoxycarboxylation reaction at the 2-position of indole, benzofuran etc.



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Chiral Carbon Dots and Their Bioconjugates: Synthesis and Optical Properties

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Abstract: Chirality in nanomaterials has emerged as a critical property for applications ranging from biosensing and enantioselective catalysis to spintronics and circularly polarized optoelectronics. Among nanoplatforms, carbon dots stand out due to their biocompatibility, tunable emission, and ease of functionalization. However, extending chirality into the red and near-infrared spectral windows, essential for deep-tissue imaging, remains challenging. Moreover, hydrophobic or organo-soluble chiral carbon systems are scarce despite their relevance in non-aqueous synthesis and device integration. Here, we report on the development of chiral carbon-based nanomaterials red- and green-emissive carbon dots (CDs) and organo-soluble carbon nanocolloids (CNCs) exhibiting strong circular dichroism, high photoluminescence quantum yields, low cytotoxicity, and enantioselective interactions with biomolecules. In one approach, N,O-doped CDs were functionalized with L-cysteine via EDC/NHS chemistry [1], yielding green- (530 nm) and red (630 nm) emissive chiral CDs with quantum yields up to 19% and 15%, respectively. These materials exhibited intense circular dichroism signals with g-factor up to 2.3×10^{-4} in the 200–300 nm range and retained stability across varying pH and metal ion concentrations (Hg^{2+}, Pb^{2+}, Cu^{2+}), with >90% cell viability at concentrations up to 16 mg/mL. A second strategy employed chiral isocyanate post-treatment of red-emissive CDs synthesized from citric acid, ethylenediamine, and formamide [2]. This approach yielded chiral CDs emitting at 640 nm with quantum yield of ≈ 13% with circular dichroism signals beyond 300 nm with $g = 8 \times 10^{-5}$ at 345 nm, which is spectrally distinct from precursor ligands. Notably, the R-enantiomer showed higher cytotoxicity than the S-form across multiple cell lines (HeLa, B16, 4T1), and enantioselective interactions with L/D-tryptophan were confirmed by circular dichroism spectroscopy and molecular dynamics simulations. Finally, organo-soluble CNCs were prepared by solvent-free heating of formamidinium salts with (R/S)-α-methylbenzylamine. The resulting quasi-spherical 3–10 nm nanoparticles displayed blue-green photoluminescence with quantum yield up to 40%, circular dichroism signals in the 250–450 nm range, and excellent dispersibility in both polar (IPA, DMSO) and nonpolar solvents (toluene). These materials are promising for bioimaging and chiral sensing.

Acknowledgement:
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Balancing Molecular Freedom: Confinement and Constraints in Supramolecular Materials Design

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Abstract: Biological systems regulate function by carefully balancing molecular freedom. They selectively restrict conformational and spatial degrees of freedom in a controlled manner to pre-organize interactions, and guide selective outcomes. My research examines how this balance can be achieved in synthetic supramolecular systems across different environments. In crystalline solids, molecular packing provides a rigid confinement that enforces geometric alignment. Such geometric restriction helps pre-organize reacting groups in topochemical reactions and the reaction outcome is governed by enforced alignment within the lattice.[1] In solution, discrete coordination cages offer well-defined nanoscale cavities that encapsulate guest molecules. Within these supramolecular hosts, spatial boundaries, shape complementarity and host-guest interactions promote structural transformations. This approach demonstrates how externally imposed confinement can modulate transformations under dynamic conditions.[2] More recently, the focus has shifted toward constraints encoded within flexible molecular systems. Short peptide systems provide an opportunity to design internal restriction through sequence. Applying constraints in the peptide backbone helps isolate the influence of side chains in the self-assembly dynamics. Even subtle variations in the sequence and sidechains alters the crystallizability and solid-state dynamics. Here, constraint is not imposed by an external factor but arises from molecular design.[3] Building on this intrinsic control, introducing molecular constraints in peptide systems that undergo liquid-liquid phase separation helps stabilize the coacervates and prevents the time-dependent ripening to ordered fibres or crystals. These stable coacervates can be further converted to microspherical containers that encapsulate cargo and useful for bio-imaging.Across crystalline lattices, coordination cages, and peptide-based assemblies, my research explores how balancing molecular freedom provides a general strategy for supramolecular materials design.

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From Bench Innovation to Clinical Impact: Nitric Oxide–Releasing Device Coatings

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Abstract: Blood/material interaction is critical to the success of implantable medical devices, ranging from simple catheters, stents, and grafts to complex extracorporeal artificial organs used in thousands of patients daily. However, there are two major limiting factors to the clinical application of blood-contacting materials: 1) platelet activation leading to thrombosis, and 2) infection. Despite a thorough understanding of the mechanisms of blood–surface interactions and decades of bioengineering research effort, the ideal non-thrombogenic prosthetic surface remains an unsolved problem. One approach to improving the hemocompatibility of blood-contacting devices is to develop materials that release nitric oxide (NO), a known potent inhibitor of platelet adhesion/activation and also an antimicrobial agent. Healthy endothelial cells sustain nitric oxide release, and materials designed to replicate this behavior are anticipated to exhibit similar antithrombotic and antimicrobial effects. The fabrication schemes, hemocompatibility, and antimicrobial testing of NO-releasing medical devices will be discussed.

Metal complexes as super-resolution microscopy cell probes, phototherapeutics and antimicrobials

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Abstract: Luminescent polypyridyl ruthenium complexes that interact with biomolecules are much studied as potential cell probes.[1] In our work we have identified multimodal cell probes for specific DNA structures; using super-resolution techniques, including SIM and STED nanoscopy, 3-D resolutions below 40 nm have been accomplished.[2] – Fig 1.

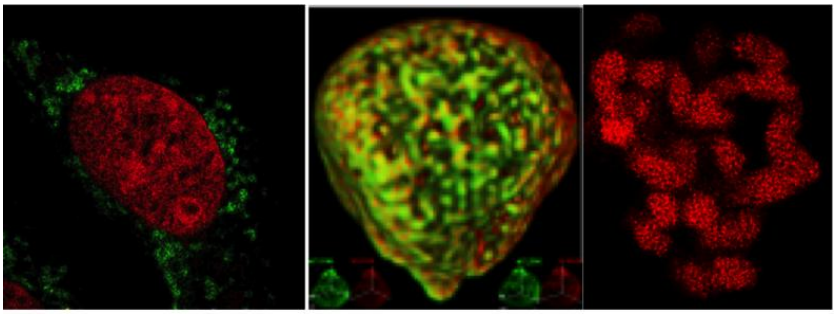

Figure 1. STED images of a single cell, nucleus and chromatin obtained using a Ru^{II} developed by the Thomas group.

Through simple structural modulations of the prototype complex, NIR STED probes and potent phototherapeutics have been synthesized.[3,4] More recently this work has led to the identification of antibacterials for multidrug resistant pathogens,[5] which are being commercially developed by the spinout company MetalloBio ltd (www.metallobio.com).

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Swelling-activated phenomenon: From thin polymer films to bulk polymer materials

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Abstract: Swelling is ubiquitous in nature. From opening and closing of pinecones in response to relative humidity, to swelling-induced changes in the geometry of articular cartilage, to controlling the motion in soft robotic, swelling plays a vital role. This talk will highlight the impact of swelling-induced processes pertaining to synthetic polymer materials ranging from polymer brushes to bulk polymer hydrogels.

Polymer brushes consist of densely grafted polymer chains tethered to a surface. When swollen in a good solvent, they acquire a stretched chain conformation away from the substrate, which imparts them with unique properties. Swollen polymer brushes are suitable candidates for several surface applications such as lubricants and anti-biofouling coatings. However, solvent exposure can also result in instabilities in the polymer brush films leading to detachment or delamination. This is believed to be a result of hydrolysis of ester, amide, and, siloxane bonds at the brush-substrate interface that are amplified by solvent-induced stretching of polymer chains. While the effects of polymer composition, grafting density, and nature of the solvent on the swelling of polymer brushes are well studied, the role of the brush-substrate interface is less known, partly due to limited chemistries available for interfacial modification.

This talk will address two questions: i) can we modulate swelling by tuning the interfacial chemistry, ii) what are the forces that act at the interface upon swelling of the brush. I will present a design of a library of probes that can be inserted at the polymer brush interface and allow for systematic modulation of interfacial properties. These probes can a) impart hydrophilic or hydrophobic characteristic to the interface depending on the functional groups involved, and b) allow us to quantify interfacial swelling-induced forces using conventional fluorescence microscopy. Furthermore, I will briefly discuss swelling-activated phenomenon in bulk polymer hydrogels.

Probes and Tracers – An Advanced Microscopy Perspective

Laura C. Zanetti-Domingues,[1] *Benji Bateman*[2], *Tom Dzelzainis*[2], *Gea van de Kerkhof*[2], *Alix Bailie*[2], *Matthew Tang*[2].

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Abstract: The chemistry of probes and tracers plays a significant role in their performance in advanced microscopy techniques, from photobleaching resistance to brightness, passing through more "exoteric" properties like partitioning coefficients, their behaviour at cryogenic temperatures and their capability to act as multimodal probes.
This presentation will provide some examples of an advanced microscopy perspective on probes and tracers, from the how partitioning coefficients influence probe selection for single-particle tracking, to how chromophore chemistry and structure influence the behaviour of fluorescent proteins and organic dyes in cryogenic imaging, to the quest to find the definitive cryo-CLEM multimodal labelling agent and fiducials. Each example will provide topics for multidisciplinary discussion between the chemistry community and the bioimaging community to break new ground in fluorophore chemistry for to meet the requirements of advanced and multimodal imaging.

Designing Sustainable Methods for the Synthesis and Functionalization of Small Molecules

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Abstract: Small molecules especially functionalized heterocycles are found in the core of pharmaceuticals, natural products, and functional materials. Therefore, the design and development of efficient and sustainable methods for their synthesis is a central objective in contemporary organic synthesis. In recent years, significant research efforts have been directed toward the development of environmentally benign, atom-economical, and resource-efficient strategies for the construction and diversification of bioactive small molecules. Such approaches align closely with the principles of green and sustainable chemistry, aiming to minimize waste generation, reduce energy consumption, and enhance overall synthetic efficiency. This presentation will highlight our recent efforts toward the sustainable synthesis and functionalization of bioactive small molecules through the development of modern catalytic methodologies.[1-3] In particular, the talk will emphasize metal-catalyzed C–H activation, multicomponent reactions (MCRs), and visible-light-driven transformations as powerful strategies for the efficient assembly of structurally diverse heterocyclic architectures. C–H activation has emerged as an enabling strategy for direct bond functionalization, allowing the streamlined construction of complex heterocyclic frameworks with enhanced step and atom economy. Similarly, multicomponent reactions provide a highly efficient platform for the one-pot generation of heterocyclic scaffolds fr]om simple and readily available starting materials, thereby improving synthetic efficiency while minimizing purification steps and waste generation. Furthermore, visible-light-mediated organic transformations has recently gained prominence as a sustainable approach for promoting challenging bond-forming processes under mild and energy-efficient conditions by utilizing visible light as a clean and renewable energy source.

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Expanding self-healing dyes towards the blue-green spectral region via modular linkers

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Abstract: Organic fluorophores are vital for various life science applications including imaging, DNA sequencing, single-molecule studies, but also biomedical assays. However, their utility is often limited by fixed photophysical properties, fast photobleaching, restricted functional versatility, and lack of modular bioconjugation options. We recently introduced a modular chemical biology approach using a 'linker' system that connects biological targets, commercial dyes, and functional moieties.[1] These linkers are synthesized via a one-pot Ugi four-component reaction, enabling rapid and diverse customization. Each linker features a bioconjugation handle, a click-compatible unit for fluorophore attachment, and a functional moiety to tune dye behaviour. This strategy converts conventional fluorophores into adaptable probes with improved photostability, controlled blinking or environmental responsiveness.[1] In this contribution we combine the linker strategy with new triplet-state quenchers relevant for blue and blue–green emitting fluorophores, where effective stabilization strategies have remained limited[2]. These self-healing systems efficiently suppress triplet-state accumulation, accelerate dark-state recovery, and significantly reduce photobleaching. Photophysical performance of the linker-dye conjugates is systematically evaluated using fluorescence correlation spectroscopy (FCS), total internal reflection fluorescence (TIRF) microscopy, and single-molecule FRET (smFRET). The results reveal substantial improvements in photobleaching lifetimes, blinking behavior, and excitation power tolerance compared to unmodified dyes and conventional buffer-based stabilizers (e.g., Trolox/DAMF systems)[2]. Importantly, implementation in smFRET experiments enables stable and high-resolution measurements in the blue-green spectral regime, expanding the accessible range of fluorophores for single-molecule studies. Overall, the modular linker platform provides a versatile toolkit for fluorophore functionalization during biolabelling and establishes a general framework for the design of next-generation functional dyes for advanced imaging applications in vitro and in vivo.

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Synthetic Strategies using C-C and C-H bond Functionalization

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Abstract: Since the beginning 21st century there has been renewed interest in functionalizing inert bonds through metal catalyst for the synthesis of many useful organic molecules. As compared to C-H bond functionalization, C-C bond functionalization is more difficult due to the high thermodynamic barrier in breaking the C-C bond. A useful strategy to overcome high thermodynamic barriers is to use strained ring systems as substrates. In our group, we have employed this strategy effectively for the synthesis of heterocycles and useful organic scaffolds. A brief overview of the works completed so far, and our ongoing works will be presented. Catellani reaction is a unique reaction wherein bicyclic olefins acts as a mediator for bi-functionalization of aromatic systems. It follows a unique mechanism wherein a bicyclic olefin transiently attaches and detaches itself with the substrate. This unusual behaviour of bicyclic olefins is believed to be due to the restricted ß -hydride elimination of the key intermediate involved in this transformation. We reasoned ourselves whether a simple monocyclic olefin can do the same job if we deprive of it from ß-hydride elimination. This indeed was found to be the case. In this talk I will also explain our efforts that led to this discovery.

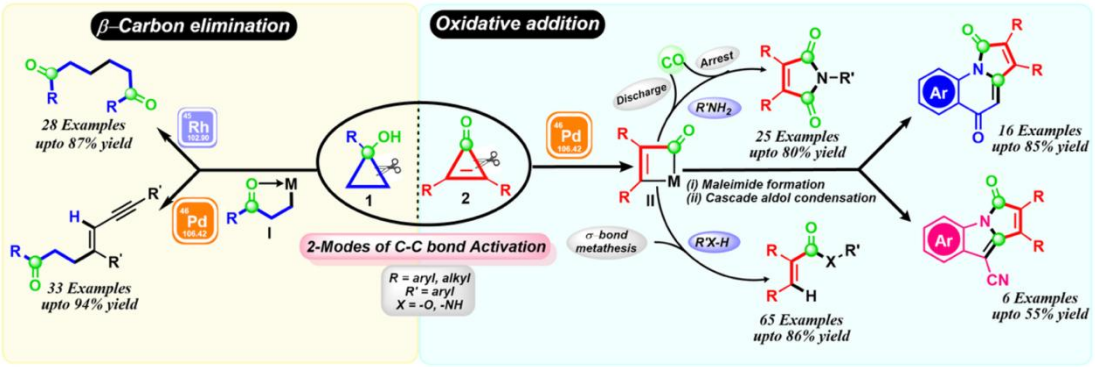

Figure 1: Transition metal-catalysed C-C bond activation of strained system

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Electrochemical Generation of Ketyl Radical Anions: Synthetic Utilization in the Construction of Diverse Cyclic and Acyclic Scaffolds.

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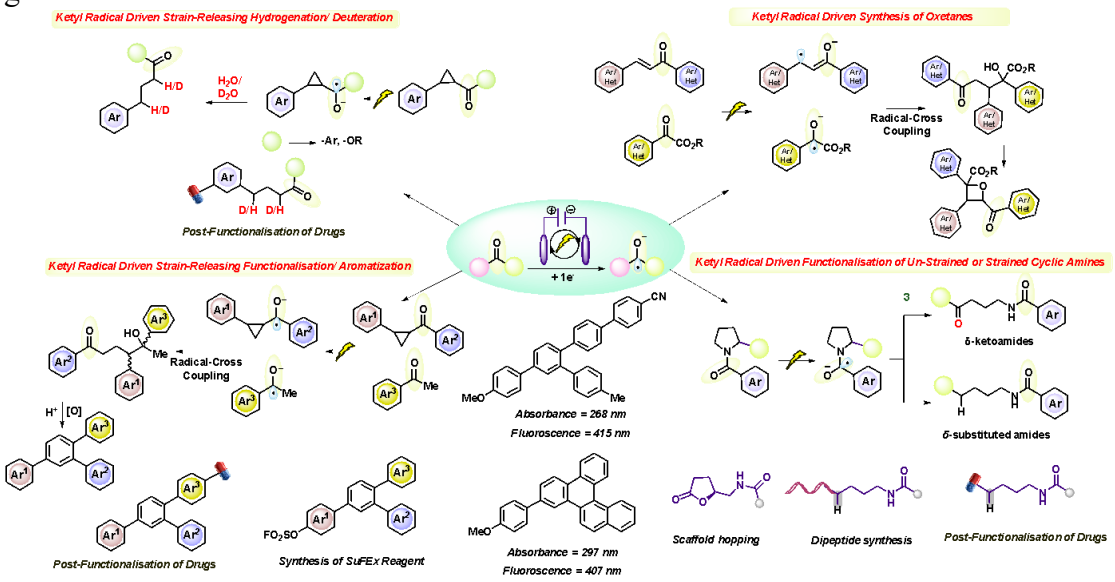
Abstract: The utilization of ketyl radicals represents a transformative paradigm in synthetic organic chemistry, enabling the construction of complex molecular architectures from simple carbonyl precursors. The "classical" generation of ketyl-type radical anion intermediates relies on the use of stoichiometric amounts of powerful chemical reductants. Recent advances (2020–2025) have focused on replacing classical, moisture-sensitive metal reductants with catalytic and sustainable methods, primarily through photoredox and electrochemical manifolds. The stability and subsequent reactivity of the generated radical anion are highly dependent on the reaction environment. The stability and subsequent reactivity of the generated radical anion are highly reliant on the reaction environment. In the absence of a proton source, these species may undergo dimerization to form pinacols or engage in radical-radical cross-coupling and functionalisation. Herein, we summarise our efforts in the electrochemical generation of ketyl-type radical anion intermediates and their corresponding utilisation in strain-releasing hydrogenation/deuteration and radical cross-coupling to synthesise 1,2,4-triarylbenzenes from donor-acceptor cyclopropanes.[1,2] Our lab also utilized the electrochemical generation of ketyl-type radical anion intermediates in the formation of all carbon-substituted oxetanes.[3] Moreover, we introduced a greener, atom-economical, and sustainable electroreductive deconstructive functionalization approach (*E*-Factor = 0.9) for transforming cyclic amines into *δ*-substituted amides *via* C-N bond cleavage, *δ*-ketoamides through the trapping of environmentally benign oxygen molecules.[4]



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Single Particle Spectroscopic and Ultrafast Dynamical Exploration of Quantum Dots and Perovskite Nanocrystals

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Abstract: Quantum dots (QDs) and perovskite nanocrystals (PNCs) have emerged as the choicest optical nanomaterials in recent years.[1,2] However, there are numerous unanswered queries regarding optical properties of QDs and PNCs.[3-5] In recent years, through alloy-shelling over the core QDs, two out of three major problems in QDs could be circumvented.[3,6] Very recently, through Zn alloying and modification of surface ligands, PNCs with extremely high brightness has been achieved.[7] However, to judge the solar cell related application potential of PNCs, it is necessary to know whether and how differently excitations at different regions of the solar spectrum control the formation, fate and dynamics of excitons. As the excitation energies vary from the blue to red region of the solar spectrum, based on steady state spectroscopic, ultrafast dynamical and single particle spectroscopic explorations, it has been observed that (i) the feasibility of exciton formation decreases >9 fold, (ii) PLQY magnitude increases >2 fold, (iii) hot exciton cooling time decreases >7 fold, (iv) normalized bleach population increases 3 fold, (v) peak maximum of ON fraction increases, from 64% to 90%, and (vi) exciton "detrapping rate/trapping rate" increases >3 fold. All these concepts and results will be discussed.

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Protein Stability and Activity in Alternate Media: An Unified explanation through Associated Water Stabilization Mechanism (AWSM)

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Abstract: The water we encounter every day and the water surrounding biomacromolecules differ significantly in behaviour and properties. Water molecules associated with a protein exhibit restricted dynamics compared to that of bulk water. This unique layer of water, known as associated water, directly interacts with the protein and impacts key protein characteristics, including stability and activity. We examined various proteins in the presence of additives; such as osmolytes, macromolecular crowders, and deep eutectic solvents, and propose Associated Water Stabilization Mechanism (AWSM). This mechanism emphasise the pivotal role of associated water in regulating the stability and activity of proteins through regulating its interior (probed through conformational fluctuation dynamics). Our proposed mechanism can successfully explain (i) protein specific response of osmolyte, (ii) counteractive effect of osmolytes towards denaturants, (iii) crowder-induced negative entropic effect, (iv) entropy-enthalpy compensation within biological systems, and (v) modulation of enzymatic activity in alternate media. Most of these observations are difficult to explain by the existing theories. Notably, the proposed mechanism was validated across various additives (osmolytes, macromolecular crowders, and deep eutectic solvents) and for different proteins (HSA, bromelain, papain and human γ-D crystallin), adding robustness to our findings.

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An artificial motor protein that walks along a DNA track

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Abstract: We demonstrate the realization of an artificial protein motor called Tumbleweed (TW) that walks directionally along a DNA track under external control. TW consists of three legs, each with a ligand-gated DNA-binding domain that enables selective interaction with specific sites along a DNA track. Using single-molecule fluorescence assays and a programmable microfluidic device, we show that TW steps directionally along a designed DNA track in response to a defined sequence of ligand inputs. We discuss the motor performance from the viewpoint of stochastic thermodynamics. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 951375).

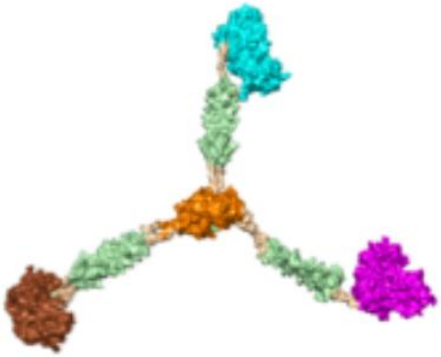

Figure 1. The Tumbleweed motor protein.

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Iridium(III) NHC Complexes: Selective C–H Bond Activation and Asymmetric Catalysis

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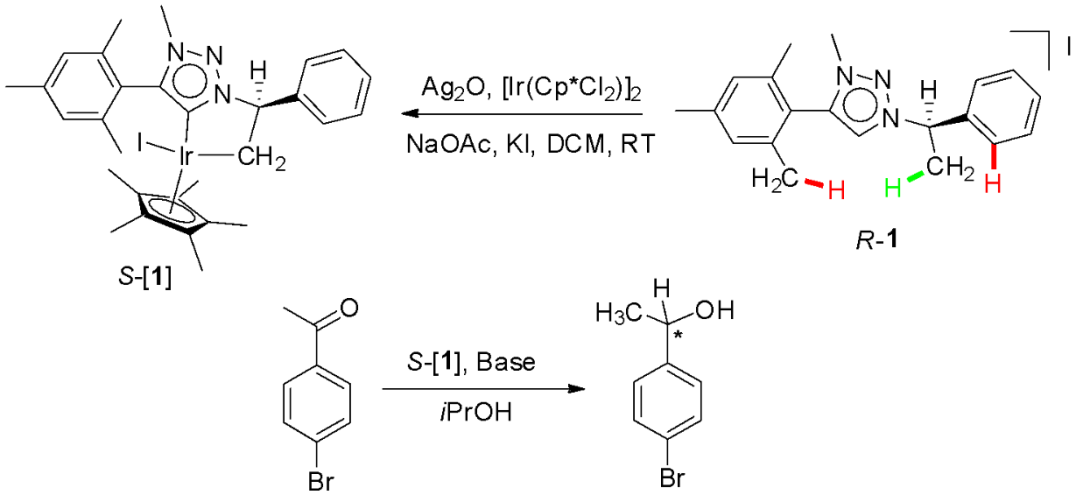
Abstract: N-Heterocyclic carbenes (NHCs) have emerged as a useful class of ligands in organometallic chemistry.[1] Although the majority of these ligands are based on imidazol-2-ylidenes or 1,2,4-triazol-5-ylidenes (normal NHCs), their mesoionic counterparts, 1,2,3-triazol-5-ylidenes, are currently gaining immense popularity.[2] The interplay between regioselective vs regiospecific C−H bond activation for the synthesis of cyclometalated Ir^{III} complexes has been demonstrated using the corresponding naphthyl-derived mono-imidazolylidene ligand. Carbene complexes synthesized via an sp^3 C–H bond activation are rare. An iridium(III) complex with a chiral mesoionic N-heterocyclic carbene (MIC) ligand, where the Ir^{III} forms an additional Ir–C bond via a regiospecific sp^3 C–H bond activation at the N-methylbenzyl wingtip, was synthesized and characterized. To our best knowledge, this represents the first example of cyclometalated iridium(III) complex possessing a chiral MIC donor ligand. This cyclometalated Ir^{III} complex was employed in the asymmetric transfer hydrogenation of 4-bromoacetophenone, and the complex was successful to transfer chirality to the final alcohol molecules (up to 92% ee).



Scheme 1. Synthesis and application of heterobimetallic complex

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Phase Separation in Active Mixtures

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Abstract: There has been intense recent interest in the physics of active matter, i.e., particles which consume energy and convert it to locomotion, e.g., birds, fish, bacteria, etc. We discuss the kinetics of phase separation in mixtures containing an active component. We highlight the important new features arising from the activity, focusing on the change in the domain growth law.

New Insight into Bistable Hofmann-Type frameworks: Kinetic Trapping and THz response

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Abstract: Temperature- and light-responsive spin-crossover (SCO) complexes offer a versatile platform for controlling electronic and structural states. However, unusual phenomena such as temperature-induced excited spin state trapping (TIESST) and their low-energy optical responses remain insufficiently understood. We investigate a series of Hofmann-type coordination frameworks to elucidate the interplay between spin-state energetics, lattice dynamics, and external stimuli. Complementary theoretical analysis reveals that the enthalpy difference between high-spin (HS) and low-spin (LS) states governs the stabilization of metastable HS states via thermal quenching, providing a mechanistic explanation. In another work, we have explored the terahertz (THz) response of a related Hofmann-type framework, $[Fe(L)_2Pt(CN)_4]$, which exhibits hysteretic SCO coupled with crystallographic symmetry breaking. THz spectroscopy reveals a strong dielectric response characterized by a phonon mode at ~0.8 THz, whose amplitude closely tracks the magnetic transition, demonstrating a direct coupling between lattice dynamics and spin-state switching. Together, these results establish a unified framework linking spin-state energetics, kinetic trapping, and THz phonon dynamics, offering new design principles for tuning metastability and enabling multifunctional SCO materials

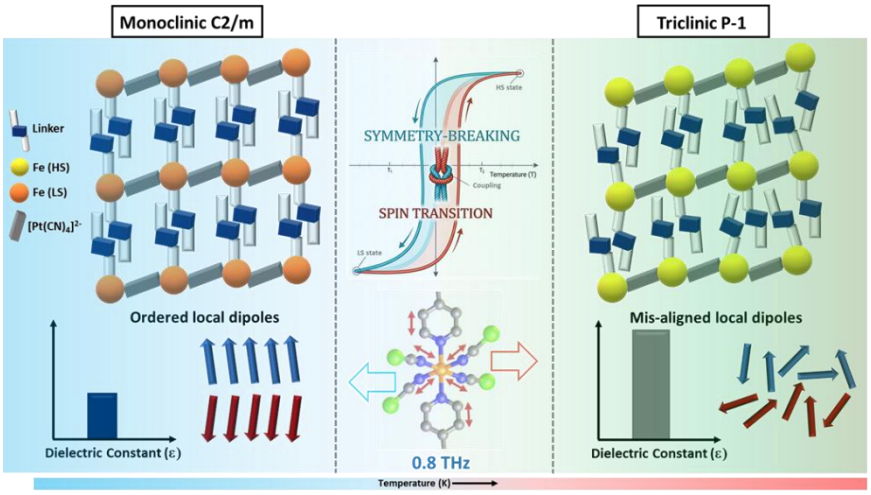

Figure 1. Schematic illustration of the mechanism underlying sub-THz switching in the Hofmann-type framework $[Fe(L)_2Pt(CN)_4]$,

Discotic Liquid Crystals as Self-assembled Molecular Semiconductors for Nanoscale Organic Electronics

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Abstract: Recent advancements in the field of organic semiconductors emphasize a challenge of achieving the perfect balance between effective charge-carrier transport and solution-processability. In this context, discotic liquid crystals (DLCs) are a class of self-assembling materials harmonizing supramolecular order and dynamics in a system that can potentially address the challenge.[1] Developing new DLCs for optoelectronic applications primarily denote the crucial role of the design and alignment for efficient movement of charge carriers in the material. To explore design and alignment in melt-processable devices, we have utilized anthraquinone as the primary motif, surrounded by ester functionalized tri-alkoxy phenyl units to develop room-temperature DLCs where the polar ester functionality stabilizes a highly ordered 2D columnar oblique (Col_{ob}) mesophase over a wide range through the involvement of dipole-dipole interaction along with the π–π stacking. Space charge limited current (SCLC) experiments revealed balanced ambipolar charge transport, with the maximum hole and electron mobilities of 5.04 and 4.93 $cm^2 V^{-1} s^{-1}$, respectively, and the high homeotropic alignment in devices were supported by conoscopic and grazing incidence small angle X-ray scattering (GISAXS) results. We also reported highest hole and electron mobility of discotic heterocoronene derivatives.[2,3] Also, to explore such properties of DLCs in solution-processable nanofilms, we have envisioned a minimalistic design strategy for a cyanovinylene-integrated pyrene-based DLC to exhibit a room-temperature columnar hexagonal mesophase and a narrow band gap for efficient semiconducting behavior. Even at low values of applied voltage, it exhibited superior charge extraction ability from the contact electrodes, achieving an electrical conductivity of 3.22×10^{-4} S/m, the highest reported value for any undoped DLC film in a vertical charge transport device. Its hole mobility values were comparable to the best organic hole transport layers (10^{-3} cm^2/Vs). In analogy with device performances, photophysical studies were correlated with carrier transport in the excited state induced by charge injection, substantially corroborated by theoretical studies on the molecular geometry, frontier orbitals and reorganization energies.[4] Again, to balance the high rigidity of the system with its fluidity, we have also developed a DLC dyad designed to induce a columnar nematic (N_{Col}) phase at room-temperature. With individual donor and acceptor components facilitating energy transfer in the excited state, the ordered nematic phase provided a defect-free nanofilm through solution-processable spin-coating. When fabricated into nanoscale two-contact devices, they displayed commendable charge-extraction property without the use of any dopant. Achieving an electrical conductivity of 10^{-4} Sm^{-1}, this is the first report of a nematic DLC nanofilms employed in a solution-processable charge-transport device.[5,6]

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Intracellular Sub degree Temperature Sensing and Dynamics by Thermoresponsive Silver Nanoclusters as Molecular Probes

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Abstract: Noble metal nanoclusters (MNCs) have emerged as promising alternatives to organic dyes and quantum dots due to their robust stability, superior biocompatibility, and tunable physicochemical properties.[1,2] However, their full potential in theranostics, sensing, and biological imaging has yet to be realized. Here, we report long-lived, red-luminescent silver nanoclusters (AgNCs) stabilized by the small-molecule ligand thiolactic acid, which exhibit exceptional stability (shelf-life exceeding three years, photostability ~100%), water-solubility, and high biocompatibility, making them suitable for diverse applications such as sensing and live-cell imaging.[3] AgNCs display extremely sensitive (>2% K^{-1}) and reversible luminescence responses to temperature, enabling subdegree (<0.5 K) precision in local thermal mapping through simultaneous monitoring of emission intensity and excited-state lifetime. Cellular assays, including MTT viability tests, confocal fluorescence imaging, and fluorescence lifetime imaging microscopy (FLIM), suggest that the non-cytotoxic AgNCs specifically stain lysosomes in live mammalian cells, functioning as an organelle-specific biomarker and providing critical insights into lysosomal dynamics and intracellular temperature fluctuations.[3] The unique properties of these AgNCs, corroborated by detailed mechanistic studies, open new avenues for studying nanoscale subcellular physiology and developing temperature-sensitive diagnostics and preservation strategies.

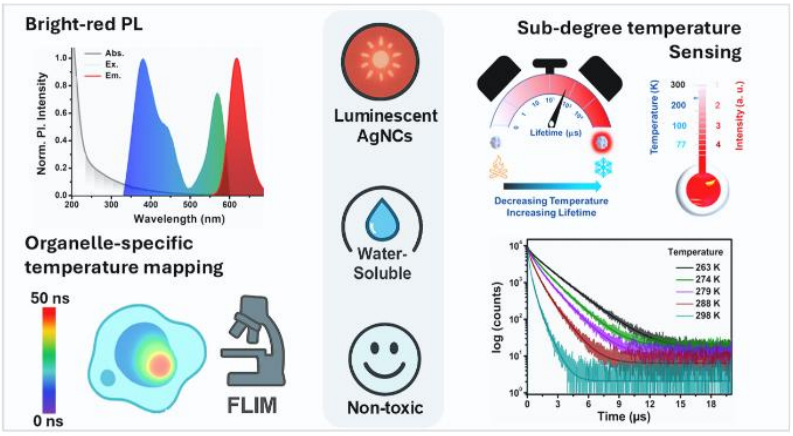

Figure: The schematic representation of the work, reflecting the salient features of the present investigation.

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DNA Target Search in Chromatin Compartments under Stochastic Resetting

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Abstract: Target search dynamics of sequence-specific DNA-binding proteins (DBPs) known as transcription factor(TF) with sequence-specific regions of DNA is a combination of 3D diffusion in bulk and 1D sliding along the DNA, commonly referred to as facilitated diffusion. In the context of target search processes, a fundamental quantity of interest is the mean first passage time (MFPT), which quantifies the average time taken before the process hits the target state for the first time.[1] Diffusion with stochastic resetting is a widely studied model where the searcher is intermittently returns to a fixed location or a location sampled from a spatial distribution and is known to reduce the mean search time.2 Interactions between intrinsically disordered regions of TF in eukaryotic cells lead to the formation of dynamic assemblies called transcription condensates. In this talk, I will discuss the search for the target within the chromatin compartments under stochastic resetting of the TF to the transcription condensates.[3] We show that intersegmental jumps and resetting can have dual effects by enhancing and reducing search efficiency depending on the resetting position of the TF. Resetting can improve search efficiency only when it occurs near the target site. We also investigate the cost associated with resetting, which increases with resetting rate and decreases with intersegmental jump rate. Our analytical results, supported by numerical simulations, provide quantitative insights into the role of chromatin architecture and TF localization in regulating the search dynamics of TF.

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Powering Solar Fuels with Next-Generation Semiconductor Heterostructures: Trends, Breakthroughs, and Mechanisms

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Abstract: Photocatalytic water splitting (PWS) is a solar-driven approach to hydrogen generation from water.[1] Despite its considerable potential, the widespread application of PEC water splitting remains hindered by limitations such as low efficiency, which arises from charge carrier recombination, and sluggish reaction kinetics. The integration of cocatalyst decoration with complementary enhancement strategies has shown promise in overcoming these challenges, offering improved efficiency and stability. A promising class of next-generation photocatalysts, conjugated polymer nanostructures (CPNs) exhibit a distinctive capacity to hybridize with other nanomaterials to form heterostructures.[2,3] Notably, femtosecond transient absorption spectroscopy has revealed that the incorporation of metal oxide and polymer nanostructures substantially enhances the separation and transfer of photoinduced charge carriers.[3] For instance, embedding polypyrrole (PPy) nanofibers within Bi_2WO_6 has been shown to markedly increase conductivity and catalytic performance, while maintaining activity through multiple operational cycles. In another example, the integration of Cu_2SnS_3 quantum dots with BiOX formed the interfacial Bi-S chemical bond, which acts as a charge migration centre, creating an internal electric field at the interface that can effectively enhance the photocatalytic H_2 evolution.[4] Very recently, atomic-scale interface engineering and built-in electric field at S-Scheme $Bi_2WO_6/ZnIn_2S_4$ heterojunctions for photocatalytic hydrogen evolution.[5] Furthermore, an indigenous prototype device incorporating a photocatalyst layer within photochemical reactor has been developed, underscoring practical advancements in this field. A deeper understanding of the photoelectrochemical behavior of emerging carbon-based nanostructures, along with elucidation of their underlying mechanisms and associated challenges, holds significant potential for scaling up solar fuel production technologies.

Keywords: Conjugated polymer nanostructures, Heterostructures, Surface engineering, S-scheme heterojunction, Photocatalytic water splitting

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Time resolved imaging of DNA labelling probe towards chromosome structural characterisation

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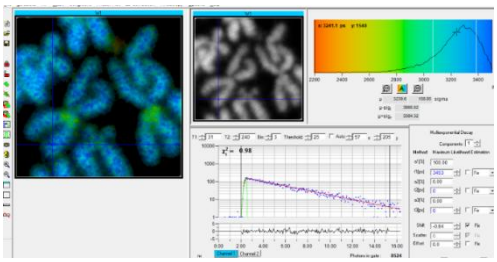
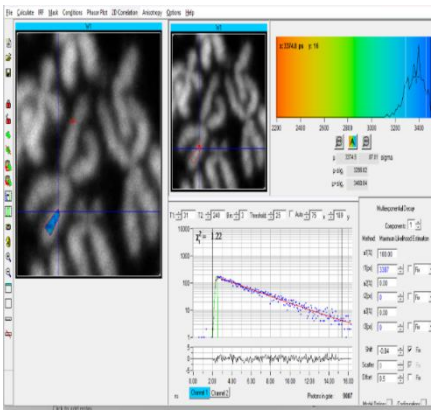
Abstract: Chromatin condensation is an important hall-mark of cell processes such as apoptosis and disease states including cancer. Research into chromatin and whole chromosomes is essential for advancing our understanding of cytogenetics, gene regulation and numerous aspects of organismal health. Chromatin condensation of whole human chromosome was followed using fluorescence lifetime imaging microscopy (FLIM), a technique that utilizes the excited state lifetime to probe changes in the fluorophore's environment. Staining metaphase chromosomes spreads with 4',6-diamidino-2-phenylindole (DAPI) and its derivatives showed differentially compacted regions of chromatin along the length of the chromosomes. Interestingly only the pericentromeric regions of human chromosomes 1, 9, and 16, short arm of chromosome 15, and distal region of chromosome Y showed statically significantly shorter DAPI lifetime values ($\tau_{1,\,16,\,Y} = 2.57 \pm 0.2$ ns, $\tau_{9a,\,15} = 2.41 \pm 0.2$ ns, and $\tau_{9b} = 2.21 \pm 0.1$ ns) than the rest of the chromosomes ($\tau = 3.0 \pm 0.1$ ns), (see figure, 1 mm scale bar). Furthermore, we show that chromosomes of cells irradiated with 0.1 Gy and 1 Gy x-rays did not show a significant change in lifetimes (2.94±0.09 ns on the arms and 2.60±0.06 ns on the pericentromeric region) of chromosome 1. Whilst irradiation with 0.5 Gy led to a noticeable and significant reduction in lifetime with 2.42±0.13 ns on the arms and 2.12±0.06 ns on the pericentromeric region of HeLa and T-cells chromosomes. Metal organic complexes were also found to have a unique long-lived (us) sensitivity to individual DNA bases. However, these sensitivities were lost in the polymeric DNA structure. These findings indicate that DAPI (a common DNA stain, minor groove binder) lifetime is a highly useful tool to measure chromosomal structural changes and further suggests that chromosome pericentric regions undergo distinct structural changes following low- and radiotherapy relevant dose of x-ray irradiation evidenced by chemical probes.





Bio-inspired, Non-Covalent Synthesis of Precision Supramolecular Polymers

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Abstract: The investigation of dynamic and adaptive supramolecular polymers, arising from monomer self-assembly, has entered a phase demanding greater structural and dynamic precision. Living supramolecular polymerization has emerged as a synthetic approach to craft assemblies with well-defined structures and dispersity. Concurrently, the pursuit of temporal control over dynamic materials is extending into the non-equilibrium realm. Despite the desirability of both controls, the strategies employed have largely been chemically distinct. Recognizing the importance of synergy between structural and temporal control, especially for the functional application of supramolecular polymers as adaptive materials, it is imperative to seek a common strategy. Drawing inspiration from the biological realm becomes crucial in navigating this conundrum.

Our laboratory is motivated by this philosophy and is actively engaged in comprehending both the thermodynamic and kinetic aspects of supramolecular polymerization. This presentation outlines our endeavors in understanding a pivotal concept in biological self-assembly: temporal control over aggregates through a chemical reaction. We believe this approach has the potential to address various challenges in supramolecular chemistry, including living supramolecular polymerization and dissipative assemblies. The talk will delve into our recent efforts to design reaction-coupled supramolecular polymers and explore bio-inspired design strategies aimed at expanding the structural diversity of supramolecular polymers

Aryl-Substituted Buta-1,3-Diene as Luminescent Core for Monomers and Copolymers: Design, Synthesis and Applications

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Abstract: Development of solid-state emissive organic moiety is promising because of the excellent optoelectronic property with versatile applications in the field of organic and polymeric light emitting diodes, ultrasensitive sensors, organic solid-state laser, and bio-imaging. However, the emissive property is substantially diminished in the solid-state owing to the molecular aggregation and it limits its use in real technological applications. To overcome this challenge, the rational molecular design is a key to develop the solid-state emissive organic moiety and 1,4-diphenylbuta-1,3-diene moiety has been judiciously picked up as the central flexible core to prepare several organic derivatives and copolymers. The effect of substituents on colour-tunability, absorption / emission properties, the band gap and energy levels have been explored. Few copolymers or donor-acceptor type small molecules linked to tetraaryl-substituted buta-1,3-diene core have been utilized as emitter to fabricate solution processed non-doped PLED or OLED devices to demonstrate the potential application as the emissive layer.

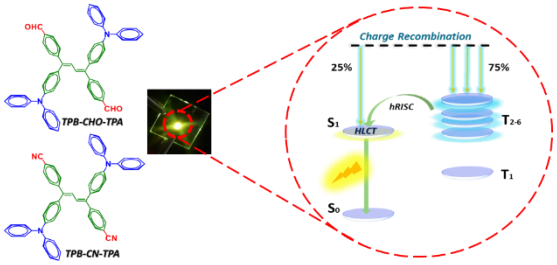

Figure 1. Representative tetraphenyl buta-1,3-diene based moieties and OLED device.

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Computational Modeling of Molecules and Materials for Applications in Energy Conversion and Storage

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Abstract: Current trend in research on molecules and materials majorly encompasses creation, conversion and storage of renewable energy. In this respect, I shall discuss our efforts in computational modeling of a few molecules and materials (i) which show electrochemical water splitting with hydrogen evolution reaction (HER) at anode and oxygen evolution reaction (OER) at the cathode end, (ii) which show bifunctional electrocatalyst with both OER and oxygen reduction reaction (ORR) [1, 2]. We have been modeling semiconducting systems for applications in Li and Na ion solid state electrolytes and cathodes. I shall discuss the modeling approach on oxygen deficient perovskite material, $Na_3MnV_2O_{7.5}$ as cathode for Na-ion battery application and on a 5V-class $LiNi_{0.5}Ge_{1.5}O_4$ Li-ion solid electrolytes which does not have any stable/metastable intermediate(s) in the wide composition domain of Li [3, 4]. We have also been working on modeling thermoelectric materials which convert waste heat into electricity using Wigner-Peierls-Boltzmann semiclassical transport equations together with density functional theory calculations. In this, I shall talk on finding thermoelectricity in 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir) and in a phonon-glass-electron-conductor, $AgGeSnSbTe_4$, which was synthesized and studied by an experimental group [5, 6]. If If time allows and scheduling permits, I shall discuss our computational efforts in understanding the very low thermal conductivities observed in two systems, TlAgSe and Tl_2AgI_3, which were synthesized and studied by an experimental group [7, 8].

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Green and Step-Economic Synthesis of Bioactive Hybrid Heterocycles

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Abstract: Heterocycles are indispensable in organic chemistry due to their widespread occurrence in natural products, pharmaceuticals, and functional materials. Developing efficient and sustainable methods for constructing complex hybrid heterocyclic frameworks using pot-, atom-, and step-economic strategies remains a central goal in modern synthesis. In this context, multicomponent reactions (MCRs) have emerged as powerful tools, enabling rapid molecular assembly with high atom economy and reduced synthetic steps. In this lecture, recent contributions from our research will be presented, focusing on the development of novel, sustainable methodologies for synthesizing biologically relevant hybrid heterocycles. These approaches employ readily available starting materials, mild conditions, and operational simplicity. Emphasis will be placed on the strategic use of MCRs to enhance efficiency, sustainability, and structural diversity, highlighting their potential in advancing modern organic and medicinal chemistry.

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New insights into photoactive earth-abundant Fe(II) complexes

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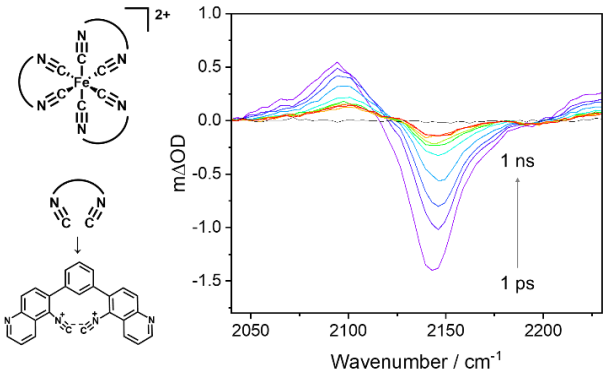
Abstract: First-row transition metal complexes gain intense attention as alternatives to photofunctional precious metal complexes. While Fe(III) complexes are now luminescent and applicable to many applications due to their nanosecond lifetimes, seeking long-lived triplet excited states of d^6 Fe(II) complexes remains important toward microsecond lifetimes as analogues of the Ru(II) polypyridyl complexes. Here, we will present two new concepts of Fe(II) complexes to extend their excited states. To create Fe(II) complexes with strong ligand fields, we aimed to synthesize an air-stable hexacarbene Fe(II) complex. As recent papers reported, strongly σ-donating hexa-N-heterocyclic carbene (NHC) ligands provide Fe(III) states under air. Here, a triazole-based NHC ligand was chosen due to its slightly weaker yet strong ligand field to stabilize the Fe(II) hexacarbene complex. We successfully isolated the air-stable Fe(II) hexacarbene complex, and its metal-to-ligand charge transfer (MLCT) excited state was analyzed by fs-transient absorption spectroscopy. Although the obtained MLCT lifetime was still short-lived (<1 ps), the ease of handling of air-stable Fe(II) hexa-NHC complexes would accelerate research on



exploring longer-lived ^{3}MLCT states.[1] As another approach, isocyanide ligands suitable for Fe(II) complexes are investigated. Aryl isocyanides are excellent ligands for Cr(0) and Mn(I) complexes; however, their π* orbital is too high for Fe(II) complexes.[2] Our Fe(II) complex with newly synthesized quinoline-based isocyanides exhibited MLCT absorption around 400 nm, and its photophysical properties were analyzed by various measurements such as UV-vis transient absorption spectroscopy, time-resolved IR spectroscopy, and Kerr-Gate luminescence spectroscopy. Interestingly, the bleach of the C-N stretching peak remains more than 1 ns in time-resolved IR spectra (Figure 1). This nanosecond-order excited state roughly matches the decay of the luminescence. This implies that potentially luminescent Fe(II) isocyanide with nanosecond lifetimes was achieved by our extended isocyanides.[3] The detailed analysis and full excited-state picture of these new Fe(II) complexes will be discussed.

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Chiral/Achiral Assemblies: Understanding the Regulation of Self-Assembly

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Abstract: Our research work aims at development of donor-acceptor building blocks which undergo self-assembly in aqueous media to generate fluorescent assemblies in aqueous media.[1] These assemblies having appropriate binding sites for interactions with specific analytes undergo guest induced morphology transformation and exhibit interesting photophysical properties. Very recently, we have developed supramolecular assemblies having chiral -handle and investigated the achiral/chiral guest induced chirality transformations in aqueous media. Furthermore, we have also developed metal based as well as metal free supramolecular catalytic ensembles for carrying out various organic transformations. In the presentation, different aspects of pathway complexity of these 'lighted' materials will be discussed.

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Metal Organic Frameworks and their hybrid for Advanced Chemical Defence Applications

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Abstract: The rapid rise in industrial emissions, toxic industrial chemicals (TICs), and chemical warfare agents (CWAs) has generated an urgent need for advanced materials capable of efficient detoxification under environmentally benign conditions. Conventional adsorbent systems, primarily based on impregnated activated carbon, largely depend on physical adsorption and often exhibit limited catalytic activity, susceptibility to humidity, and risks associated with secondary desorption of toxic species. In this context, metal organic frameworks (MOFs) have emerged as highly promising next-generation materials owing to their exceptionally high surface area, tunable pore architecture, and abundance of catalytically active sites. This presentation will show recent advances in the development of MOF-based hybrid materials for the adsorption and catalytic degradation of toxic gases and CWAs. Particular emphasis will be placed on defect-engineered zirconium-based MOFs and MOF carbon composites designed to enhance gas uptake capacity, diffusion pathways, and catalytic hydrolysis efficiency. Comprehensive physicochemical characterization using FTIR, PXRD, BET, SEM, TEM, and XPS provided critical insights into the structural evolution, surface chemistry, and active site engineering of the developed MOF-based materials. The presentation will highlight how these engineered materials exhibit superior adsorption behavior and rapid *in-situ* catalytic detoxification of hazardous toxicants under ambient conditions compared to conventional adsorbent systems. Particular emphasis will be placed on the role of defect engineering, enhanced porosity, accessible metal active sites, and surface functionalities in achieving efficient and sustainable detoxification performance. In summary, the potential integration of these advanced MOF-based materials into next-generation NBC protection platforms, offering improved protection efficiency, reduced secondary contamination risks, lightweight design, enhanced wearer comfort, and extended operational life. These findings provide new insights into the design of multifunctional protective materials for defense, industrial safety, and environmental remediation applications.

Hydrogels/ gels and nanomaterials for biomedical applications

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Abstract: Biomaterials are designed to interact with the living systems, and different types of biomaterials, like polymeric hydrogels, self-assembled peptide gels, and nanomaterials have been used for sensing, drug delivery, antibacterial, wound healing, and tissue engineering applications, owing to their excellent biocompatibility and/or extracellular matrix (ECM)-mimicking properties. Our group has been engaged in the development of hydrogels/ gels/ nanomaterials for drug delivery, medical devise-associated infection, chronic wound management, biocatalyst, and tissue regeneration applications. Our group has successfully developed cyclic peptide nanotubes for bone mineralization and osteogenic differentiation. The nanotubes mimic alkaline phosphatase, an enzyme crucial for bone remineralization, and also possess excellent cell migration, anti-inflammatory, and antioxidant properties. Another work in the field of bone tissue regeneration employs hydrogels loaded with MgO nanoparticles exhibiting anti-inflammatory and antioxidant properties, thus, promoting the regeneration of damaged bone tissue in rheumatoid arthritis. These hydrogels also induced the removal of fibroblast-like synoviocytes by apoptosis, further aiding in the mitigation of the disease. Currently, we are working with self-assembled bioactive peptide gels containing melatonin functionalization, with potential for wound healing along with antibacterial properties. The biomaterials developed show excellent potential for tissue engineering applications.

Abstracts

Poster

Synthesis of Imine- linked Covalent Organic Frameworks for Photocatalytic glycerol reforming

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Abstract: Sustainable materials development is central to addressing global challenges in energy, environment, and climate change. Imine-linked Covalent Organic Frameworks (COFs) — crystalline porous materials with high surface areas and tunable pore architectures — have emerged as promising platforms for advanced catalysis and biomass reforming. However, their conventional solvothermal synthesis remains energy-intensive, time-consuming, and difficult to scale, limiting broader deployment. In this work, we report the synthesis of an imine-linked COF via three green and scalable routes: mechanochemical synthesis, co-precipitation, and continuous-flow processing. Mechanochemical synthesis enables rapid COF formation under minimal solvent conditions; co-precipitation offers a straightforward ambient-temperature pathway; and continuous-flow synthesis affords precise control over residence time and mixing, ensuring high reproducibility and scalability. The optical and electronic properties of the resulting COFs are systematically tuned to enhance photocatalytic performance towards green hydrogen evolution and value-added product generation. The synthesized materials are being evaluated for solar-driven photocatalytic reforming of biomass-derived substrates, demonstrating efficient utilization of solar energy under mild conditions. This work establishes green synthesis strategies as key enablers for next-generation COF-based photocatalysts, contributing scalable and sustainable solutions to the intersecting challenges of energy conversion and climate change.

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Multifunctional Porous Polymer Networks for Efficient Capture of Radioactive Nuclides

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Abstract: The efficient sequestration of radioactive contaminants generated from nuclear energy production and associated industrial processes remains a major environmental and public health challenge. Among these, volatile iodine species and soluble uranium ions are particularly hazardous due to their long-term radiotoxicity, high mobility, and persistence in environmental matrices. In this context, the development of robust porous materials with high adsorption capacity, rapid kinetics, and selective binding functionalities is of significant importance for nuclear waste remediation. Herein, we report two strategically engineered porous polymer platforms designed for the ultrafast and efficient capture of radioactive waste species. In the first system, a poly(aminoamide)-based mesoporous polymer was synthesized through an Aza–Michael addition reaction, followed by in situ endo-templating using piperazine to generate a crosslinked porous framework.[1] The lyophilized polymer exhibited a high surface area of 143 m^2 g^{-1} and demonstrated exceptionally rapid iodine uptake, reaching adsorption saturation within 1 minute in batch mode. Remarkably, the material achieved adsorption capacities of 8.5 g g^{-1} in aqueous medium and 12.4 g g^{-1} in the vapor phase, highlighting its outstanding potential for ultrafast radioactive iodine capture. In the second system, a triazolinedione (TAD)-based porous polymer network was developed to introduce urazole as a novel multifunctional binding site for uranium sequestration.[2] The porous framework was synthesized via ultrafast click chemistry using an indole-derived trifunctional monomer and MDI-bisTAD linker, generating a chemically robust mesoporous polymer enriched with urazole, imine, and amine functionalities. This rationally designed functionality enabled strong and selective coordination with U(VI) ions, resulting in an exceptionally high adsorption capacity of 956 mg g^{-1}, with 99.6% uptake achieved within 50 minutes and excellent recyclability over multiple cycles. Overall, this study presents a unified porous polymer platform for the rapid and selective capture of radioactive iodine and uranium species for nuclear waste remediation.

Keywords: Nuclear waste remediation, Mesoporous polymer, Poly(aminoamide), Iodine adsorption, Uranium capture

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Supercritical Fluid–Engineered Pt/TiO_2 Photocatalysts for Enhanced Natural Sunlight-Driven Hydrogen Evolution: A Comparative Study with Chemical Reduction

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Abstract: The growing global energy demand and the environmental concerns associated with fossil fuel consumption have accelerated the search for sustainable and renewable energy alternatives. Among them, green hydrogen has emerged as a promising clean fuel for future energy systems. In line with this vision, the Government of India has recently launched the National Green Hydrogen Mission to promote research and technological advancements in hydrogen production. Photocatalytic hydrogen evolution using semiconductor materials offers a sustainable pathway for solar-to-hydrogen conversion; however, its practical application is limited by rapid charge carrier recombination and low surface reaction efficiency. In this work, glycerol-assisted photocatalytic hydrogen production over Pt/TiO_2 photocatalysts has been investigated. Biomass-derived glycerol, an abundant by-product of biodiesel industries, was utilised as a sacrificial agent to suppress electron-hole recombination and enhance hydrogen generation. Platinum was deposited onto TiO_2 using two different approaches: supercritical fluid reactive deposition (SFRD) and conventional chemical reduction deposition (CRD). The influence of deposition strategy on the physicochemical and photocatalytic properties of Pt/TiO_2 was systematically studied. SFRD is expected to provide uniform nanoparticle dispersion, controlled nucleation and stronger metal support interaction compared to CRD, which often results in particle agglomeration and non uniform growth. These structural and electronic differences significantly affect photocatalytic performance by influencing charge separation efficiency, surface active sites, light absorption behaviour and catalyst stability. The present study focuses on identifying the critical parameters governing hydrogen evolution, including Pt loading, particle size, dispersion, oxidation state and interfacial interaction between Pt and TiO_2. This comparative investigation provides valuable insights into the design of efficient and durable Pt-based photocatalysts for sustainable hydrogen production and highlights the potential of supercritical fluid deposition techniques for photocatalytic applications.

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Cobalt (III) Catalysed Annulation of Indoles With Phenylethynyl ether For the Synthesis of ABC Ring System of Ergot Alkaloids

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Abstract: The synthesis of ergot alkaloids, a diverse family of natural products with significant pharmacological importance, has long been considered a synthetic challenge due to their complex polycyclic framework. Traditional strategies often involve lengthy, stepwise procedures, which limit efficiency and scalability. In this work, we present a rational and streamlined approach that directly addresses these challenges by employing a C–H activation strategy for the rapid assembly of the ABC ring system of the ergot alkaloid skeleton. Our method begins with the C4-alkenylation of indole, which serves as a key step in functionalizing the indole core. This transformation is followed by an annulation process driven by *β*-carbon elimination, leading efficiently to the construction of the fused tricyclic (ABC) system. Remarkably, this sequence represents the first reported one-step synthesis of the ergot alkaloid ABC ring framework via C–H activation,[1] highlighting the novelty and synthetic utility of the strategy.

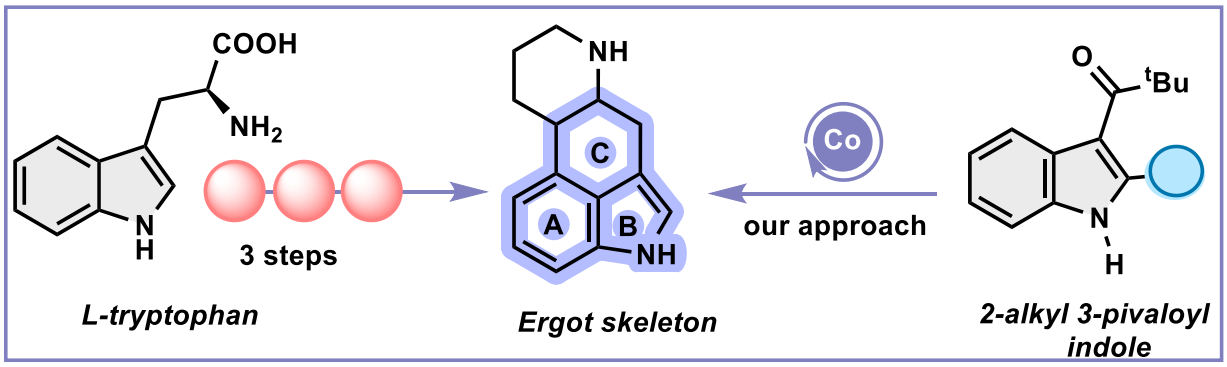

Figure 1. Classical synthesis vs catalytic method to synthesise ABC ring system of Ergot skeleton

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COF-Electrospun Nanofiber Membranes with Engineered Pore Environments for Superior Iodine Capture and Confinement

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Abstract: Radioactive iodine isotopes released from nuclear waste streams pose severe environmental and health risks, making their stable long-term confinement a critical challenge.[1,2] Here, we report the in-situ growth of a systematically designed series of imine-linked Covalent Organic Frameworks (COFs) TAPB-TA, TAPB-DHTA, TAPB-DMTA, and TAPB-DETA - on electrospun polyacrylonitrile nanofiber membranes (EPNMs) to produce a high-performance COF-EPNM platform for iodine capture and retention. By varying the aldehyde linker while keeping the amine component fixed, we demonstrate that introducing hydrophobic substituents at the ortho position of the aldehyde creates a nonpolar pore environment that thermodynamically stabilizes captured iodine while simultaneously shielding the imine linkage from hydrolytic degradation by nuclear off-gases. The EPNM architecture plays a decisive role - not only accelerating iodine adsorption kinetics by 2.4-4.3X relative to pristine COF particles through enhanced pore accessibility, but also significantly improving long-term retention, with TAPB-DMTA-EPNM achieving 80% retention over 10 days. These results establish COF-EPNMs as a robust and tuneable membrane platform where substituent engineering and nanofiber architecture act synergistically to overcome the fundamental trade-off between rapid uptake and stable iodine confinement.

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Strong metal-support interaction for enhanced photocatalytic synthesis of H_2O_2

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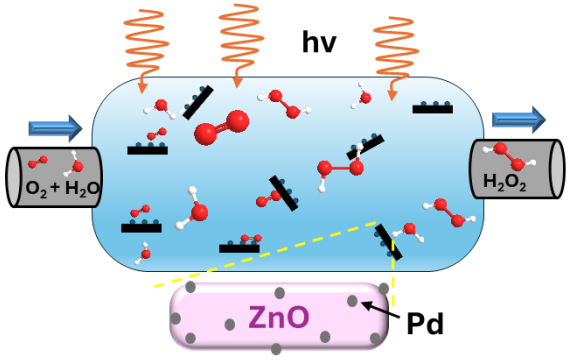
Abstract: Contrary to the centralised anthraquinone oxidation process, localised synthesis of H_2O_2 at the site of its need can reduce the cost of transport and storage.[1] Therefore, light-assisted conversion of O_2 and H_2O to H_2O_2 is an eco-friendly and cost-effective way of its production. However, the slow photocatalytic kinetics limit the production of high concentrations of this compound. Metal oxides are promising candidates as photocatalysts due to their abundance, stability, and low cost.[2] Here we show that Pd colloids supported on ZnO are capable of producing high concentrations of H_2O_2 (Fig. 1). Most reports on the photoproduction of H_2O_2 use a sacrificial agent (e.g., alcohol) as an electron donor, which complicates the photocatalytic system and adds cost.[3] A very low amount of Pd loading on ZnO improves the concentration of H_2O_2 tremendously compared to pristine ZnO without an extra sacrificial agent. This remarkably high photocatalytic activity is attributed to the strong electronic metal-support interaction. This work reveals the potential of designing efficient photocatalysts for H_2O_2 production through an electronic modulation strategy.

Keywords: Metal-support interaction, H_2O_2, photocatalysis



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Naphthalimide based Dual Fluorescence sensor for the detection of Co(II) and Zn(II)

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Abstract: The selective and sensitive detection of biologically and industrially important metal ions has attracted significant research interest in recent years. Zinc is essential for gene expression, cell division, and enzyme activity, while cobalt is required for vitamin B12 synthesis and has important industrial applications.[1-3] 1,8-naphthalimide-based fluorophores are effective platforms for detecting Zn(II) and Co(II) ions due to their excellent photophysical properties and stability. Here in this work, a novel 3-amino-1,8-naphthalimide hydrazine fluorophore (Nap-NH_2) was produced in quantitative yield through a one-pot imidation process between 3-nitro-1,8-naphthalic anhydride and hydrazine hydrate ($N_2H_4 \cdot H_2O$), and this fluorescent "turn-on" chemosensor for metal cations demonstrated positive solvatochromism and remarkable selectivity toward Zn(II) and Co(II) ions with nanomolar (10 nM) sensitivity, as exhibited by fluorescence titration studies. Interestingly, the presence of commonly coexisting different metal cations [Fe(II), Cu(II), Mg(II), Cd(II), Ni (II), Mn(II), Ba(II), Al(III) Ce(III), Pb(II), Cr(III) and Ca(II)] showed negligible changes in the emission intensity and thus weak binding interactions with Nap-NH_2. These studies demonstrate that Nap-NH_2 is a potential fluorescence "turn-on" chemosensor for selective, sensitive detection and quantification of bio-logically relevant metal cations.[4,5]

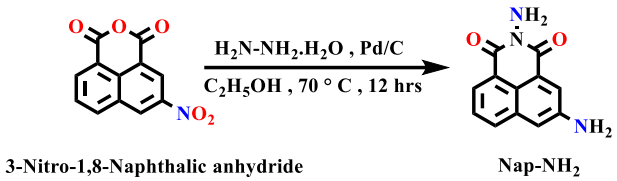

Figure 1. Synthesis of Nap-NH_2

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Reaction Energy Landscape for the Methane and Propane Conversion Over the Catalytic Active Sites generated Over Liquid Boron Oxide

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Abstract: Recently, oxidative dehydrogenation of light alkanes over metal-free boron-based catalysts, such as boron oxide (B_2O_3)[1],[2] and hexagonal boron nitride (*h*-BN)[3], have gained significant attention. However, these reactions typically proceed at very high temperatures (~700–800 K), limiting their practical applicability. In this direction, Rousseau and co-workers reported the formation of catalytically active sites in liquid boron oxide at 850 K using *ab-initio* molecular dynamics (AIMD) simulations. Despite this progress, the catalytic activity of these active sites toward the activation of light alkanes, such as methane[4] and propane, remains unclear. Furthermore, detailed mechanistic insights into the formation of value-added products, such as formaldehyde (HCHO) and olefins (propylene and ethylene), as well as undesired side products, including CO and CO_2, are still lacking. Herein, we employ *ab-initio* CASSCF/NEVPT2 and density functional theory (DFT)-based mechanistic investigations to explore methane and propane conversion over these structural motifs in the presence of singlet ($^1O_2$) and triplet ($^3O_2$) oxygen. Additionally, intrinsic bonding orbital (IBO) and quasi-restricted orbital (QRO) analyses are utilized to elucidate the associated electron-transfer events. Our results reveal that B–B sites serve as the most catalytically active motifs, facilitating HCHO formation during methane conversion and propene and ethene formation during propane conversion. In contrast, cyclic B–O–B motifs exhibit substantially higher activation barriers (~50-78 kcal mol^{-1}), indicating comparatively lower catalytic efficiency. Orbital analyses further highlight distinct electron-transfer pathways, involving oxygen lone-pair donation in B–O–B rings versus σ(B–B) bond donation at B–B sites.

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Au/Defected-TiO_2 Photoelectrodes for Overall Water Splitting

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Abstract: Photoelectrochemical water splitting using plasmonic nanoparticle–integrated semiconductors has attracted growing interest for solar-driven hydrogen production.[1] This work examines the roles of defects and surface plasmon resonance using self-standing Au/bare-TiO_2 and Au/defected-TiO_2 nanorod arrays grown on FTO substrates. Mott–Schottky and UPS analyses reveal enhanced carrier density, valence band shifts, and Schottky junction formation upon Au loading or defect introduction. The Au_{10}@TiO_2 electrode achieved a photocurrent density of 4.8 mA cm^{-2} at 1.23 V vs. RHE and a hydrogen evolution rate of 279.76 µmol h^{-1} cm^{-2}. While oxygen vacancies improve TiO_2's OER activity, Au incorporation drives efficient HER, demonstrating a synergistic effect that enables bifunctional photoelectrodes for overall water splitting.[2]

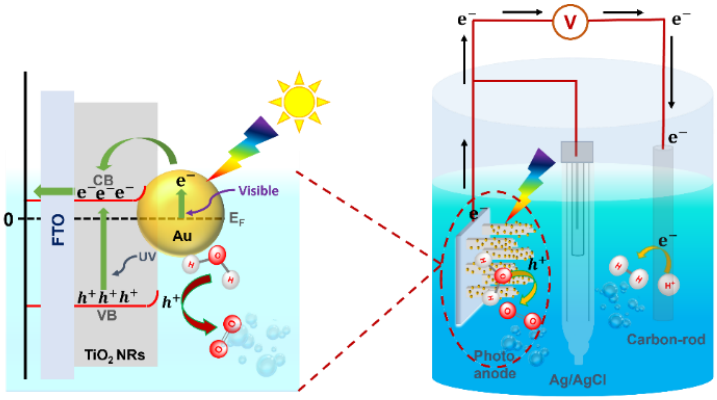

Figure 1. Synergistic effect of oxygen vacancies and noble metal loading for overall performance of photoelectrochemical water splitting.

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Development of a cost-effective paper-based disposable microextraction device for rapid detection of pesticides from dry fruit

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Abstract: The persistence occurrence of organochlorine pesticides (OCPs) found in dry fruits led to serious environmental and health risks because of their toxicity and bioaccumulation. In order to guarantee food safety, there is a need for an efficient and rapid analytical tool for monitoring and detecting the OCP residues from the dry fruit matrices. In this study a thin-film solid phase microextraction (TF-SPME) patch was fabricated using the synthesized metal-organic framework (MOF-199) which was incorporated with polydimethylsiloxane (PDMS) for the extraction of OCPs from the cashew samples. The developed TF-SPME patch's performance was evaluated by optimizing the various experimental parameters such as solvent profiling, concentration, stirring rate, temperature, reusability, extraction and desorption. The optimized TF-SPME patch exhibited high extraction efficiency and good reproducibility for OCPs followed by the quantification using gas chromatography-mass spectrometry (GC-MS). The fabricated MOF-199/PDMS patch showed excellent selectivity and sensitivity, indicating its potential as a simple, cost-effective and environmentally friendly analytical tool for the detection of the trace-level OCPs in the complex lipid rich cashew sample. This work highlights the feasibility of MOF-199 coated microextraction patch as a simple sample preparation tool for extraction of pesticide residues from dry fruit.

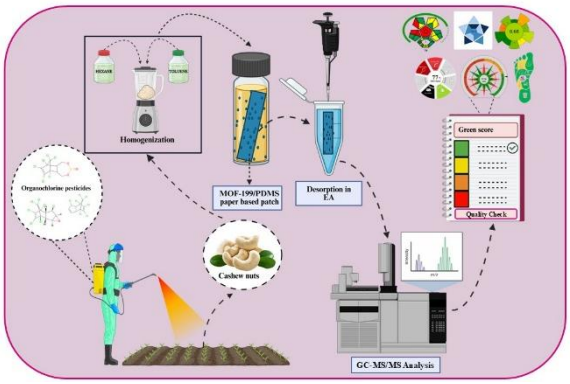

Figure 1. Extraction of OCPs from Cashew nuts using the developed MOF-199/PDMS patch

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Ultrasound-assisted ring opening of epoxides in HFIP: THF: Synthesis, characterization, computational studies and molecular docking of novel 2-hydroxy dithiocarbamates

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Abstract: Under the influence of ultrasonic irradiation, pyridazinone, triazinone, or phthalimide containing 2-hydroxy dithiocarbamates, a biologically relevant novel organo-sulphur compound, was synthesized. Detailed characterization, computational, and molecular docking studies are being investigated. Molecular interactions were studied using 3D Hirshfeld surfaces and corresponding 2D fingerprint plots. Theoretical (DFT) studies on the molecular structure, HOMO, LUMO, and quantum chemical descriptors were performed at the B3LYP/ 6–311++G(d,p) level of theory. At the same time, the interaction energy was computed using the B3LYP/6–31G (d,p) level of theory. The FMO study revealed that molecules 4a and 4p in the gas phase have 3.545 eV and 3.263 eV HOMO-LUMO energy gaps, respectively, and they are hence kinetically stable. Quantum chemical calculations confirm the electrophilic character of compounds 4a and 4p, as the molecule is stable and highly electrophilic.

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Dual Reaction Pathway Catalysis: Base free transfer hydrogenation of aromatic aldehydes by NiAl LDH catalyst via in situ Ni(0) formation

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Abstract: Formulating environmentally friendly and sustainable protocols for catalytic transfer hydrogenation (CTH) utilizing non-noble metal catalysts presents a considerable difficulty owing to their diminished activity relative to noble metals.[1, 2] This study presents a highly effective NiAl layered double hydroxide (LDH) catalyst produced by a traditional co-precipitation technique and activated in situ by isopropanol (IPA), functioning as both a hydrogen donor and a reducing agent. The CTH of benzaldehyde to benzyl alcohol proceeds efficiently under base-free conditions. Notably, during the reaction, a unique in situ transformation of Ni^{2+} species in the LDH to metallic Ni^{0} particles was observed, fundamentally shifting the reaction mechanism. Initial cycles proceed via a Meerwein–Ponndorf–Verley (MPV) pathway mediated by Lewis acidic and basic sites of the LDH. However, upon repeated use, the formation of Ni^{0} introduces a new metal-hydride-based pathway, wherein IPA dehydrogenation and aldehyde hydrogenation are facilitated by metallic Ni^{0} and Lewis acid sites. This dual mechanistic pathway results in the dynamic evolution of the catalyst during the reaction. Control and poisoning studies further confirm the pivotal role of basic sites in the initial CTH process. This protocol provides an environmentally friendly and chemoselective method for synthesizing aromatic alcohols, demonstrating exceptional substrate tolerance and advantageous environmental metrics.

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Synergistic Role of Sulfur Vacancies and Intergranular Cracks in Variable Resistive Switching of WS_2 Monolayers

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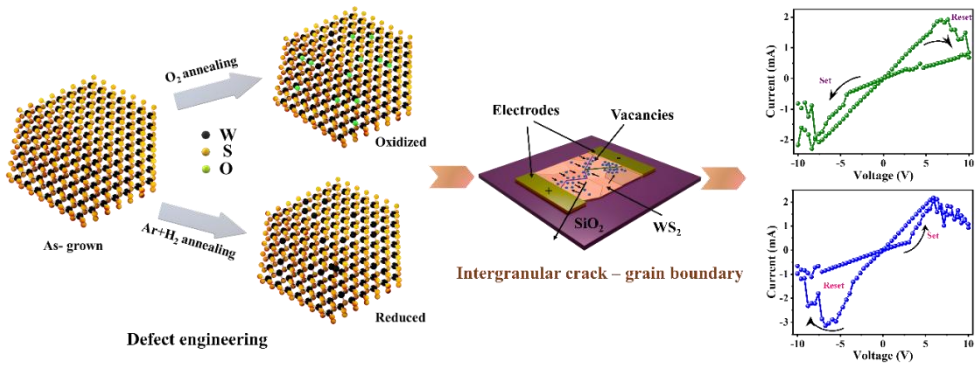
Abstract: Achieving reliable defect-engineered neural connections in 2D materials requires resistive switching that remains stable over prolonged cycling, demanding a deeper understanding of electrically driven defect evolution. Here, we demonstrate that the memristive behavior of monolayer WS_2 lateral devices is strongly governed by the interplay between point defects and intergranular crack networks. Controlled thermal annealing enables systematic tuning of WS_2 stoichiometry, varying sulfur vacancy concentrations from near-stoichiometric to ~10^{14} cm^{-2}, as confirmed by aberration-corrected HR-TEM and Raman spectroscopy[1]. Electron microscopy further reveals interconnected crack boundaries that act as energetically favorable channels for vacancy migration and localized conduction. The defects play a vital role in the observed rectification and conductance switching, arising from Schottky barrier modulation at the WS_2–metal interface and the redistribution of vacancies along crack-assisted transport channels. These findings establish a direct correlation between stoichiometry, defect-mediated transport, and memristive stability in monolayer WS_2.



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Waste to Wealth: Low-cost Carbon based Electrocatalysts for Water Splitting

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Abstract: The development of cost-effective, efficient, and durable electrocatalysts for the hydrogen evolution reaction is essential for advancing sustainable hydrogen production via water splitting. In this study, commonly discarded waste materials were transformed into conductive carbon-based supports and evaluated for their electrocatalytic performance in overall water splitting. Waste-derived precursors, including human hair, plastic bottles, and newspapers, were systematically converted into functional carbon materials and further engineered into single-atom catalyst systems. The resulting materials exhibit promising catalytic activity, highlighting their potential as low-cost alternatives to conventional noble-metal-based electrocatalysts. This approach not only addresses the economic limitations associated with large-scale hydrogen production but also promotes waste valorization and environmental sustainability. The findings demonstrate a viable pathway toward scalable and eco-friendly electrocatalyst design for hydrogen generation.

Ball-Milling Driven Regio- and Stereospecific Strain Release of Chiral Activated Spiro-aziridine Oxindoles with Alkyl Amines

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Abstract: An eco-friendly mechanochemical strain-release strategy for the regio and stereospecific amination of spiro-aziridine oxindoles is unveiled, yielding a, b-diamino oxindoles bearing chiral N-alkyl tertiary amine with excellent enantiopurity upto >99%. This carefully designed approach leverages the use of primary and secondary amines, especially water-miscible ones, which were limited in conventional methods. Aromatic amines also delivered desired product with high yield and enantioselectivity. This protocol functioning at ambient temperature with 100% atom economy requires no chromatographic purification. The potential of mechanochemistry is demonstrated by comparative studies showing superior kinetics and significantly improved green metrics (RME = 90%, E-factor = 0.05) in comparison to solution-based methods. Moreover, this orchestrated approach working under solvent as well as catalyst free condition, offers a sustainable option.

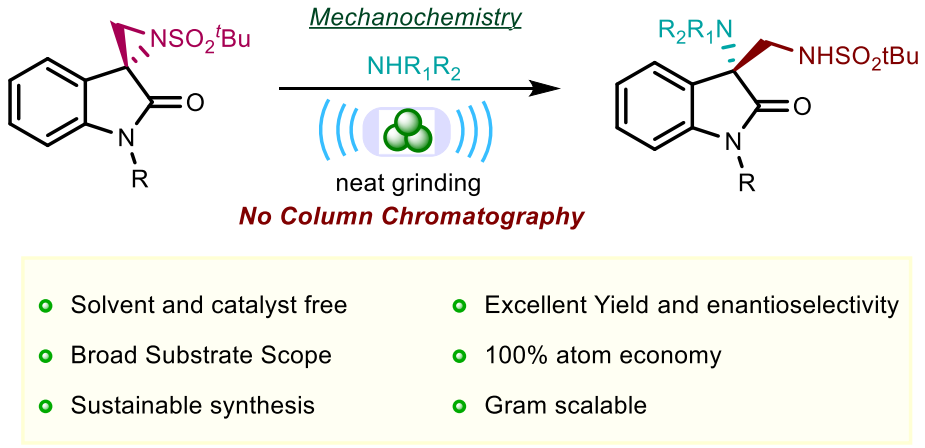

Figure 1: Mechanochemical amination in spiro-aziridine oxindoles.

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A water-soluble fluorescent probe for selective detection of palladium (II) ions

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Abstract: Palladium contamination poses significant environmental and biological risks, underscoring the need for highly efficient sensing tools that can detect trace Pd^{2+} in aqueous media.[1] In this study, water-soluble fluorescent probe 1-(3-(1-methylimidazol-3-ium-3-yl)propyl)-2-(8-quinolinyl)-1H-benzimidazole bromide (QBIm) incorporating an imidazolium–quinoline framework was synthesized for the selective recognition of Pd^{2+}.Spectroscopic investigations revealed that QBIm exhibits a rapid and significant fluorescence quenching response upon the addition of Pd^{2+} ions in aqueous solution. This quenching behavior can be attributed to the coordination of Pd^{2+} with the nitrogen donor sites present in the probe, leading to perturbation of the electronic structure and suppression of the emissive excited state. The sensing process is highly efficient and enables straightforward monitoring via fluorescence measurements without the need for additional reagents or complex procedures. QBIm exhibits rapid and pronounced fluorescence quenching upon coordination to Pd^{2+} in aqueous solution. QBIm demonstrates excellent selectivity for Pd^{2+} over a wide range of competing metal ions and provides a strong linear response over the low nanomolar concentration range, with a detection limit (36nM) suitable for environmental and analytical applications.[2]

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Electro-Redox-Mediated Formal (3+2) Cycloaddition: Sustainable Synthesis of Tetrazoloquinoxalinones

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Abstract: In this work we have discussed about a sustainable electrochemical protocol for the synthesis of tetrazolo[1,5-*a*]quinoxalin-4(5*H*)-one derivatives. A key feature of this method is the use of the electro-redox mediator 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), which enables the efficient utilization of sodium azide as a cost-effective azide source. Moreover nitrogen-based heterocycles such as tetrazole and quinoxalinone scaffolds have attracted considerable attention owing to their significant roles in medicinal chemistry, drug design, and materials science. This formal (3 + 2) cycloaddition strategy provides access to a wide range of functionalized tetrazoloquinoxalinone derivatives with potential biological significance. Comprehensive synthetic and electrochemical investigations reveal a mediator-assisted electrocatalytic mechanism, underscoring the advantages of this transition-metal-free electrochemical approach.

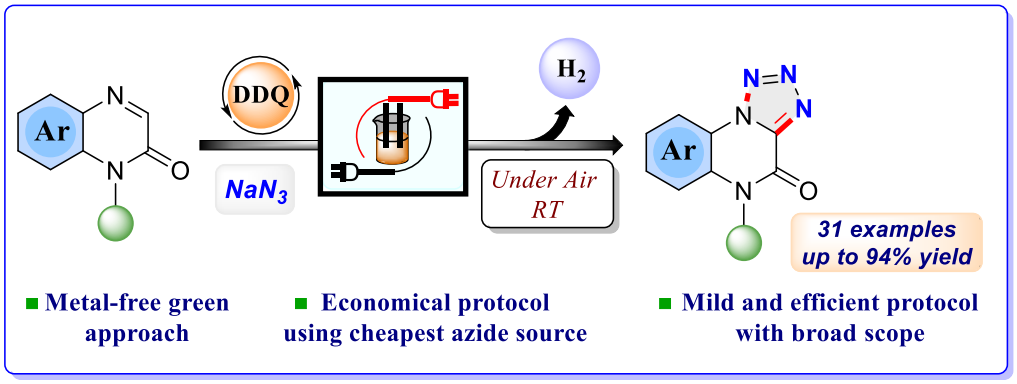

Figure 1. A schematic illustration of our methodology.

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Engineering Defects and Thermal Effects in Vanadium Oxides for High-Performance Energy Storage Applications

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Abstract: Vanadium oxides are a versatile class of materials for electrochemical energy storage due to their multiple oxidation states and layered structures; however, their practical application is often limited by poor electronic conductivity and sluggish kinetics. In this work, we demonstrate a combined defect and thermal engineering strategy using V_2O_5 as a model system to enhance electrochemical performance. Vanadium oxide nanoparticles were synthesized from commercial V_2O_5 via controlled oxalic acid reduction, where optimization of the precursor-to-reductant ratio (1:2) resulted in uniform nanostructures enriched with oxygen vacancies. These defects facilitate enhanced Li^+ diffusion and improved charge transport. Furthermore, annealing at optimised temperature (400 °C) effectively tunes crystallinity, oxidation states, and surface area without external additives, leading to improved electrochemical kinetics. The optimised electrode exhibits a high specific capacitance of 432 F/g at 5 mV/s with improved rate capability. A two-electrode device delivers an energy density of up to 20.8 Wh/kg at a power density of 480 W/kg. This study highlights that defect chemistry and thermal treatment synergistically govern the electrochemical behaviour of vanadium oxides, providing a simple and scalable pathway toward high-performance electrode materials and offering insights relevant to the broader design of next-generation energy storage systems.

Mono(Silylene)-Stabilized Borylenes for Small Molecule Activation

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Abstract: Although base-stabilized borylenes are now a decade old concept, the number of experimentally isolable mono(Lewis base)-stabilized borylenes are scarce and all of them feature carbenes as the stabilizing agent. Silylenes with an energetically accessible lone pair and a vacant orbital may be promising alternatives to carbenes. In this work, we have designed a few mono(Lewis base)-stabilized borylenes with silylenes as the Lewis base. Quantum chemical calculations revealed that the designed systems possess appreciable donor and acceptor properties that motivated us to investigate their potential towards the splitting of enthalpically strong E–H bonds (E= H, CH_3, NHPh) as well as binding of CO and N_2. All the activation and binding processes by the proposed borylenes were found to possess either better or comparable activation barriers compared to that obtained for cyclic (alkyl)(amino)carbene-stabilized borylene.

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Lewis Acid-Catalyzed Switchable Functionalization of *C*,*N*-Cyclic Ketimines with Vinyl Azides: Access to Diverse C(2)-Alkylated Pseudoindoxyls

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Abstract: Herein, a divergent coupling of indole-derived *C*,*N*-cyclic ketimines with vinyl azides is described for the synthesis of structurally diverse C(2)–Alkylated pseudoindoxyls, especially α–indoxyl acetamides, ketones, and acetonitrile derivatives. The Lewis acid-catalyzed divergent Schmidt and interrupted Schmidt–type pathways of the transient iminodiazonium ion intermediate enable vinyl azides to effectively function as surrogates for amides, ketones, and cyanomethanides. Furthermore, α–indoxylacetamides exhibited fluorescent properties, demonstrating an impressive fluorescence quantum yield.[1]

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From Nonemissive to Bright Green Luminescent: Eu^{3+}-Induced Clusterization of L-Cysteine

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Abstract: Clusteroluminescence (CL) offers an effective strategy for generating emission from nonconjugated, heteroatom-rich molecules, yet simple, biocompatible CL systems derived from natural building blocks remain scarce. Here, we report that coordination of Eu^{3+} with intrinsically non-emissive L-cysteine induces spontaneous clusterization and activates intense green emission. Under basic conditions, Eu^{3+} templates the formation of hierarchical Eu–Cys clusters that display a broad emission centerd at ~525 nm, a large Stokes shift (~150 nm), excitation-dependent emission, and a 56-fold enhancement in quantum yield (14%) compared to Eu^{3+} alone. Control experiments with other metal ions and amino acids reveal a pronounced coordination specificity, highlighting the unique cooperative interplay between Eu^{3+}'s high coordination propensity and cysteine's thiol-containing ligand topology. Combined spectroscopic and microscopic analyses reveal that the emission originates from clustered Cys domains rather than Eu-centered excited states, with Eu^{3+} functioning primarily as a structural node that rigidifies heteroatom-rich assemblies and suppresses nonradiative decay. This rare-earth-ion-induced clusterization strategy extends CL to single, non-aromatic amino acids, providing a general route to biocompatible luminophores from simple biomolecules

Small molecule-driven sensitization of insensitive inorganic salt: An approach for photoresist composition

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Abstract: Although many inorganic salts are readily available in bulk at high purity, they generally show little to no sensitivity towards electron-beam (e-beam) or photon exposure, limiting their applicability as photoresist materials.[1] Zinc(II) acetate, a well-known salt, is a representative example of a compound with negligible sensitivity. In our ongoing work to develop inorganic-organic hybrid resist materials, we hypothesize that introducing heterocyclic compounds with suitable metal-chelating functionality could enhance the sensitivity of such inorganic salts through potential complexation and interaction with exposure radiation. To validate our hypothesis, we designed and developed substituted pyrazole-based carboxylic acids and investigated their role as small-molecule sensitizers for zinc acetate dihydrate. The resulting zinc-metal-based resist composition (ZnNH) exhibited significant improvements in sensitivity. Results show efficient responses to both deep-ultraviolet (DUV) photon and e-beam exposure. In e-beam lithography, the resist composition shows an onset of response in e-beam at a dose as low as ~20 μC cm^{-2} and achieves a complete polarity switching, as supported by the normalized remaining thickness (NRT) curve, at doses ~115 μC cm^{-2} under an 18.0 kV electron acceleration voltage and a beam current of 56.3 pA. We can pattern the silicon surface to as small as 50 nm with a very low dose. Importantly, the composition of the resist system is well-suited to practical scalability for high-volume manufacturing. The current findings highlight a promising pathway to scalable, highly sensitive zinc-based resist systems for nanopatterning applications, with further potential as an extreme ultraviolet lithography (EUV) hybrid resist platform.[2]

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Lewis Acid-Catalyzed and Sulfur Ylide-Promoted Epoxide Ring Expansion for the Synthesis of Spiro-Oxetane Oxindoles Followed by Their Strain Release with Indoles: An Access to Mixed 3,3'-Bisindoles

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Abstract: C3-spirooxindoles are one of the privileged cores in synthetic chemistry. Three-membered cyclic structures, such as cyclopropane, epoxide, and aziridine, containing C3-spirooxindoles are well studied.[1] This time, in pursuit of our consistent research objective, we have developed a robust Lewis acid-catalyzed protocol to obtain spiro-oxetane oxindoles from spiro-epoxide oxindoles. To date, the only reported procedure for unsubstituted spiro-oxetane oxindoles suffers from several challenges, like limited substrate scope, use of expensive and potentially toxic selenium reagent, etc.[2] We have successfully designed a Corey-Chaykovsky reaction[3] that achieves regioselective ring opening of spiro-epoxide oxindoles by judicious choice of reagents and reaction conditions, thereby paving the way for spiro-oxetane oxindoles by effectively suppressing the previously unavoidable cyclopropanation.[4] An easy and efficient synthetic route to spiro-oxetane oxindoles brings up the opportunity to study the strain release chemistry of the same. We have successfully orchestrated the first-ever strain release of unsubstituted spiro-oxetane oxindoles using indole as nucleophile. This strategy provides us with an alternative way to mixed 3,3'-bisindoles. Multiple dimeric hexahydropyrroloindole (HPI) alkaloids are achievable from this ring-opening product core. We have also demonstrated the total synthesis of (±)-Folicanthine.

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Amplification of Self-Sensitization at Nanoscale in NIR-Upconverting NaErF4 Core-Shell Crystals: Implications for Energy Applications

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Abstract: Enhancement of self-sensitized near-infrared responsive (NIR)-upconversion (UC) process was examined on core-shell (CS) type of $NaErF_4$ crystals in the form of micron-sized particles mimicking bulk dimension and nanosized particles via three approaches. The manipulation of pristine $NaErF_4$ core, inert shelling of the unmanipulated pristine core and a combination of both core-manipulation and inert shelling were undertaken. The effect of the third or combined process appeared to be synergistic leading to an unprecedented augmentation of UC photoluminescence intensity, when the core particle was taken at nanoscale. To understand the basis of such magnified optical property at nanoscale, synchrotron X-ray diffraction (SXRD) based on synchrotron source and theoretical modelling using density functional theory (DFT) were conducted. Assessment of local disorder by atomic pair distribution function (PDF) analysis and microstrain by Williamson−Hall's analysis of SXRD revealed a relatively higher atomic level disorder and microstrain existing in the manipulated (Li^+ doped) nanosized core. Results obtained from DFT supported the structural feasibility of the Li^+-doped engineered core and indicated a progressive increase in misfit strain with increasing Li^+ concentration. The experimental misfit strain calculation obtained by differential lattice parameter analysis from Rietveld refinement of SXRD confirmed a hyper augmentation of misfit strain, at nanoscale domain, while no discernible difference of the same was observed at microscale domain. For the first time, the extent of lattice mismatch was shown to get amplified at nanoscale for a CS crystal system using SXRD aided with DFT. The atomic level study herein, appeared to highlight fundamental properties at nanoscale. Such engineered nanocrystals may be suitable for potential energy applications.

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An Unprecedented Photocatalyst- and Workup-Free Visible- Light-Mediated Oxidative Cyclization of Enynes Enabling Atom-Economic Synthesis of Indeno-Fused Furan Derivatives

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Abstract: A sustainable and economical visible-light-mediated intramolecular radical oxidative cyclization of enynes has been developed under mild, metal-, additive-, and workup-free conditions at room temperature. This protocol employs an inexpensive selenium catalyst to deliver indeno-fused furan derivatives in good to excellent yields with high regioselectivity.[i] Notably, the catalyst can be recycled and reused for up to six consecutive cycles without any significant loss of efficiency, highlighting the robustness and sustainability of the method. The transformation exhibits broad substrate scope and excellent functional group tolerance, demonstrating its versatility. Furthermore, green metrics evaluation confirms the environmental friendliness, operational simplicity, and atom economy of the process, making it a practical and efficient strategy for the synthesis of valuable heteroaromatic frameworks relevant to organic synthesis and medicinal chemistry.[ii]

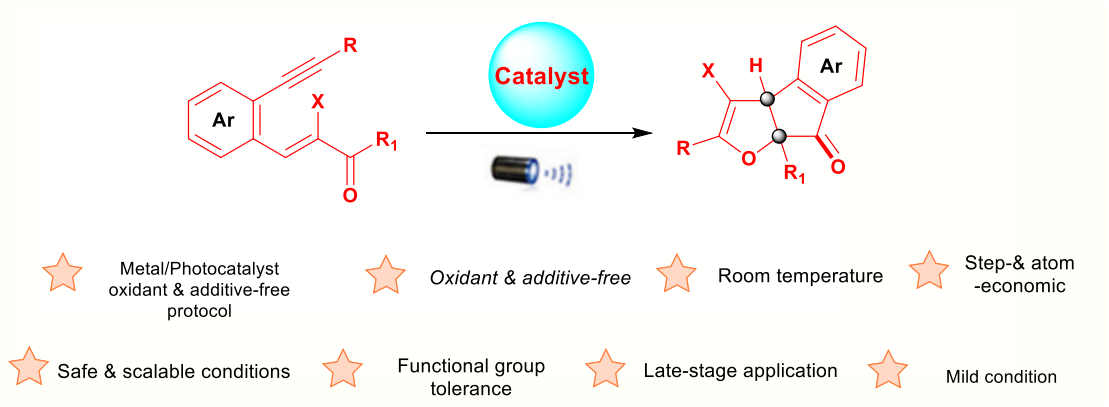

Figure 1. Visible-light-driven cyclization of enynes to indeno-fused furans.

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Carbodiborylenes: Computational Discovery of 1,3-Diboraallenes Capable of Multiple Complexation of CO_2 and CS_2

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Abstract: In this work, we provide computational evidence for the possible existence of metal-free diboraallenes in which the central carbon atom is supported by two base-stabilized borylenes. An evaluation of their proton affinity values and binding with AuCl suggests that they possess hidden C(0) character and hence can also be referred to as 'carbodiborylenes'. Owing to the presence of two lone pairs at the central carbon atom and vacant orbitals at the boron as well as carbenic carbon of the neighboring borylenes, these compounds demonstrate ambiphilic reactivity. Calculations suggest that the proposed compounds are not only capable of activating inert bonds such as N–H bond of ammonia but also hold promise for multiple complexation of CO_2 and CS_2.

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Zinc Phthalocyanine modified Polypyrrole sheets for Mechanistic Investigation of Neurodegenerative Oxidative Stress

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Abstract: According to the World Health Organization's global demographic data, neurological disorders affected 3.4 billion people in 2024, representing a major health concern.[1] Notably, neurodegenerative disorders like Alzheimer's, Parkinson's, Amyotrophic Lateral Sclerosis, etc. are contributing significantly in this domain. Among four nitrogenous bases in DNA, guanine plays a central role since its lowest oxidation potential leads to the formation of toxic 8-hydroxyguanine (8-oxoG).[2] 8-oxoG is one of the most extensively investigated oxidative DNA damage biomarkers due to its miscoding properties. Elevated levels of 8-oxoG are observed in both nuclear and mitochondrial DNA in the brains of patients with Alzheimer's and Parkinson's diseases.[3,4] Considering these findings, herein, we aim to design an electrochemical probe to understand the underlying effect of amino acid neurotransmitters in the oxidative damage of guanine, leading to the neurodegeneration. In this regard, zinc phthalocyanine (ZnPc) is employed as the electrochemical probe owing to its favorable binding affinity toward guanine, as revealed by density functional theory (DFT) analysis. ZnPc is supported on conductive polypyrrole (PPy) sheets via interfacial synthesis to obtain the electrochemical probe. This selective and sensitive ZnPc/PPy probe has the potential to elucidate the role of the oxidative lesion 8-oxoG in neuronal death.

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Interfacially Engineered Pd-Ni/ZnO Nanostructures for Selective Glycolysis of PET Waste into Bis(hydroxyethyl) Terephthalate

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Abstract: PET (poly (ethylene terephthalate)), is a very popular polymer because of its many useful properties and low production costs. But serious environmental problems, such the occurrence of "white pollution," have resulted from the improper handling of PET waste. To overcome this obstacle, shape-engineered heterogeneous ZnO nanostructures in the form of hexagons, rods, and cylinders were hydrothermally synthesised and then surface-modified using a wet impregnation technique with metals like Pd, Ni, and Pd-Ni. The catalytic efficiency of PET glycolysis was increased using this approach. The ZnO catalyst's shape was adjusted by adjusting variables like pH, precursor concentration, and reaction time. One of the byproducts of glycolysis is bis(2-hydroxyethyl) terephthalate, or BHET. This monomer has significant practical use in the manufacturing of jet fuels and other important fuels, as well as in the manufacture of polymers. With full (100%) PET conversion and an optimised catalyst operating under reflux conditions, the BHET yield was 90%. Mass spectrometry, ^{13}C-NMR, and ^{1}H-NMR were used to characterise the very pure monomer, while BET, TGA, UV-DRS, XRD, XPS, TEM, and SEM were employed to conduct a thorough analysis of the catalyst. The results of the BET test showed that the pore volumes varied between 0.19 and 0.015 cm³/g. With strong activity maintained after 13 consecutive cycles, the catalyst proved to be recyclable. There was also a successful recovery of the ethylene glycol used in the glycolysis step, and gas chromatography verified its purity. The results show that shape-engineered, metal-modified ZnO catalysts can be used to depolymerise PET in an efficient and recyclable way, which could lead to more sustainable monomer recovery and better chemical upcycling methods.

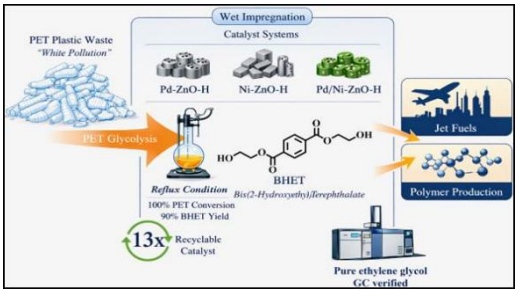

Fig. 1. Efficient PET glycolysis to BHET over the Pd-Ni supported ZnO nanocatalysts.

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Computational modeling to achieve targeted, effective delivery and theranostic capabilities

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Abstract: TBI remains a major therapeutic challenge due to poor blood brain barrier permeability and off-target toxicity of promising anti-amyloid agents [1]. Chalcone-based composites exhibit potent amyloid-β (Aβ) target capability [2]. Most anti-amyloid drugs have limitations, which necessitates sophisticated nanocarriers like PLGA nanoparticles as carriers [3]. Computational modeling offers a cost-effective, mechanistically rigorous method to design and optimize polymeric nanoparticle formulations [4]. The small molecule amyloid inhibitors were taken, each modeled against a chalcone-conjugated PLGA nanoparticle. This study aims to predict drug affinity and effective drug loading in nanoparticles using in silico tools. A hierarchical computational workflow was implemented in Material Studio. First, Monte Carlo adsorption simulation using the adsorption locator module assessed drug adsorption on the polymer carrier [5]. Next, Flory-Huggins-based blend docking rapidly screened polymer drug miscibility, generating interaction parameters (χ) to rank carrier systems. Systems with $\chi < 50$ and more negative adsorption energies were advanced to 500 ps NPT molecular dynamics. The multistage computation filtered the promising polymeric drug carrier candidates, reducing overall computational expense while preserving dynamic realism. Blend docking identifies high-miscibility candidates, and MD simulations validate encapsulation stability, binding affinity, and also controlled-release behavior. Drug-polymer interaction mechanism and nanocarrier flexibility were characterized, providing molecular-level insights into drug loading capacity. This work provides integrated in silico approaches combining adsorption modeling, blend docking, and molecular dynamics to systematically analyze the rational design of nanocarrier materials, a targeted drug delivery system for CNS disorders.

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Effect of Cation Substitution in Spinel MFe_2O_4 and Its Integration with NiCo LDH toward Efficient Hydrogen Evolution Catalysis

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Abstract: Developing efficient and affordable electrocatalysts for green hydrogen production is essential to address rising energy demands and environmental challenges. In this work, a $MnFe_2O_4$/NiCo layered double hydroxide (LDH) heterostructure electrocatalyst was synthesized on Ni foam through a simple in situ hydrothermal method for enhanced hydrogen evolution reaction (HER) performance. Comparative analysis of cation-substituted ferrites ($MnFe_2O_4$, $NiFe_2O_4$, $ZnFe_2O_4$) revealed that $MnFe_2O_4$ offers superior catalytic activity due to its favorable cation distribution, improved conductivity, and abundant redox-active sites. Integrating $MnFe_2O_4$ with NiCo LDH nanosheets significantly boosted charge transfer, active site exposure, and proton adsorption–desorption kinetics. The optimized $MnFe_2O_4$/NiCo LDH (30 wt%) composite achieved an overpotential of 240 mV at 10 mA cm^{-2} and a low Tafel slope of 56 mV dec^{-1} in 1.0 M KOH. This strong synergistic coupling and robust structural stability highlight its potential as a high-performance, non-noble metal electrocatalyst for sustainable water splitting and green hydrogen production.

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Intervention of hIAPP amyloid aggregation by smart post-transmuting anti-amyloidogenic peptidomimetics

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Abstract: hIAPP, human islet amyloid polypeptide, aggregates have been implicated in the development of type 2 diabetes mellitus (T2DM). As a prelude to developing a potential cure for T2DM, researchers worldwide have employed various strategic molecular entities to target β-sheet-rich hIAPP aggregates, known as disruptors, or to prevent the self-assembly of hIAPP, known as inhibitors. Peptide-based strategies are at the forefront. Most β-sheet breakers have a pre-installed breaker element, notably Proline. Here, we describe a different approach that works in a pro-drug fashion—the use of the infamous aspartimide formation. The designed smart peptides sneak into the aggregating system as standard peptides and undergo various aspartimide-induced chemical transformations, developing into an anti-amyloidogenic agent. The peptide develops a pre-programmed kink via aspartimide formation. The kink misaligns the β-sheet topology of the hIAPP aggregates, significantly disrupting them. The reaction cascade is followed by racemization and nucleophilic ring opening by water, resulting in the formation of L-α/β and D-α/β aspartyl peptides. The L-peptides and D-isopeptides are anti-amyloidogenic. Moreover, the negative charges on such peptidomimetics improve solubility and recognisability. The strategy could be a promising leap toward developing therapeutics for amyloidogenic type 2 diabetes mellitus (T2DM). This study will also help to understand the aggregation-disaggregation mechanism of hIAPP.

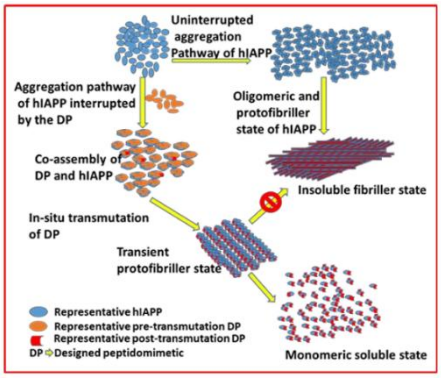

Figure 1: Graphical representation of the probable mode of action of the designed smart peptidomimetics

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Static Magnetic Fields Reverse High Glucose-Induced Cellular Damage and Pathological Protein Aggregation In Vivo

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Abstract: Hyperglycaemia disrupts mitochondrial function, elevates oxidative stress, and impairs proteostasis, thereby promoting metabolic dysfunction and neurodegenerative complications. Using an in vivo Caenorhabditis elegans model, we found that hyperglycaemia significantly reduced mitochondrial area, perimeter, and branching, accompanied by developmental delay, reduced body size, and impaired organismal fitness. Exposure to a 70 mT static magnetic field completely restored mitochondrial network morphology and normalized growth. This recovery was associated with a marked reduction in reactive oxygen species to near-control levels, indicating ROS attenuation as a central underlying mechanism. In addition, magnetic field treatment significantly reduced lysosomal enlargement, lysosomal aggregation, and the accumulation of pathogenic protein aggregates, including α-synuclein and huntingtin. Collectively, these findings demonstrate that static magnetic fields restore organelle homeostasis, alleviate proteotoxic stress, and represent a promising non-invasive therapeutic strategy for hyperglycaemia-induced cellular dysfunction and neurodegenerative pathology.

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Hydrogen-Bond Gating of Interfacial Capacitance in Amine-Rich Hybrid Interfaces for Redox-Free Ionic Recognition

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Abstract: Continuous, selective ion detection in aqueous media without redox mediation remains an outstanding challenge in electrochemical sensing. Here, we introduce a hydrogen-bond-gated, non-faradaic charge-transduction mechanism that enables real-time selective halide detection (F- ion) under ambient conditions. The amine-rich electroactive interface, constructed by integrating polyethyleneimine (PEI) onto UiO-66-NH_2 MOF (metal-organic framework), functions as a redox-inactive yet ion-responsive hybrid platform. Under applied bias, $F^{-}\cdots H$ interactions at the interface modulate interfacial capacitance, producing a distinct, reversible signal that allows continuous monitoring at pH 7. The optimized hybrid achieves a detection limit of 0.2 ppm with exceptional selectivity for F^- over competing anions (Cl^-, Br^-, I^-, NO_3^-, CO_3^{2-}, CH_3COO^-), supported by DFT-derived charge-polarization analysis confirming H-bond driven stabilization. The system maintains stable operation over >25 h (250 cycles) and accurately quantifies F- ions in real water samples (real-time detection of F- ions in tap and drinking water down to ~1 ppm). This study establishes H-bond mediated modulation of interfacial capacitance as a design principle for redox-free amperometric electrochemical sensing, offering a versatile platform for responsive hybrid materials and adaptive ionic interfaces.

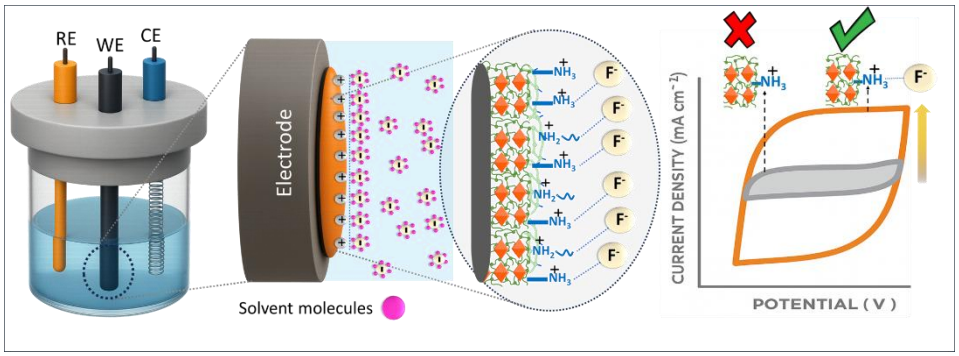

Figure 1: Schematic representation showing the electrochemical capacitive F^- sensing on the UiO-66-NH_2/PEI electrode surface.

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Copper nanocluster-mediated degradation of toxic organic dyes: a sustainable approach to water remediation

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Abstract: Organic pollutants, particularly toxic dyes discharged in large quantities by the textile and food industries, have attracted considerable scientific attention due to their environmental persistence and detrimental effects. Metal nanoclusters (NCs), owing to their redox-active metal cores and tunable surface properties, represent promising candidates for the efficient degradation of such pollutants. In this study, we report an efficient protocol for the degradation of Rhodamine B (RhB) and Methylene Blue (MB) using cysteine-capped copper nanoclusters (Cys-Cu NCs) in the presence of hydrogen peroxide (H_2O_2), without any external stimuli. The degradation, carried out under neutral pH and aqueous conditions, was monitored using UV-visible spectroscopy and showed approximately 97% degradation of both dyes (20mM) within 90 minutes, accompanied by complete decolourization of the solutions. Characterization of the degradation products using LC-MS, ^{1}H NMR, and ion chromatography confirmed the complete mineralization of the dyes into non-toxic species. Control and free-radical scavenging experiments confirmed that the process proceeds through the synergistic action of Cys-Cu NCs and H_2O_2, primarily involving reactive oxygen species (ROS) such as hydroxyl ($^{\cdot}OH$) and superoxide ($^{\cdot}O_2^-$) radicals, thereby elucidating the underlying degradation mechanism. Comparative studies with other metal nanoclusters highlight that the superior activity of Cys-Cu NCs arises from the intrinsic redox property of copper, which plays a pivotal role in ROS generation and dye degradation. Kinetic analyses revealed that RhB and MB follow distinct degradation pathways. Furthermore, degradation studies performed at varying dye concentrations, larger reaction volumes, and in real water samples demonstrated the robustness and practical applicability of the developed method. Overall, the Cys-Cu NC-mediated degradation offers a sustainable and efficient approach for the remediation of dye-contaminated water.

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σ-Aromaticity in Trinuclear and Tetranuclear Transition Metal Carbonyl Clusters: A Comprehensive Magnetic and Electronic Analysis

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Abstract: Metal carbonyl complexes and clusters gain stability through aromaticity.[1,2] In this study, a series of trinuclear and tetranuclear metal carbonyl clusters with the general formulas $M_3(CO)_{12}$, $M_4(CO)_{14}$, $M_4(CO)_{15}$, $M_4(CO)_{16}$, (where M = Fe, Ru, and Os), and isolobal trinuclear clusters $[M_3(CO)_{12}]^{3-}$ (where M = Mn, Tc, Re), and $[M_3(CO)_{12}]^{3+}$ (where M= Co, Rh, Ir) are considered. Density Functional Theory (DFT) was employed for all the geometry optimisation. Aromaticity was assessed using magnetic criteria, specifically Nucleus-Independent Chemical Shifts (NICS)[3] and Gauge-Including Magnetic-Induced Ring Currents (GIMIC). Our findings indicate that all cluster types exhibit σ-aromaticity. Among all the clusters studied, the $Fe_3(CO)_{12}$ cluster displayed exceptionally strong σ-aromaticity, evidenced by highly negative NICS values and a significant diatropic current, as confirmed by GIMIC analysis. Further analysis, utilising NICS-scan, Electron Density of Delocalized Bonds (EDDB), Energy Decomposition Analysis with Natural Orbitals for Chemical Valence (EDA-NOCV), confirmed the presence of pronounced σ-aromaticity in these metal carbonyl clusters.

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Surface-Selective PbTe Passivation for Suppressing Halide Segregation and Enhancing Environmental Stability of Mixed-Halide Perovskites

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Abstract: Mixed-halide lead perovskites are promising materials for optoelectronic applications; however, their practical implementation is hindered by light- and moisture-induced halide segregation, which leads to spectral instability and performance degradation. In this work, a surface-selective PbTe passivation strategy is employed to suppress halide segregation and enhance the environmental stability of mixed-halide perovskites. The incorporation of PbTe at the surface is found to significantly influence the photophysical behavior of the material. Under continuous UV illumination, the passivated films exhibit reduced spectral shifts and improved photostability, indicating effective suppression of light-induced halide migration. Furthermore, stability studies under moisture exposure demonstrate enhanced resistance to environmental degradation, suggesting improved structural robustness. These improvements are attributed to effective passivation of surface and grain-boundary defects, which are known to act as initiation sites for halide migration. By minimizing defect-assisted ion movement, the PbTe treatment stabilizes the emission characteristics of the material. This study highlights the importance of surface engineering as a viable route to control halide segregation and improve the operational stability of mixed-halide perovskites.

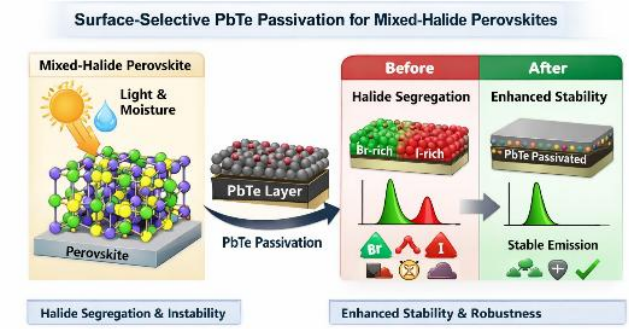

Figure 1. Graphical representation of PbTe-mediated passivation suppresses halide migration and phase segregation, enhancing photostability and moisture resistance in mixed-halide perovskites.

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Carbon Dioxide Absorption in Deep Eutectic Solvents as a Function of Water: A Molecular Dynamics Simulation Study

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Abstract: Carbon dioxide (CO_2) is one of the major components of flue gases, contributing 10-15 vol% of all gases. Aqueous amine solvents are typically used for carbon capture through absorption. However, there are major shortcomings to such a process, including high energy cost during regeneration, corrosiveness, and solvent loss. Hence, new-generation solvents, such as ionic liquids (ILs) and deep eutectic solvents (DESs), are now being studied extensively to replace them. DESs are easy to prepare, less hazardous, and less expensive than ILs, and can therefore be used as solvents in the gas-capturing process. However, the high viscosity of DESs is a major hindrance to their widespread applications, which can be overcome by adding water. The main challenge is to find the balance between DES viscosity and CO_2 solubility, as increased water content in the DES can reduce both. Molecular dynamics (MD) simulation can be used to calculate gas solubility in various solvents using the free-energy perturbation method and to provide insights into the interactions within the system. Herein, we studied the CO_2 absorption in two DESs, one hydrophilic and one hydrophobic, at three different water contents (5 wt%, 10wt% and 15 wt%) through MD simulations. The free energy of solvation decreases gradually with addition of water and becomes positive at 15 wt% of water. The interaction of anion with CO_2 is prominent in both the systems.

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Decoding Nitrogen Reduction Pathways on Transition Metal Electrocatalysts: A DFT Study

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Abstract: The conventional Haber–Bosch process for ammonia synthesis operates at extreme temperatures and pressures, contributing significantly to global energy consumption. As a sustainable alternative, the nitrogen reduction reaction (NRR) enables the electrocatalytic, photocatalytic, or enzymatic production of ammonia under ambient conditions. Among these, electrochemical NRR using transition metal catalysts has emerged as a promising route due to its tunability and potential for decentralized synthesis. NRR can proceed via two primary mechanisms: dissociative, in which the N≡N bond is cleaved before hydrogenation, and associative, in which hydrogenation occurs before bond dissociation. The associative mechanism further divides into alternating and distal pathways, depending on the sequence of hydrogen addition to the nitrogen atoms. In this work, the adsorption energies of important NRR intermediates on different transition metals on the (111) and (110) surfaces for the FCC crystal structure and on the (0001) surface for the HCP crystal structure are determined using density functional theory (DFT). The chemical route is predicted by the adsorption energies of intermediates, including 2*N, *NNH, *NHNH, and *NNH_2. Comparing the adsorption values of 2*N and *NNH reveals whether the N_2 molecule has a propensity to dissociate or not before hydrogenation. The more stable intermediate between *NHNH and *NNH_2 requires that the associative mechanism's route be either distal or alternating. These energies serve as descriptors to predict the most favorable reaction pathway. The insights from this computational analysis deepen understanding of NRR mechanisms and guide the rational design of efficient electrocatalysts for ambient-condition ammonia synthesis.

Keywords: Nitrogen Reduction Reaction (NRR), Ammonia, DFT, Adsorption Energy

Bio-based Materials for Female Hygiene: Advancing Sustainability in Menstrual Hygiene Products

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Abstract: Synthetic sanitary napkins, an indispensable part of women's menstrual hygiene, are chemically composed of acrylates.[1] They generally have four layers: the top layer, the acquisition and distribution layer, the absorbent core and the backsheet. The layers other than the absorbent core are, typically composed of polyethylene and polypropylene. Conventional disposable sanitary napkins are 90% plastic, which takes approximately 700-800 years to decompose.[2] Moreover, these products can release various chemicals like volatile organic compounds, fluorides, phthalates, and dioxins, which may trigger hormonal imbalances, reproductive health issues, and even cancer. On the contrary, bio-based materials offer a viable solution, owing to their biocompatibility, biodegradability, absorbency, and cost-effectiveness. Bio-based materials like polysaccharides and proteins show remarkable absorbance and retention properties that make them potential candidates in this field. In addition to them, the lignocellulosic fibres, such as banana, bamboo, jute, water hyacinth and hemp fibres, are biodegradable and possess good absorption properties, leveraging their high cellulosic content.[3] Switching to bio-based alternatives will reduce the environmental burden and CO_2 emissions, and provide women with the *right to safe periods*.

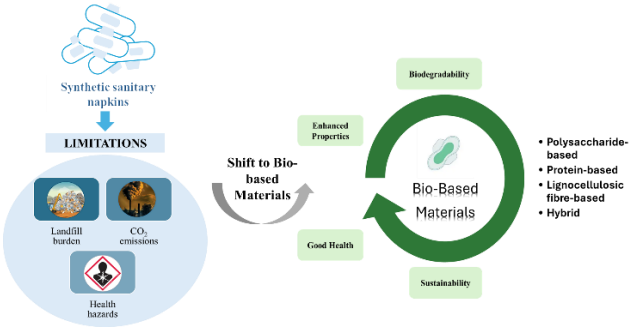

Figure 1. Transition from synthetic to bio-based sanitary napkins for menstrual hygiene.

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Cyclodextrin-Assisted L-Cysteine–Capped Copper Nanoclusters for Dual Detection of Hg^{2+} and Ag^{+}

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Abstract: The sensitive and selective detection of toxic heavy metal ions in aqueous matrices remains an important analytical challenge. Here, a rapid and environmentally benign photoluminescence (PL) sensing platform was reported for the dual detection of Hg^{2+} and Ag^{+} ions using γ-cyclodextrin-assisted L-cysteine-capped copper nanoclusters (γ-CD–Cys–Cu NCs). Introduction of γ-cyclodextrin into pre-synthesized Cys-Cu NCs instantaneously induced controlled aggregation, resulting in pronounced emission enhancement with intense blue-green PL (λ_{em} = 500 nm) upon excitation at 370 nm. Exploiting the strong coordination affinity of exposed thiol groups toward soft heavy metal ions, the aggregation-enhanced γ-CD–Cys–Cu NCs were employed as a single-fluorophore probe for the selective sensing of Hg^{2+} and Ag^{+} ions. Both analytes induced efficient PL quenching (~90% at 250 μM), with limits of detection as low as 25 nM, well below the permissible limits for drinking water. Intensity-based and time-resolved PL studies revealed a combined static and dynamic quenching mechanism, consistent with metal–thiolate complex formation and concentration-dependent collisional processes. Dynamic light scattering (DLS) and high-resolution transmission electron microscopy (HRTEM) analyses further indicated that the metal-ion-triggered disassembly of the aggregated nanoclusters correlated with structural reorganization and PL quenching. Notably, Ag^{+} additionally induced a distinct colorimetric response enabling complementary visual identification. The sensing platform enabled accurate quantification of Ag^{+} and Hg^{2+} in real water samples, demonstrating reliable analytical performance in real matrices. Overall, this work establishes γ-CD–Cys–Cu NCs as an efficient, selective, and practical single-fluorophore platform for dual heavy-metal detection in complex aqueous environments.

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Biochemical And Mechanistic Characterization of Enzymes Involved in Gourgerotin Biosynthetic Pathway

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Abstract: Natural products and their derivatives remain vital sources of antibacterial, antiviral, anticancer, and antifungal agents, yet the rise of antimicrobial resistance (AMR) threatens their effectiveness. This underscores the urgent need for antibiotics with new structures and mechanisms. Gougerotin is a broad-spectrum dipeptidyl nucleoside antibiotic that inhibits bacterial protein synthesis and also exhibits anticancer, antiviral, anthelmintic, antimycoplasma, and acaricidal activities. Structurally, it consists of cytosine, 4-amino-4-deoxyglucuronamide, and a sarcosyl-D-serine dipeptide. A biosynthetic gene cluster (BGC) for gougerotin has been identified in *Streptomyces graminearus*, and a preliminary pathway has been proposed, though none of the enzymes has been characterized in vitro. The pathway suggests that GouF catalyzes formation of cytosylglucuronic acid (CGA), followed by oxidation (GouA) and transamination (GouH) to yield 4′-amino-CGA. In parallel, D-serine is derived from 3-phosphoglycerate via GouL, GouI, and GouG, while GouN methylates glycine to sarcosine. These amino acids are activated by GouK and sequentially transferred by GouJ to form yunnanmycin, which is finally converted to gougerotin by GouB.

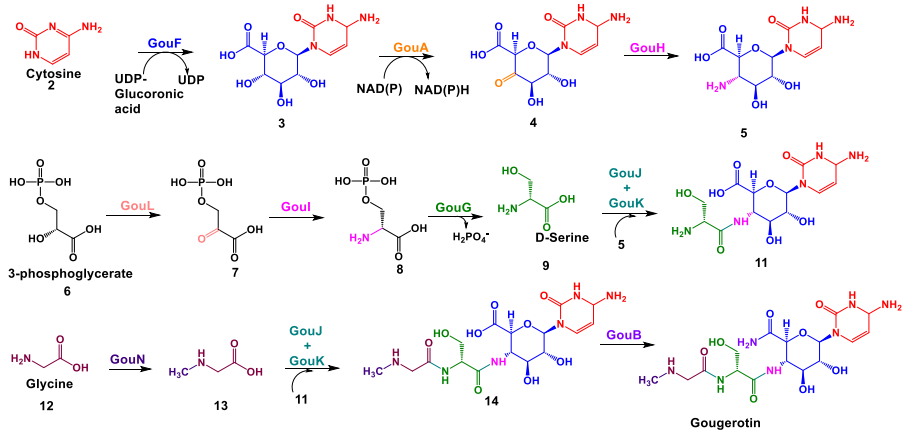

Figure 1. Proposed biochemical pathway of gougerotin

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Oxygen vacancy-engineered WO_{3-x} for light-assisted hydrogen evolution from ammonia-borane

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Abstract: Hydrogen (H_2) is a clean and sustainable energy carrier that plays a pivotal role in the development of renewable energy technologies. This study focuses on the development of tungsten oxide-based hybrid plasmonic catalysts for hydrogen production from catalytic dehydrogenation of ammonia borane (AB). The introduction of oxygen vacancies in WO_3 improves the photocatalytic performance through the generation of localized surface plasmon resonance (LSPR) effects, enhanced light absorption, and reduced charge recombination.[1] In this study, the incorporation of Pd nanoparticles on WO_{3-x} further improves the catalytic efficiency due to the synergistic interaction between WO_{3-x} and Pd nanoparticles.[2] The catalyst demonstrated stable activity for up to four cycles. To gain deeper insights into the mechanistic pathway, trapping experiments were carried out and the plausible mechanism is shown in Fig. 1. This study offers a sustainable and efficient pathway for hydrogen production, contributing to the advancement of renewable energy solutions.

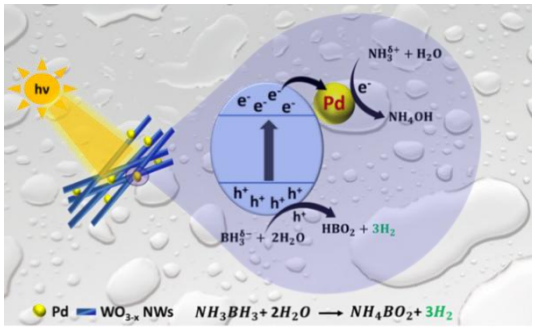

Figure 1. Schematics of hydrogen generation from AB on Pd/WO_{3-x}.

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From Multifunctional Hydrogels to Intelligent Bilayer Dressings: Advanced Strategies for Infected Wound Care

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Abstract: Advanced wound dressings capable of simultaneously managing infection, oxidative stress, tissue regeneration, and real-time wound monitoring are highly desirable for effective wound care. In this work, a series of multifunctional wound dressing platforms with enhanced therapeutic and diagnostic capabilities are developed for infected wound management. Initially, a disulfide-crosslinked chitosan/alginate hydrogel incorporated with iron oxide/selenium nanocomposite (SeIO) and ursodeoxycholic acid (UDC) is fabricated. The developed film exhibits suitable mechanical strength, swelling behavior, and porosity. Furthermore, the system demonstrates significant antioxidant, antibacterial, and cell growth-promoting features. Subsequently, to better mimic the hierarchical structure of native skin, a multifunctional bilayer dressing is developed by integrating a chitosan/gelatin-based electrospun nanofibrous layer with a UDC/carbon dots-loaded chitosan/alginate-based hydrogel layer. The bilayer architecture significantly improves the therapeutic features compared to the monolayer. Finally, the work is extended toward the development of an intelligent bilayer wound dressing with real-time monitoring capability. The system consists of an ionic liquid-loaded polycaprolactone nanofibrous layer and a hydrogel layer incorporated with UDC and a Himalayan flower extract. Besides exhibiting therapeutic features, the dressing displays pH-responsive colorimetric behavior, enabling non-invasive wound monitoring. Overall, this work demonstrates the progressive development of multifunctional and intelligent wound dressing platforms that combine therapeutic efficacy with biomimetic architecture and real-time monitoring capability, highlighting their potential for advanced wound management applications.

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Implications of CeO2 on physical, optical, spectroscopic and thermal properties of alkali Zinco-boro-tellurite Glasse for optical display applications

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Abstract: A new set of glass containing zinc oxide, borate, tellurite and Sodium oxide doped with CeO2 were prepared by applying melt quenching method. The prepared glasses (BTZNC) analysed thoroughly to check their suitability for the display applications in terms of XRD, SEM, EDAX, FTIR, Physical and optical properties, thermal and photoluminescence properties. The nanocrystalline and the transparency nature of the glasses were revealed by XRD and UV-Visible spectroscopy, respectively. The thermal study by DSC denotes the good thermal stability of BTZNC glasses which ranges from 90 to 121 ℃. Microstructural properties and purity of glasses are revealed by the SEM and EDAX. Physical properties like density, molar volume were determined by using mathematical equations. The density of the glasses varied from 2.920 to 2.990 g/cm3. The FT-IR confirms the conversions BO3 to BO4 units and presence of non-bridging oxygens. The energy bandgap and refractive index of the glasses are varied from 3.079 to 2.793 eV and 2.365 to 2.455, respectively. The distinct emission peak was seen for the BTZNC -3 glass at 454 nm. The influence of CeO2 was properly noticed for the thermal, optical, physical properties of glass. The variations in the optical properties such as optical basicity, metallization criterion and electronic oxide polarizability are caused with addition of CeO^2. The found outcomes of this novel set of glass indicates that BTZNC glasses are suitable for light-emitting devices.

Key Words: Alkali zinco-tellurium borate glasses; FT-IR, Optical basicity, Metallization criterion; light-emitting devices.

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Electrochemical sensors based on MXene-Laser Induced Graphene (LIG) Heterostructures for Ultra-sensitive Fluoride Detection in Drinking Water

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Abstract: Fluoride contamination in groundwater is a significant public health issue. As per WHO standards, excessive fluoride levels (>1.5 mg/l) lead to severe health issues such as dental fluorosis (dark yellow pigmentation of teeth), skeletal fluorosis (bone deformities), pain in back and joints, weakened bones, bending of bones and stiffs joints with difficulties in walking along with other health problems such as low hemoglobin levels, gastrointestinal problems, neurological disorders, bone resorption, skin rashes, urinary tract malfunctioning, etc. Therefore, detecting fluoride in water is highly important. Several methods, such as ion-selective electrode (ISE), graphene-based fluorescent sensors, colourimetric sensors etc have been developed for the detection of fluoride in water. Fluoride ion-selective electrode (ISE)-based sensors are commercially available and used widely, but these ISEs typically use solid-contact electrodes that may suffer from low stability and low detection limits. Graphene-based fluorescent sensors are not used widely in practice and do not meet practical requirements such as stability and low detection limits. Therefore, alternative methods are needed for the detection of fluoride. 2D MXenes and laser-induced graphene (LIG) have drawn significant attention as nanomaterials for sensing applications. MXenes exhibit unique properties such as hydrophilicity, surface chemistry with abundant surface functional groups, high electrical conductivity, and the ability to form colloidal dispersions and thus hold great potential for sensing applications. Graphene, a well-known 2D material, is also extensively studied and used for sensing applications. The advantages of MXenes over graphene for sensing applications include greater electrical conductivity, higher chemical activity, and transfer of analyte ions through interlayer spaces. The heterostructure of MXene with graphene (MXene-G) combines the merits of both materials and promises enhanced flexibility and improved sensing performance. In this study, LIG has been prepared directly onto solid and flexible substrates using a simple CO_2 laser writing system. MXene was drop-casted onto it to form MXene -LIG heterostructure and was demonstrated as an ultra-sensitive Electrochemical sensor. The sensor exhibits outstanding performance in the detection of fluoride in drinking water. In phosphate buffer solution, the MXene-LIG heterostructure achieves a remarkable LOD of 0.01 µM for fluoride, with high sensitivity (1.268µA μM^{-1}). The electrode demonstrates excellent selectivity, repeatability, and reproducibility, underscoring its potential as a ultrasensitive, robust and versatile electrochemical sensing platform, establishing MXene-LIG heterostructure as a promising candidate for real-time detection of fluoride in drinking water.

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Facile Development of Hierarchical Carbon Nanostructure for Energy Storage Applications

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Abstract: The Development of high surface area electrodes at low cost remains a critical challenge in advanced energy storage systems. Metal-organic frameworks (MOFs) have emerged as promising precursors for designing next-generation electrode materials due to their tunable porosity and structural versatility.[1] In this study, we report the fabrication of binder-free, self-supported, highly porous and cost-effective electrode with a significantly enhanced specific surface area. A porous graphitic nanoleaf (P-GNL) architecture was synthesized from Co-MOF grown on carbon cloth (Co-MOF@CC), followed by acid etching to induce hierarchical porosity. Subsequently, a bimetallic Zn-Cu MOF[2] was directly grown on the P-GNL substrate (Zn-Cu/P-GNL@CC) and subject to secondary pyrolysis process to further improve electrical conductivity and structural stability. The as-prepared electrode was evaluated in a symmetric supercapacitor configuration, demonstrating a high areal capacitance of 60 mF cm^{-2} at a scan rate of 10 mV s^{-1}. The enhanced electrochemical performance is attributed to the synergistic effects of the hierarchical porous structure, high surface area, and improved charge transport pathways. These findings highlight the potential of MOF-derived hierarchical nanostructures for the development of efficient, scalable and low-cost energy storage devices.

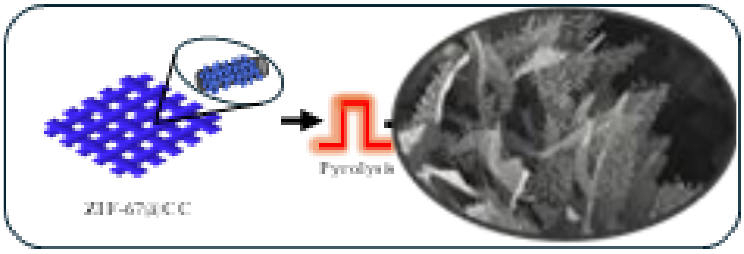

Figure 1. Schematic of P-GNL Catalyst Synthesis.

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Development of a cost-effective thin-film microextraction device for the detection of agrochemicals from water

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Abstract: Agrochemicals are widely used during the farming process to protect crops from pests and improve agricultural productivity. These pesticides accumulate in regular water sources, posing potential hazards to the environment and human health. To simplify the detection of agrochemicals, thin-film solid-phase microextraction (TF-SPME) analytical devices were developed which is both cost effective and sensitive. The results showed that TF-SPME patches were able to extract pesticides with a LOD of 0.1 ng/mL. The developed technique aligned with the green analytical principles due to low solvent use, minimal waste generation, and energy efficiency. The AGREE score emphasized its strong connection with green chemistry, while complex GAPI and BAGI validated its environmental compatibility and user safety. This microextraction TF-SPME device may be applicable for the rapid quantification of agrochemicals from water resources to safeguard human lives.

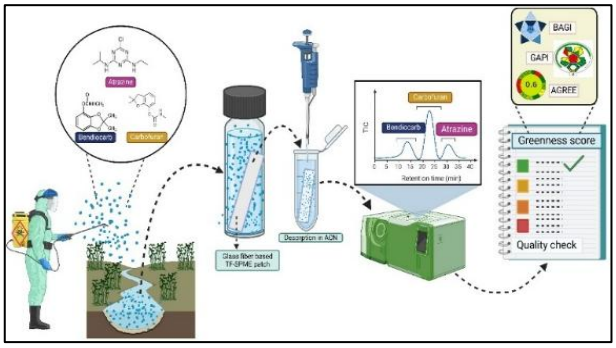

Figure 1. Graphical illustration of pesticide extraction and detection from water using a thin film microextraction device

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Development of an Efficient Ru/CoO_x Electrocatalyst for Alkaline Hydrogen Evolution

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Abstract: Efficient electrocatalysts for the hydrogen evolution reaction (HER) are critical for the advancement of sustainable water splitting technologies. Despite the mature infrastructure of alkaline electrolyzers, widespread commercialization is hindered by high hydrogen production costs, primarily due to reliance on expensive electrocatalysts.[1] Recently, noble metal-dispersed catalysts (single atom or cluster) have gained significant attention due to their maximum atom utilization, offering a promising pathway to reduce costs.[2] Herein, we report a robust synthetic strategy utilizing graphene oxide as a template and precursor to prepare well-dispersed metal oxide nanoparticles embedded within a carbon network. Using this approach, we developed a highly active electrocatalyst, ruthenium-anchored cobalt oxide (Ru/CoOx), for alkaline HER. The resulting Ru/CoO_x catalyst exhibits outstanding performance, requiring an overpotential of just 40 mV to achieve a benchmark current density of 10 mA cm^{-2} in alkaline conditions. Furthermore, owing to the optimized low noble-metal content, the catalyst delivers an exceptional mass activity of ~6 A mg^{-1} at an overpotential of 166 mV, surpassing that of commercial Pt/C. This research highlights that the strong synergistic effects between the metal and the metal oxide can significantly accelerate electrocatalytic hydrogen evolution in an alkaline medium.

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A Fast Route to Fluorinated Branched Aliphatic Amino Acids and Their Radiofluorinated Analogues

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Abstract: Fluorinated branched aliphatic amino acids are valuable targets in both synthetic chemistry and PET tracer development.[1] We have identified a fast fluoride-based synthesis of fluorinated branched aliphatic amino acid derivatives that is also amenable to radiofluorination. This approach enables efficient access to radiolabeled amino acid scaffolds relevant to PET imaging and is applicable to homoleucine and related branched aliphatic amino acid substrates. The short reaction time and useful radiochemical yield demonstrate the potential of this platform for practical radiotracer synthesis. Overall, this work provides a streamlined route to fluorinated branched aliphatic amino acids with relevance to both synthetic and radiochemical applications.

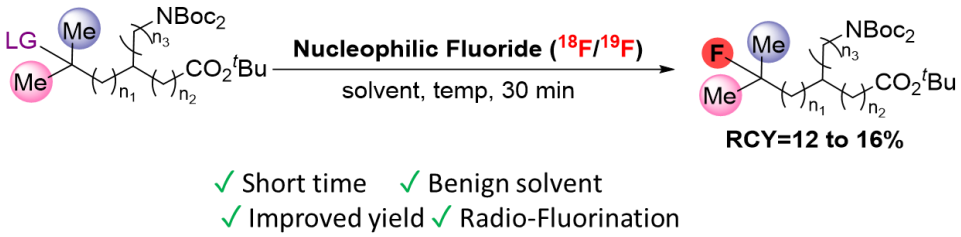

Figure 1. Cold fluorination and radiofluorination

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Influences of Hydrophobic Groups on Intermolecular Interactions and Terahertz Response of Urea and Its Derivatives in Water

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Abstract: Intermolecular interactions in aqueous solutions of small organic solutes play crucial roles in many aspects [1]. Terahertz (THz) spectroscopy has proven to be a useful tool for probing these intermolecular interactions in aqueous solutions [2,3]. Theoretically, THz spectra of aqueous solutions have been reported in previous studies [4-7]. In this work, we have investigated the terahertz absorption spectra of aqueous solutions of urea and its dimethyl derivatives (1,1-DMU and 1,3-DMU) through molecular dynamics simulations using polarizable AMOEBA forcefields for both water and the solutes. We calculated the total THz absorption spectra for these systems, including the difference absorption spectra of the solutions and dissected the total spectra into their individual components. The water-only contribution shows negative features in the THz spectrum due to disruption of the hydrogen bond network of water, and the effects are more pronounced for the aqueous solution of 1,1-DMU. In the THz spectra arising from solute-water interactions, the aqueous solution of 1,1-DMU and 1,3-DMU exhibit lower intensities than urea, which shows that the dimethyl substitution of urea decreases the interaction of the solutes with water. The vibrational density of states (VDOS) of center of mass of the solutes in the solutions, and atom-specific VDOS, provided further insights into how individual solute atoms contribute to the observed spectral features. Aqueous solutions of the three solutes are found to exhibit distinct spectral behaviors originating from dimethyl substitution in the urea molecule.

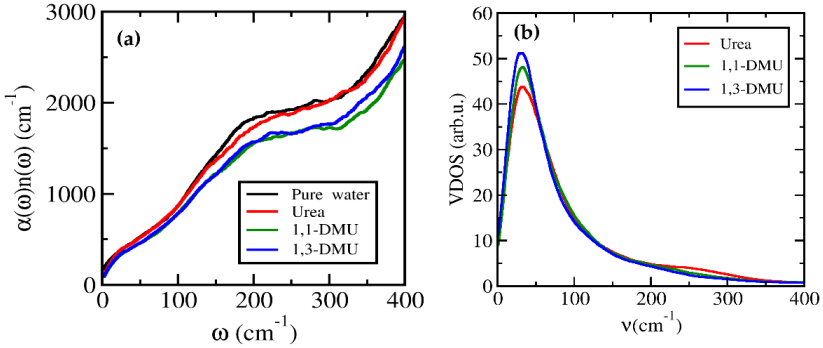

Figure 1. (a) Total terahertz absorption spectrum of water and aqueous solutions of urea, 1,1-DMU and 1,3-DMU. (b) Center of mass vibrational density of states of urea, 1,1-DMU, and 1,3-DMU in their aqueous solutions.

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Electrochemical immunosensing of AQP-4 IgG biomarkers using SnS_2@gC_3N_4 nanocomposite for Neuromyelitis Optica diagnosis

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Abstract: Neuromyelitis Optica (NMO) is a rare autoimmune disorder affecting the optic nerves and spinal cord, with aquaporin-4 (AQP4) antibodies serving as a specific diagnostic biomarker. Early detection of AQP4-IgG is essential for effective disease management.1 In this work, an electrochemical immunosensor based on a SnS2@g-C3N4 nanocomposite-modified electrode was developed for sensitive AQP4-IgG detection. The nanocomposite was synthesized via a one-step hydrothermal method and characterized using XRD, Raman, FTIR, SEM, and TEM. The modified electrode showed enhanced electrochemical performance due to improved conductivity and increased surface area. Cyclic voltammetry (CV) analysis revealed a low limit of detection (LOD) of 0.046886 µM/mL. The sensor demonstrated excellent stability for up to 60 days, rapid response time (20 s), and good reusability over 15 cycles. Interference studies with biomolecules such as glucose, urea, and ascorbic acid showed high selectivity.2 Additionally, real sample analysis in spiked human serum indicated good recovery with minimal matrix effects. Overall, the developed immunosensor shows strong potential for reliable detection of AQP4 antibodies in NMO diagnosis.

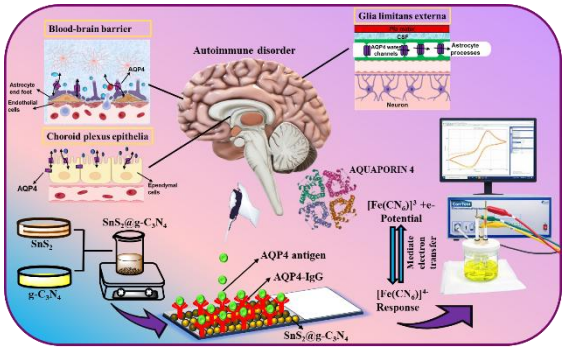

Figure 1. Graphical abstract of the process performed for this electrochemical sensing

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UiO-66(Zr):Tb^{3+},Eu^{3+}/PVDF Composite Films as Optical Thermometers for Temperature Sensing above Room Temperature

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Abstract: Luminescent thermometry enables remote, non-contact temperature sensing in environments where conventional thermometers are ineffective[1]. Here, a self-referenced nanothermometer was developed by incorporating terbium (Tb^{3+}) and europium (Eu^{3+}) ions into the zirconium-based UiO-66 metal–organic framework (MOF). Crystalline UiO-66 nanoparticles (~60 nm) showed characteristic Tb^{3+} and Eu^{3+} emissions. Temperature-dependent photoluminescence (80–400 K) exhibited a linear Tb/Eu intensity ratio with a maximum relative sensitivity of 0.8 % K^{-1} at 400 K. PVDF composite films showed enhanced sensitivity of 1.2 % K^{-1} at 353 K, attributed to reduced nanoparticle aggregation. The UiO-66(Zr):Tb,Eu nanothermometers enable lanthanide-based, sensitive temperature detection above 300 K, with better sensitivity compared to previously reported lanthanide-terephthalate frameworks[2]. Further, embedding the nanoparticles in a PVDF polymer matrix improves sensitivity and stability and enables potential applications in microfluidic and lab-on-a-chip systems.

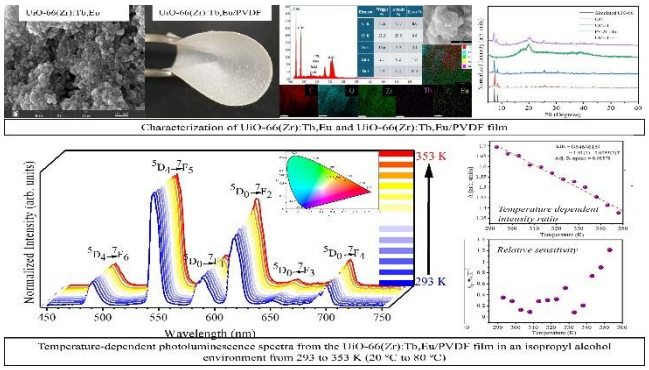

Figure 1. UiO-66(Zr):Tb,Eu nanothermometers and their temperature sensing performance in a composite PVDF film.

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PPh_3-Promoted Sulfa-Michael Addition-Driven Cyclization: A Divergent Route to Access Spirothiochromanone Derivatives

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Abstract: A novel triphenylphosphine-mediated sulfa-Michael addition-triggered cascade reaction has been developed for an efficient synthesis of spirothiochromanone derivatives using 3H-benzo[c][1,2]dithiol-3-one as sulfur surrogate. This transformation initiates with reductive S–S bond cleavage, smoothly delivering a diverse array of spiro 1,3-dimethylbarbiturate thiochromanones and spiro 1,3-indanedione thiochromanones under mild conditions. Current synthetic route features key advantages including operational simplicity, scalability, and excellent functional group compatibility with good to excellent conversions across substrates. Furthermore, this protocol obviates the purification techniques such as column chromatography for the isolation of spiro-adducts, making it a valuable strategy for the construction of complex sulfur-containing spirocyclic scaffolds.[1]

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Highly Diastereoselective Synthesis of *N*,*S*-polyheterocyclic Scaffolds *via* [3+2] Cycloaddition of *N*-phenacylbenzothiazolium Bromides

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Abstract: A highly efficient, metal-free, atom-economical green protocol for the synthesis of *N*,*S*-polyheterocycles *via* dearomative [3+2] cycloaddition of *N*-phenacylbenzothiazolium salts with alkylidene acenaphthylenones and barbiturate-derived alkenes. This reaction tolerates diverse substituents on the acenaphthylenone and barbiturate partners, underscoring its broad scope and providing an efficient method to construct desired cycloadducts in good to excellent yields with high diastereoselectivity. This strategy provides the formation of two C–C bonds with multiple contiguous stereocenters, including one spiro-center, in a one-pot reaction. Significantly, no hydro-quenching, solvent separations, or chromatographic/ recrystallization purifications are required. Overall, this efficient, selective, and eco-friendly strategy offers rapid access to *N*,*S*-frameworks relevant to medicinal chemistry and materials science.

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Tuning the Optoelectronic properties of $MoSe_2$ Nanosheets through Heterostructure Formation with Ag_2Se Nanoparticles

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Abstract: Heterostructure engineering is a powerful strategy for overcoming the intrinsic trade-off between spectral range and carrier transport in photodetectors.[1] Here, we demonstrate a broadband, solution-processable photodetector based on a two-dimensional $MoSe_2$–Ag_2Se heterostructure, which integrates the strong visible absorption and high photogain of semiconducting 2H-$MoSe_2$ with the narrow-bandgap, high-mobility characteristics of Ag_2Se.[2] Structural analysis by X-ray diffraction and transmission electron microscopy confirms intimate heterointerfacing without compromising crystallinity. The resulting type-II band alignment enables ultrafast electron transfer from $MoSe_2$ to Ag_2Se and efficient hole confinement in $MoSe_2$, thereby promoting long-lived carrier populations. Devices exhibit a broad spectral response from 400 nm to 900 nm, a peak responsivity of 1.2 A W^{-1} at -3 V bias, a high detectivity of 8.5×10^{10} Jones, and rise/decay times of 150/268 ms. The synergistic combination of broadband absorption, low dark current, and efficient charge extraction highlights the $MoSe_2$–Ag_2Se heterostructure as a promising candidate for next-generation, low-cost, and scalable photodetection technologies.

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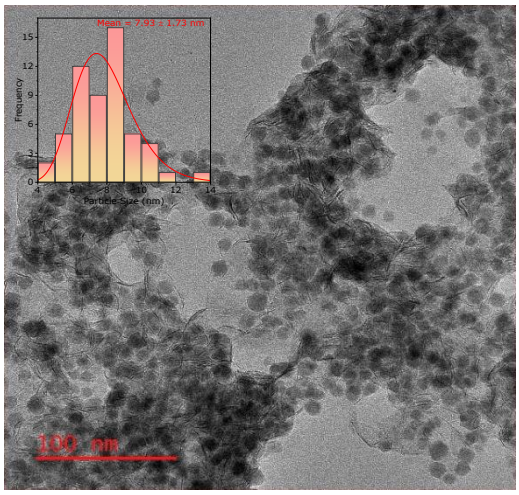

Figure 1. TEM image showing Ag_2Se nanoparticles uniformly distributed on $MoSe_2$ sheet.

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Ru-N^{H}NP Pincer Complex for CO_2 Reduction: Conversion Towards Value-added C_1 Feedstocks

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Abstract: Here in, we prepared a series of Ru-pincer complexes and check their catalytic activity towards CO_2 hydrogenation to formic acid/formate. Highest TON for CO_2 hydrogenation was 1,40,000 achieved using Ru-N$^{t\text{Bu}}$NP$^{i\text{Pr}}$ hydride complex. Mechanistic study highlighted Metal ligand cooperativity plays important role for activation pre-catalyst to form dearomatized active Ru-H species. Active catalyst having dual binding site facilitate the CO_2 hydrogenation by maintaining oxidation sate of central metal ion. Further, organometallic study and DFT calculation supported the formation of reactive dihydride species followed by MLC pathway.

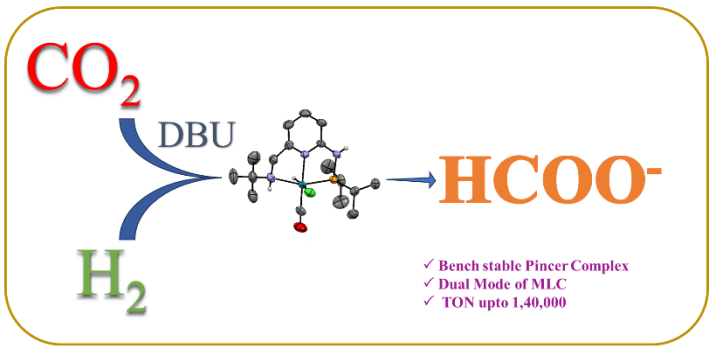

Figure 1. CO_2 to hydrogenation to Formate using Ru-N^{H}NP pincer Complex

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Aqueous Zinc Ion Batteries: A Safer Sustainable Future

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Abstract: Lithium-Ion Batteries are the best player in the field of energy storage devices but its widespread application is constrained by toxic components, high production costs, and safety concerns.[1] Aqueous Zinc-Ion Batteries have emerged as promising alternatives to lithium-ion batteries owing to their high theoretical volumetric capacity (5851 $mAhcm^{-3}$), abundant zinc resources, enhanced sustainability, and the intrinsic safety associated with non-flammable aqueous electrolytes.[2] In the present study, MnO_2 is investigated as a cathode material for Aqueous Zinc-Ion Batteries with the aim of improving specific capacity and overall electrochemical performance. To further enhance the cathodic properties, the MnO_2 is engineered on Graphitic Carbon Nitride (g-C_3N_4), which possesses a layered aromatic polymeric framework.[3] The resulting composite, MnO_2@g-C_3N_4 has delivered a specific capacity of 246 $mAhg^{-1}$, which is higher than that of pristine MnO_2 (221 $mAhg^{-1}$). Moreover, the composite exhibited significant enhancement in reaction kinetics and ion diffusion coefficient. Overall, the enhanced electrochemical performance and improved kinetics of the MnO_2@g-C_3N_4 illustrates its potential as a promising cathode material for Aqueous Zinc-Ion Batteries.

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Chemical Depolymerization of Polylactic acid into Methyl Lactate using Copper Supported Ceria as an Efficient and Reusable Catalyst

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Abstract: Chemical upcycling of plastic waste has attracted attention from all around the world because it offers a sustainable solution to the issue of plastic waste accumulation and helps create a circular plastic economy.[1] One sustainable method of conserving resources and protecting the environment is by the chemical depolymerization and recycling of polylactic acid (PLA). The chemical depolymerization of PLA was investigated using Cu-CeO_2 as a catalyst, yielding methyl lactate (ML) as the product under relatively mild conditions to achieve closed-loop recycling of PLA waste as shown in Figure 1. In this work, we present an environmentally friendly and cost-effective approach for the methanolysis of polylactic acid. The PLA is completely depolymerized in the presence of Cu-CeO_2 catalyst at 140 °C for 8 h. In order to get the best catalytic activity and product selectivity, the reaction condition was optimized. ^{1}H NMR spectroscopy is used to support the detailed depolymerization mechanism. Experiments on a larger scale were also carried out to demonstrate the synthetic utility of the designed reaction protocols. The effectiveness and sustainability of the designed protocols were demonstrated by the evaluation of the green metrics parameters, paving the way for the industrial upscaling of plastic depolymerization. This study offers a sustainable, low chemical input and environmentally friendly method for chemically recycling these plastics.[2]

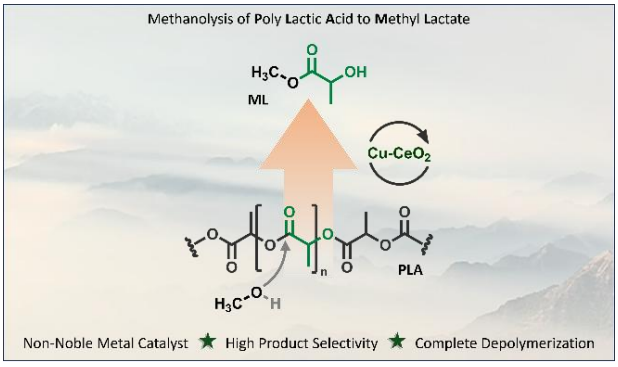

Figure 1. Chemical depolymerization of PLA to ML using Cu-CeO_2 catalyst.

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Tuning surface redox chemistry through trace Ni doping in Cobalt Pyrophosphate ($Co_2P_2O_7$) for high-performance supercapacitors: Experimental and theoretical insights

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Abstract: In The electrochemical performance of cobalt pyrophosphate (Co2P2O7) as a supercapacitor electrode can be markedly improved by trace nickel doping. The optimized Ni-doped $Co_2P_2O_7$ (Ni:Co = 0.1 stoichiometric ratio) electrode exhibits an impressive specific capacitance of 490.2 F g-1 at 1.5 A g-1, significantly surpassing that of pristine Co2P2O7, reflecting enhanced charge-storage capability. To elucidate the underlying mechanism, in situ Raman spectroscopy and X-ray photoelectron spectroscopy (XPS) depth profiling were employed, revealing that the formation of surface Co3+ species promotes reversible redox transitions and accelerates ionic diffusion. However, excessive Ni doping (beyond 0.2 stoichiometric ratio) disrupts this balance, leading to diminished capacitance. These combined experimental and theoretical insights demonstrate that minimal Ni doping effectively tunes the surface chemistry and electronic structure of Co2P2O7, thereby enabling superior pseudocapacitive behaviour. Furthermore, an assembled asymmetric supercapacitor device delivered a high energy density of 26.23 W h kg-1and a power density of 1859.22 W kg-1, underscoring the material's potential for high-performance energy.

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Photo-Biocatalytic Hydrogen Production with Coenzyme Regeneration via Cascade Catalysis

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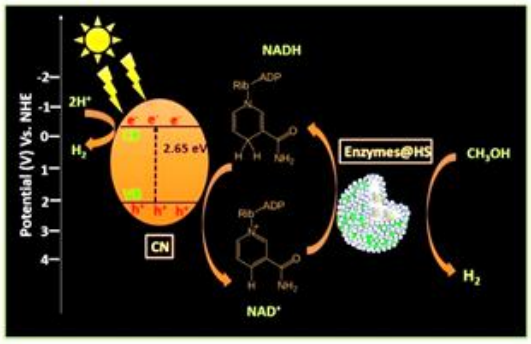
Abstract: The depletion of fossil fuels and increasing CO_2 emissions demand sustainable energy alternatives. Hydrogen (H_2) is a promising green fuel, and methanol reforming offers a relatively cleaner production route. However, conventional thermocatalytic methods require high temperatures and produce CO, while electrocatalytic approaches depend on external electricity, limiting sustainability. Photo-biocatalytic systems, inspired by natural photosynthesis, combine the selectivity of enzymes with light-driven processes, offering an efficient alternative. Yet, challenges such as enzyme instability and the high cost of coenzymes (NAD^+) restrict their practical application. This work proposes hybrid microreactors that integrate enzyme cascades-alcohol dehydrogenase, formaldehyde dehydrogenase, and formate dehydrogenase with visible-light photocatalysts (e.g., carbon nitride or CdS) for methanol-to-hydrogen conversion under ambient conditions. The enzymes drive sequential oxidation steps, while the photocatalyst regenerates NAD^+ from NADH, enabling continuous and cost-effective operation. Encapsulation of enzymes and photocatalysts enhances stability, improves cascade efficiency, and drives reactions toward completion. This integrated strategy offers a sustainable, efficient approach to hydrogen production.



Scheme 1. Schematic illustration of the proposed biocatalytic conversion of methanol to H_2 and photocatalytic regeneration of NAD^+.

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Supramolecular Chemical Ligation (SCL): Synthesis of Functional Protein from Peptide Fragments

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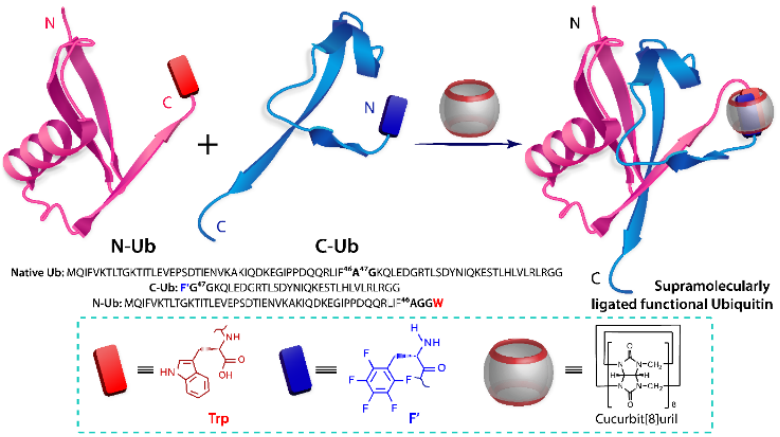
Abstract: The invention of Native Chemical Ligation (NCL)[1] revolutionized chemical biology by enabling precise, site-specific assembly and modification of proteins for functional and mechanistic studies. However, among many other limitations, one major drawback of NCL is the irreversibility of the synthesised protein. To overcome this limitation, in the present work we utilised the host-guest chemistry of Cucurbit[8]uril (CB[8])[2] to develop a new strategy for reconstructing fully functional proteins from their peptide fragments, called Supramolecular Chemical Ligation (SCL). As a proof-of-concept, two fragments of Ubiquitin are synthesised and functionalized with two guests for CB[8]. Under appropriate conditions, the guests form a ternary complex with CB[8] that conjugates the two fragments (Scheme 1). The conjugated protein showed folding similar to that of native Ubiquitin. The activity assay confirmed that the reconstructed protein is fully functional. The developed SCL was further extended to a larger protein, KRAS-4B. The newly developed SCL enables the generation of fully functional proteins from peptide fragments for important biological applications.



Scheme 1. Graphical presentation of the SCL of Ubiquitin.

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Biheteroaryl : Pyridyl-Thiazole

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Abstract: Biheteroarene pyridyl-thiazole is an important class of heterocyclic compounds which find broad applications in many fields of chemistry and physics. Derivatization and an atom economy is an important principle of green chemistry. In recent years an enormous attention of pyridyl-thiazole in pharmaceutical sector, in the world of natural products, thiopepetide antibiotics, luminescence and as a ligand in coordination chemistry and many more. We have reported synthesis of Biheteroaryl Pyridyl - thiazole, attached at all the three positions of pyridine that is not only the reactive C-2 and C-4 but also the non-reactive C-3, without using any metal catalyst. Many new derivatives of pyridyl-thiazole were synthesized by the reaction of thioamides using Hantzsch Thiazole route.

Keywords: Biheteroaryl, pyridyl-thiazole, thiopeptide, ligand, Hantzsch.

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Esterase-responsive Self-immolative Prodrugs for the Sustained Delivery of the Anticancer Drug 5-Fluorouracil with Turn-on Fluorescence

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Abstract: The FDA-approved chemotherapeutic drug 5-Fluorouracil (5-FU) is an antineoplastic antimetabolite of the uracil anabolic pathway.[1] 5-FU has been widely used to treat various types of cancer including lung cancer. It exhibits cytotoxicity by inhibiting the activity of nucleotide synthesizing enzyme thymidylate synthase (TS) to prevent the conversion of deoxyuridylic acid to thymidylic acid in the DNA synthesis pathway.[2] However, 5-FU possesses some limitations and side effects, such as short half-life, readily converted into inactive form by dihydropyrimidine dehydrogenase (DPD), myelosuppression, central neurotoxicity, gastrointestinal toxicity.[3] To overcome the limitations of 5-FU, stimuli-responsive prodrugs of 5-FU are advantageous for the selective delivery of drug to cancer cells with minimized off-target side effects.[4] In the present study, esterase-activatable fluorogenic prodrugs of the chemotherapeutic drug 5-FU have been rationally designed and synthesized using multi-step organic synthesis. While 5-FU was connected directly with the fluorophore via a C-N bond in the prodrug BJ-50, an additional self-immolative benzylic spacer with a carbonate linker was incorporated in the prodrug BJ-92. Although absorption and emission spectroscopic studies revealed the activation of both the prodrugs by porcine liver esterase (PLE), reverse-phase HPLC studies confirmed the inability of BJ-50 to release the active drug 5-FU. In contrast, a sustained release of 5-FU and Cou-OH was observed from BJ-92 in the presence of PLE. The endogenous esterase-mediated activation of the prodrug BJ-92 was validated by the turn-on fluorescence in A549 cells and the anti-proliferative activities in A549, and HEK-293 cells. Modulation of the expression of a few cancer marker proteins by BJ-92 and 5-FU was studied to evaluate their anticancer activities. As esterases are overexpressed in cancer cells, the prodrug in the present study would be helpful in selectively delivering 5-FU to cancer cells with reduced off-target side-effects.

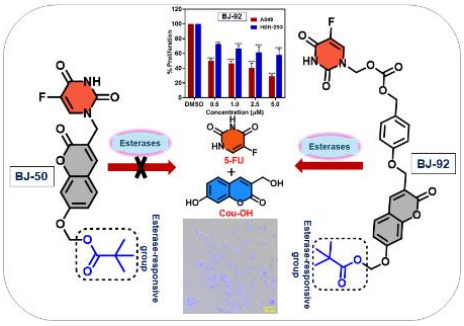

Figure 1. Graphical abstract representing the esterase-responsive activation of prodrugs BJ-50 and BJ-92 for the delivery of 5-FU with turn-on fluorescence.

Carbazole-Dansyl Conjugate as a Single Molecular System for Latent Fingerprint Imaging and on-site Date Rape Drug Detection

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Abstract: Drug-facilitated sexual assault (DFSA) investigations critically depend on two major forensic analyses: identification of illicit "date rape drugs" such as γ-butyrolactone (GBL) and γ-valerolactone (GVL), and detection of latent fingerprints as legally admissible evidence. Conventional fluorescent probes often address these applications independently, requiring multiple materials and delayed analysis. We recently reported the design and synthesis of a carbazole-dansyl conjugate (DASH) as a single multifunctional probe for dual forensic applications. DASH exhibits strong solid-state emission and hydrogen-bonding interactions, enabling sensitive *on-site* detection of GBL and GVL at concentrations lower than p-reviously reported systems. Simultaneously, the conjugated dansyl and carbazole fluorophores provide high contrast latent fingerprint visualization with confirmed biocompatibility. DASH represents the first single molecular system capable of addressing both DFSA drug detection and fingerprint analysis, offering a portable and efficient solution for forensic investigations.[1] The synthesis, photophysical properties and applications of DASH will be presented in the conference.

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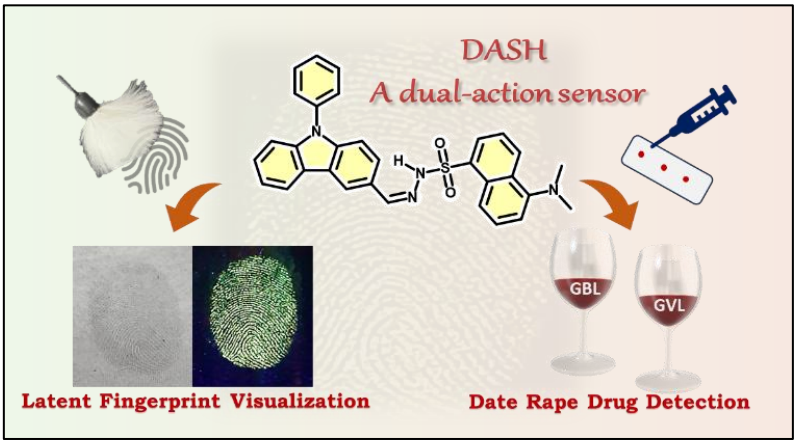

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2D Confinement as Control Parameter for Efficient Organic Transformations

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Abstract: Investigating molecular congestion within 2D nanometric confinement as primary control parameter for boosting the kinetics of chemical transformations is of prime importance. Our work demonstrates the reversible assembly of nanosheets to form 2D nanoreactors that showed enhanced conversion rate for the conversion of arylboronic acids to phenols and aryl iodides to biphenyls. The observed rate enhancement is mechanistically attributed to the synergistic effects of local concentration of reactants, nanoparticles, altered vibrational patterns of the reactants and the influential electrostatic forces exerted by the atomically thin channel walls. The kinetics boosted by ~4 times for the hydroxylation reaction and for Suzuki-Miyaura Coupling (SMC) by ~10^4 times inside the 2D nanoconfinement when compared to bulk (surface) reaction under identical conditions.

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Biochemical characterization of enzymes involved in synthesis and activation of α-methylserine fragment in amicetin biosynthesis pathway

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Abstract: Nucleoside antibiotics are important therapeutic agents with unique structures and mechanisms to combat antimicrobial resistance. Amicetin is a potent disaccharide nucleoside antibiotic active against a broad spectrum of bacteria, including Mycobacterium tuberculosis. Its biosynthesis involves the assembly of cytosine, para-aminobenzoic acid (PABA), deoxysugar units, and a key (2S)-α-methylserine moiety. AmiS, a PLP-dependent enzyme homologous to serine hydroxymethyltransferases, catalyzes the formation of (2S)-α-methylserine from L-alanine using tetrahydrofolate (THF). AmiT, an NRPS-like enzyme containing adenylation and thiolation domains, activates and loads this intermediate onto a carrier domain for subsequent incorporation. Together AmiS and AmiT enable a critical biosynthetic step, highlighting a unique enzymatic strategy and providing opportunities for engineering novel nucleoside antibiotics. we have purified and reconstituted the activity of AmiS in-vitro and mechanistic investigation is in progress.

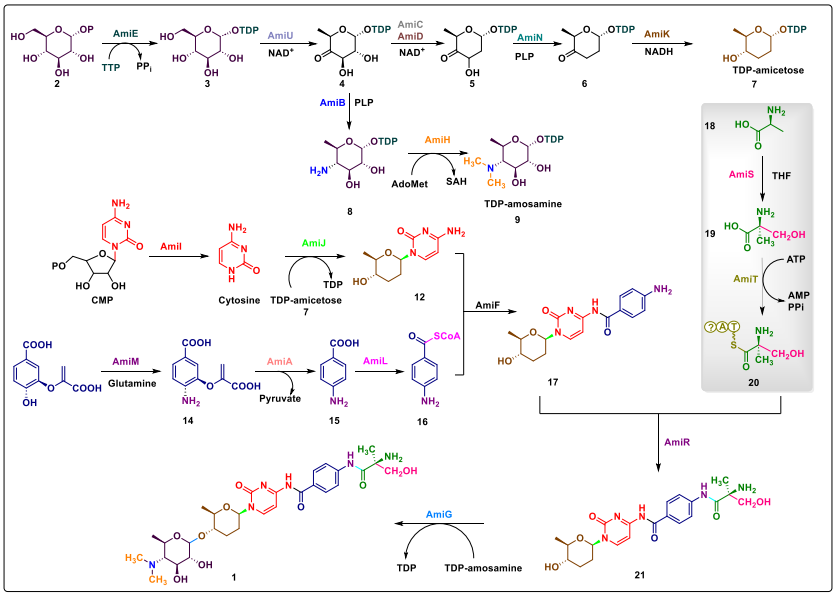

Figure 1. Proposed biochemical pathway of Amicetin

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Self-Assisted Q-COF@Ti_3C_2-MWCNT Ternary Membrane for Ultrafast and Flexible Hydrogen Sensing at Room Temperature

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Abstract: The development of flexible and highly sensitive hydrogen (H_2) sensors operating at room temperature is crucial for next-generation energy and safety applications.[1,2] Herein, we report a self-assisted membrane-based ternary composite including quinone-functionalized covalent organic frameworks integrated with Ti_3C_2 MXene and multi-walled carbon nanotubes (Q-COF@Ti_3C_2 - MWCNT) for efficient H_2 sensing. The self-assembled, binder-free membrane structure provides enhanced mechanical flexibility, continuous conductive pathways, and abundant accessible active sites for gas adsorption. The fabricated sensor exhibits an ultrafast response time of 6 s and a recovery time of 8 s toward 1 ppm H_2, exhibiting excellent sensitivity at low concentrations. Notably, the device retains stable sensing performance under mechanical deformation, showing response and recovery times of 14 s and 20 s, respectively, at a bending angle of 98.6°, confirming its robustness for flexible sensor applications. Density Functional Theory (DFT) calculations performed using VASP reveal a strong interaction between H_2 molecules and the composite, with a binding energy of -40.6 kcal mol^{-1}, indicating favourable adsorption-desorption kinetics[3]. This work demonstrates that self-assisted membrane-engineered Q-COF@Ti_3C_2-MWCNT composites are promising candidates for high-performance, flexible, and room-temperature hydrogen sensing applications.

Keywords: Quinoline; COF; Ti_3C_2; MWCNT; H_2;VASP; and Ambient Temperature

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Electrochemical Divergent Synthesis of Azetidines via Strain Release of 1-Azabicyclo[1.1.0]butanes

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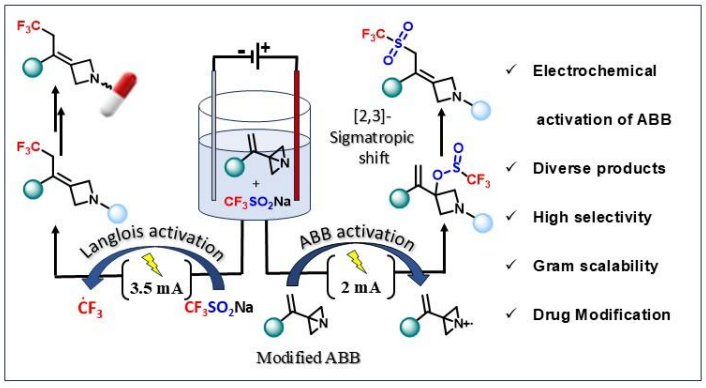
Abstract: Due to the favourable pharmaceutical properties of the azetidine ring, it can serve as a bioisostere to replace saturated heterocycles such as piperazines, piperidines, and pyrrolidines in drug discovery. The diverse methods for azetidine synthesis are still limited and challenging. Herein, we design a new class of 1-azabicyclo[1.1.0]butanes (ABBs) and report the first electrochemical protocol for the synthesis of chemo-selective trifluoromethanesulfonylated and trifluoromethylated azetidine derivatives via direct anodic oxidation. The key features of this strategy involve: (i) electrochemical anodic oxidation of ABB to form a *N*-centered radical cation, (ii) a rare [2,3]-sigmatropic shift of sulfone, (iii) selective oxidation of Langlois' reagent ($NaSO_2CF_3$), and (iv) the kinetic study of the developed methodology. The strategy exhibits broad substrate scope and scalability, making it practical. Installation of generated azetidines into marketed drug motifs, including ibuprofen, naproxen, and olaparib derivative, demonstrates the method's utility. Mechanistic investigations, supported by control experiments, cyclic voltammetry, and electrochemical impedance spectroscopy (EIS), provided key insights into the reaction pathway. This electrochemical approach advances the strain-release chemistry of ABBs and offers a promising platform for future developments.



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Ultrathin 2D Ni-Co-OH Nanowalls on Activated Carbon Cloth: A Scalable Route to High-Performance Battery-Type Supercapacitors

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Abstract: Flexible, wearable, and customizable electrodes with high electrochemical performance and cost-effective synthesis have become a key focus in energy storage research for next-generation portable and wearable electronic applications. In this work, a scalable two-step strategy is implemented to synthesize hollow and ultrathin Ni-Co hydroxide nanowall arrays on functionally activated hydrophilic carbon cloth for energy storage applications. This ultrathin electrode delivers a high specific capacitance of 2563.62 F g^{-1} at a current density of 1 A g^{-1}, along with excellent rate capability and cyclic stability. The superior electrochemical performance arises from the enhanced surface wettability, efficient charge transport, and the presence of numerous electroactive sites provided by the electrochemically activated carbon cloth, together with the hollow and ultrathin morphology of the Ni-Co-OH nanosheets. This renders the material highly promising for the industrial development of high-performance supercapacitors and advanced energy storage systems.

Probing interfacial charge dynamics via *EIS* in column-purified *Petunia* flower extract based DSSC

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Abstract: Electrochemical impedance spectroscopy (EIS) has emerged as crucial characterization tool for investigating charge transport dynamics at the interfaces of various IoT devices, solar cell, and electro-optical devices[1,2]. In this work, EIS studies have been made under both dark and illuminated conditions to investigate the interfacial charge dynamics of a dye-sensitized solar cell (DSSC)[3] using column-purified Petunia (a rich source of Anthocyanin) flower extract (CPE) as a natural sensitizer[4] [Fig.1]. Importantly, EIS analysis combined with appropriate equivalent circuit modelling, provides quantitative insights into interfacial charge processes. The recombination resistance (R_{rec}) for the CPE-based DSSC has been significantly enhanced (~134 Ω) relative to the crude extract (~52 Ω), indicating effective suppression of electron recombination pathways i.e., the back transferring of photoexcited electron at the electrode/electrolyte interface. Furthermore, the charge collection efficiency (η_{coll}) has also got improved to 0.77 from 0.58. These results demonstrate that EIS enables quantitative evaluation of interfacial charge dynamics, confirming the superior performance of purified natural dyes over crude extracts in DSSC applications.

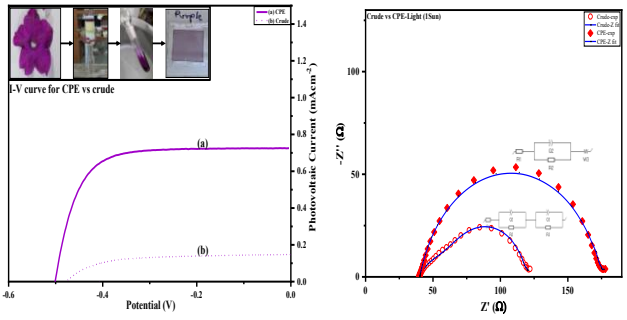

Figure 1. The schematic procedure and corresponding photovoltaic curve, along with Nyquist plot obtained via EIS analysis.

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$ZnFe_2O_4$/g-C_3N_4 Nanohybrid-Reinforced PVDF Composites for Wearable Piezoelectric Energy Harvesting Applications

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Abstract: The advancement of high-performance, self-poled piezoelectric nanogenerators[1] is important for the future of self-powered devices. Here, we introduce a $ZnFe_2O_4$/g-C_3N_4 (ZFG) nanohybrid-reinforced PVDF composite film to harvest mechanical energy,[2] fabricated by a simple casting method. The ZFG nanohybrid, composed of spinel $ZnFe_2O_4$ nanoparticles dispersed on two-dimensional g-C_3N_4 nanosheets, provides a high surface area and a substantial quantity of interfacial active sites. The structural and spectroscopic study indicates robust ion-dipole and electrostatic interactions between the nanohybrid and PVDF chains, which effectively inhibit the nonpolar α-phase and facilitate the nucleation of the electroactive β-phase. At an optimal loading of 9 Wt% ZFG_{30}, the composite exhibits a significant β-phase fraction (~88%), increased dielectric constant (21 at 100 Hz frequency), and substantially improved ferroelectric characteristics (P_r ~ 0.51 μC cm^{-2}, P_s ~ 2.7μC cm^{-2}). The fabricated nanogenerator attains a peak power density of approximately 15 μW cm^{-2} at 4 MΩ load resistance, producing an output voltage of 41 V and a short-circuit current of around ~0.9 μA under 16 N mechanical stimulation without external electrical poling. Throughout four weeks, the gadget demonstrates sustained operational stability. An effective method to improve dipole alignment and piezoelectric conversion in polymer matrices is created using a nanohybrid in a synergistic interfacial engineering technique. This provides a scalable and environmentally friendly base for wearable energy harvesting applications.

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Exploiting the Electronic Influence of Polyfluorinated N-Heterocyclic Carbene Ligands in Highly Efficient and Regioselective Copper-Catalyzed Hydroboration Reactions

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Abstract: N-heterocyclic carbenes (NHCs) are well known for their strong σ- donation.[1] This property of NHC is capitalized in past for enhancement of the catalytic abilities of various metal catalysts. Steric environment of these NHC have also played a crucial role in enhancement of the catalytic abilities of metal catalysts. But the π–accepting tendency of the NHC have not be exploited yet to a very large extent. This property is crucial in some specific catalytic processes where the metal needs to be electron deficient in nature for better results.[2] $BIPr^F$ & $BIMes^F$ comes out to be an excellent example of π-acceptor NHCs having tetraflurobenzene group attached to backbone of traditional IPr and IMes ligands. This leads to a significant decrease in LUMO energy levels.[3] This ligand system in combination with copper system yields an enhanced reactivity and selectivity in hydroboration reaction of alkynes and alkenes.

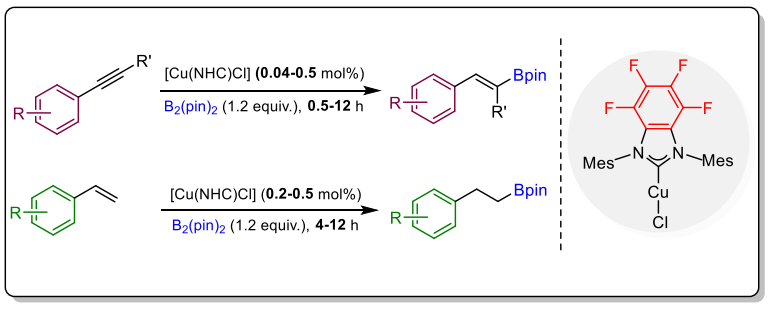

Figure 1. New fluorinated Cu(I) NHC complex for efficient hydroboration of alkyne and alkene

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Ruthenium (II)-N-Heterocyclic Carbene Complexes Having Extended Ligand Backbone with Record Metal-to-Ligand Charge Transfer Lifetimes

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Abstract: Complexes of Ru(II) and its congeners such as Os(II) and Ir(III), are extensively studied in the field of photocatalysis, solar energy harvesting, LEDs and photodynamic therapy.[1] $[Ru(bpy)^3]^{2+}$, which is considered as the benchmark complex, has the ^{3}MLCT (metal-to-ligand charge transfer) excited state lifetime of 890 ns in deaerated acetonitrile at room temperature. But when the tridentate ligand ,2':6',2''-terpyridine (tpy) is used instead of 2,2'-bipyridine (bpy), the resultant complex $[Ru(tpy)^2]^{2+}$ has the ^{3}MLCT lifetime of only 0.25 ns. This is due to the poor bite angle of tpy-ligand which results in weaker metal-ligand overlap, and hence the ^{3}MLCT state decays non-radiatively through the low lying ^{3}MC (metal-centered) states.[2] When two terminal pyridine units in the tpy-ligand are replaced by two strong s-donating N-heterocyclic carbene (NHC) units, the new Ru(II) complex, $[Ru(L^{CNC})_2]^{2+}$ forms and features ^{3}MLCT lifetime of 820 ns in deaerated acetonitrile at room temperature.[3] Herein we have synthesized three new Ru(II)-NHC complexes with extended backbones featuring ^{3}MLCT lifetimes up to 11.2 ms. Detailed photophysical studies have been done. These Ru(II)-NHC complexes also feature high triplet state energies (~2.4 to 2.6 eV) and can be used in challenging [2+2] cycloaddition and dearomatization reactions.

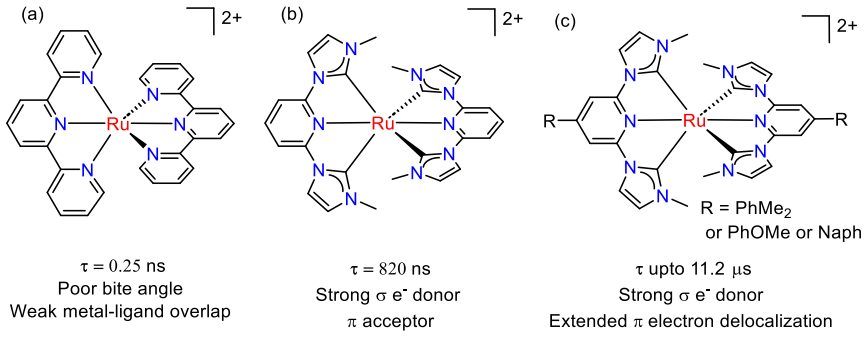

Figure 1. Previous reports (a-b) and newly synthesized Ru(II)-NHC complexes (c)

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Electrochemical Mapping of Catecholamine-Copper Redox Cycling Induced DNA Damage Using a MXene–HOF Hybrid Platform

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Abstract: Oxidative DNA damage induced by reactive oxygen species (ROS) plays a critical role in mutagenesis and the progression of neurodegenerative disorders, with guanine being the most oxidation-susceptible nucleobase forming 8-oxoguanine (8-oxoG) lesions. Catecholamine neurotransmitters, particularly in the presence of transition metals such as Cu^{2+}, can undergo redox cycling to generate ROS, thereby accelerating oxidative DNA damage. In this work, we report a novel electrochemical DNA damage probe based on a poly-L-lysine electropolymerized Nb_2CT_x MXene-hydrogen-bonded organic framework nanocomposite modified carbon yarn electrode (pLy-HOF-Nb_2CT_x/CY) for monitoring catecholamine-mediated oxidative guanine damage and evaluating antioxidant protection. The nanocomposite electrode exhibited enhanced electron transfer kinetics and increased electroactive surface area, enabling sensitive detection of 8-oxoG generated at the electrode interface. The voltammetric experiments was demonstrated to characterize the catecholamine (dopamine, epinephrine, norepinephrine, and L-DOPA) and copper ion (Cu^{2+}) mediated guanine oxidation, with further, confirming synergistic metal-mediated oxidative damage. The 8-oxoG peak currents increased markedly in catecholamine-Cu^{2+} systems, indicating enhanced ROS-driven DNA oxidation. The platform was further employed to investigate the protective effects of antioxidants including ascorbic acid, quercetin, curcumin, resveratrol, glutathione, EGCG, N-acetyl cysteine, and α-lipoic acid, which substantially suppressed the 8-oxoG signal, with several compounds exhibiting >90% inhibition of oxidative damage. These findings demonstrate that the developed MXene-HOF-polylysine electrochemical probe provides a robust and sensitive approach for studying metal-mediated oxidative DNA damage and evaluating antioxidant efficacy. The proposed strategy offers valuable insight into catecholamine-induced genotoxicity and holds promise for screening protective agents against oxidative stress-related diseases.

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Doxorubicin and Curcumin Controlled Release using Heterocyclic-based Metal Organic Frameworks

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Abstract: Metal-organic frameworks (MOFs) are porous crystalline materials composed of metal ions coordinated to organic ligands, having high surface area, tunable pore size, and the ability to encapsulate a variety of therapeutic agents. In cancer therapy, MOFs can load anticancer drugs and target tumour cells effectively, thereby enhancing treatment efficacy while minimizing side effects. So to evaluate this, the present work focuses on the synthesis, characterization, and drug delivery characteristics of two Cu^{2+} coordinated magnetic MOFs with heterocycle 1,4-bisimidazolylmethylene Benzene and Sodium pyromellitic, formed as Fe_3O_4@MRCU201 and Fe_3O_4@MRCU301 MOFs, respectively. XRD, FESEM, FTIR, XPS, EDX, and Zeta potential were used to characterize these MOFs. XRD confirmed the crystalline nature of MOFs, and the presence of coordinated metals was verified by using EDX. Drug loading and release studies with doxorubicin (DOX) and curcumin (Cur) showed that Fe_3O_4@MRCU301 loading capacities 200 mg/g for DOX and 19.89 mg/g Cur and exhibited strong pH-responsive release up to 81.2% DOX at pH 5.5. Fe_3O_4@MRCU201 showed a loading capacity of 100 mg/g DOX; 65.96 mg/g Cur) with controlled release under acidic conditions. Overall, the magnetic MOFs demonstrate promising potential for pH-responsive targeted anticancer drug delivery.

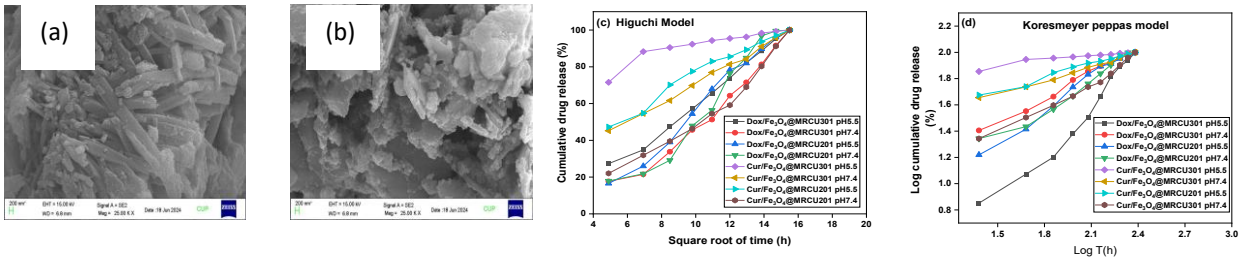

Figure 1: FESEM image of (a) Fe_3O_4@MRCU301 (b) Fe_3O_4@MRCU201 (c) Higuchi Model and (d) Koresmeyer-Peppas model fit for Drug release by MOFs

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Dicationic Molecular Probe for Detecting Altered NADH Levels in NAFLD Cell Model and Diseased Liver Tissues

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Abstract: NADH is a crucial coenzyme that plays an important role in various biological processes.[1,2] To diagnose various pathological conditions, it is crucial to detect changes in NADH levels at an early stage.[3] Towards this, we reported an organoselenium-based molecular probe MQ-SeZ, which is weakly emissive in nature. However, it emits strongly at ~574 nm (λ_{ex} = 543 nm) upon NADH addition.[4] The enhancement in the fluorescence emission is possibly due to intramolecular charge transfer from donor to acceptor moiety. Further, the probe has been explored for detecting altered NADH levels in nonalcoholic fatty liver disease cell models associated with hyperglycemia, hyperlipidemia, and hyperinsulinemia conditions. Next, the MQ-SeZ was utilized for imaging elevated NADH levels in high-fat-high-sucrose diet (HFHS) fed liver-tissue sections. Overall, the study demonstrates the utility of a small molecular probe for imaging altered NADH levels in various pathological conditions.[4]

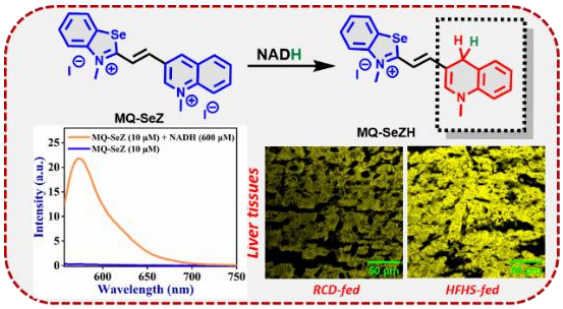

Figure 1: Schematic representation of NADH-mediated reduction of MQ-SeZ and its application in bioimaging.

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Ferric Nitrate Promoted Highly Regiospecific *ortho*-Nitration of *N*-Nitrosoanilines Under Mild Conditions

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Abstract: Nitroaromatic compounds are key intermediates in dyes[1], explosives[2], agrochemicals[3], pharmaceuticals[4], and other value-added compounds. However, conventional acid-mediated nitration suffers from poor selectivity, limited functional group tolerance, and hazardous NO_x emissions, driving the need for milder, sustainable methods. *N*-Nitrosoanilines are valuable intermediates in medicinal and synthetic chemistry, their modifiable nitroso group enables access to diverse functional molecules including diazonium salts, α-carbanion equivalents and bioactive compounds[5]. Herein, we report a practical, highly regiospecific *ortho*-nitration of *N*-nitrosoanilines using $Fe(NO_3)_3.9H_2O$ under neutral, acid-free conditions. The method proceeds via electrophilic aromatic substitution with Fe(III) coordination to the nitroso group (N=O) enabling efficient synthesis of *N*-nitroso-*N*-alkyl nitroanilines in good to excellent yields. The protocol exhibits a broad substrate scope, high functional group tolerance, and enables regioselective nitration of heteroaromatic frameworks. The reaction is operationally simple, moisture and air-tolerant and readily scalable.

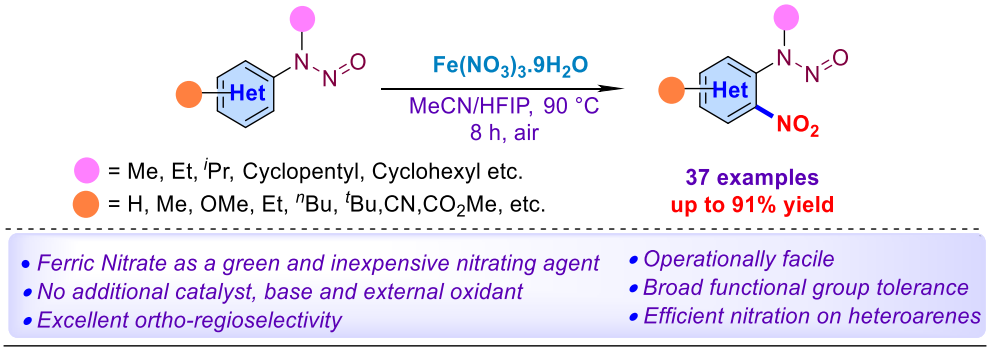

Figure 1. Regiospecific *ortho*-nitration of *N*-Nitrosoanilines

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Long-life rechargeable aqueous zinc-ion battery anodes enabled by regulation of interfacial zinc deposition kinetics through alkyl chain engineering of nitrile additives

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Abstract: Rechargeable aqueous zinc-ion batteries (AZIBs) are gaining attention as promising alternatives of lithium-ion batteries, owing to their high ionic conductivity, inherent safety, environmental compatibility, and competitive energy density. Zinc metal, with its high theoretical capacity and low reduction potential, is an attractive anode material. However, its practical application is hindered by challenges such as dendrite growth, hydrogen evolution, and corrosion, which degrade its performance and stability. Several key strategies have been employed to date to address the issue, however additive engineering offers the more straightforward and commercially viable strategy. It works via reconstructing the solvation structure of Zn^{2+} ions and/or tailoring the zinc–electrolyte interface, thereby effectively regulating zinc deposition kinetics. Within the class of alkyl nitriles, only acetonitrile, containing a single nitrile (-CN) group bonded to a methyl ($-CH_3$) group, has been explored as an electrolyte additive to date, where it functions through preferential adsorption on the zinc surface. Surprisingly, the potential of other nitrile molecules with longer alkyl chain lengths as electrolyte additives has not been thoroughly explored, likely due to their reduced solubility in aqueous media.[1] In this study, we have systematically investigated the roles of the alkyl chain length in straight-chain nitrile series from acetonitrile to hexanenitrile in modulating the behaviour of nitrile groups in a multitude of interfacial effects to increase the cycle life of AZIB. We have found that pentanenitrile with an optimized alkyl chain length delivers a prolonged cycle life of up to 1400 h under 5 mA cm^{-2} current density and 5 mAh cm^{-2} capacity in Zn//Zn cells, which is markedly superior to acetonitrile, exhibiting only 165 h stability under identical current density and capacity.

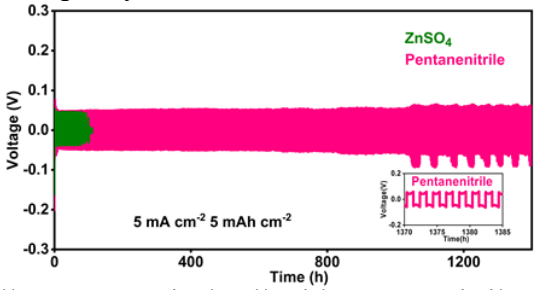

Figure 1. Cycle life of Zn//Zn symmetrical cell with pentanenitrile additive

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Mechanochromism induced polymorphism and the role of different interactions: double encryption-decryption applications

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Abstract: A pyrene-based carbohydrazide derivative (PYH) is reported to display mechanochromism, acidochromism and aggregation induced emission (AIE). Herein, a relatively rare occurring reversible red-shifted enhanced emission upon mechanical force is observed. The mechanochromism induced crystal to crystal transition is reported and the structural changes at molecular level are explored using PXRD, SCXRD, DSC and Hirshfeld surface analysis. The single crystals of both polymorphs in pyrene-based material (PYH) have been successfully obtained. The mechanically-induced enhancement of molecular planarity facilitates ICT processes and changes the supramolecular arrangement from robust π–π stacking to C–H···π interactions leading to red-shifted enhanced emission. The acid sensitive property of PYH has been successfully utilized in devising portable sensor kit for acidic fumes. Additionally, the acidochromism and mechanochromism has been synergistically exploited to design a multi-level data encryption decryption system. The PYH-coated papers enable the practical utility in pressure sensing and rewritable pressure printing technologies.

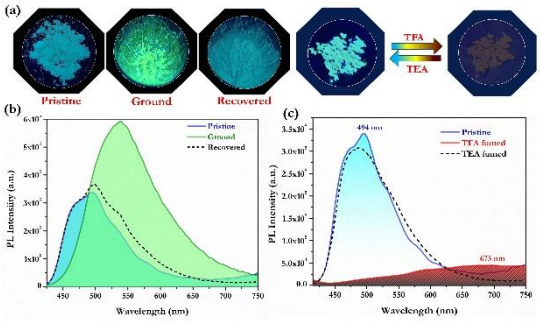

Figure 1: (a) PYH powder samples under UV-illumination. (b) Solid PL spectra of pristine, ground, recovered, TFA fumed and TEA fumed PYH powder.

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Engineering Ti- MXene / $LaNiO_3$ Perovskite Composites for Efficient HER and OER Electrocatalytic Performance

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Abstract: The demand for renewable energy has driven interest in water splitting, where HER and OER require efficient electrocatalysts due to sluggish kinetics. Although $LaNiO_3$ perovskite offers good redox activity and stability, its poor conductivity and low surface area limit performance. To address this, a $Ti_3C_2T_x$ MXene -supported $LaNiO_3$ composite was developed. MXene was synthesized via HF etching and $LaNiO_3$ via coprecipitation, followed by ultrasonication and stirring to form the composite. FESEM confirmed nano cube $LaNiO_3$ uniformly distributed on layered MXene, while XPS verified oxidation states and surface terminations (F, O). Electrochemical studies (CV, LSV, and EIS) conducted in 1 M KOH using a Ni foam electrode demonstrated excellent bifunctional performance of the $Ti_3C_2T_x$ @$LaNiO_3$ composite. It exhibited low overpotentials of 90 mV for HER and 350 mV for OER at a current density of 10 mA cm^{-2}, along with Tafel slopes of 59 mV dec^{-1} (HER) and 100 mV dec^{-1} (OER), indicating favorable kinetics. The composite also showed higher Cdl (larger ECSA) and lower charge transfer resistance (Rct) compared to pristine $LaNiO_3$. Stability tests confirmed its strong durability under alkaline conditions.

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Development of Highly Efficient Electrocatalyst Derived from ZIF-67 for the Synthesis of Green Ammonia from Nitrate

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Abstract: Ammonia is not only a crucial component in nitrogen-based fertilizers to ensure food security but also serves as a versatile energy carrier with efficient storage and transportation capabilities. The traditional Haber-Bosch process dominates industrial ammonia production; however, it operates under extremely harsh conditions and is associated with substantial CO_2 emissions, raising significant environmental concerns.[1] In contrast, electrochemical nitrate reduction (NO_3RR) offers a green alternative to Haber–Bosch by simultaneously treating wastewater and producing ammonia.[2] In this work, we developed a binder-free, self-supported, low-cost electrocatalyst with high surface area derived from the pyrolysis of Zeolitic imidazolate framework (ZIF-67) to a graphitic nanowall (GNW) structure which acts as a promising electrocatalyst for the reduction of NO_3^- to ammonia. This study also explores the profound impact of graphitization levels of GNW and highlights the crucial significance of in-situ nitrogen doping on carbon substrate for ammonia synthesis. The prepared catalyst shows a high yield rate of 36.2 mg $h^{-1}cm^{-2}$ with a faradaic efficiency of 96.5 % at -1.1 V Vs RHE. This work will provide new insights and open avenues for future electrocatalyst development.

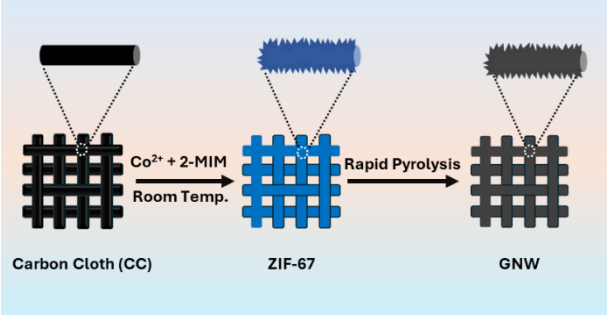

Figure 1. Schematic of GNW catalyst preparation.

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Molecularly Engineered Organic Single Crystals for Stimuli-Responsive Luminescence and Unconventional Photoconductivity

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Abstract: Stimuli-responsive organic single crystals offer a powerful platform that efficiently translates molecular-level design into adaptive optical and electronic functionalities. In this work, we demonstrate how rational molecular engineering of donor-acceptor boron-based Schiff base complexes allow for precise control over charge-transfer interactions in organic single crystals, enabling a variety of distinct yet interconnected stimulus-driven responses. In the first part, tunable fluorescence is reported for naphthalidenimine-boron single crystals, which selectively respond to pH and temperature variations. Crystallographic and spectroscopic analyses revealed that protonation of the donor moiety mediates intramolecular charge transfer, altering the photophysical performance while inducing controlled, sustained proton release. This proton-mediated process enables an in-situ synthesis of metal nanoparticles that facilitates surface passivation and regulated growth kinetics with well-defined morphologies.[1] Following the same design principles of the charge-transfer approach, we further expand this molecular strategy into electronic functionality by realizing negative photoconductivity (NPC) in long, flexible organic single crystals, an effect that has never been reported in such systems. A salicylideneimine–boron single crystal, engineered with optimized donor-acceptor interactions, promotes deep-level trap-state formation under light irradiation, leading to a counterintuitive decrease in conductivity under both UV and visible illumination. The crystals exhibit a detection sensitivity of ~45% and a photoresponsivity of 7.18 μA/W, enabling stable light-modulated switching. Leveraging these properties, a human–machine interface for secure user authentication was successfully demonstrated. Together, these studies establish molecularly engineered organic single crystals as a unified and versatile platform in which tailored charge-transfer interactions govern both stimulus-responsive luminescence and unconventional photoconductive behavior. This integrated approach highlights the potential of organic single crystals for next-generation smart materials, adaptive optoelectronics, and intelligent sensing technologies.[2]

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Superabsorbent Hydrogel for Antibacterial Drug Delivery Capable of Infectious Wound Healing

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Abstract: Chronic wounds and secondary bacterial infections present significant challenges in clinical wound management, necessitating the development of advanced drugs and biomaterials that offer both protective coverage and therapeutic intervention. Antimicrobial molecules developed as substitutes of antimicrobial peptides and lipopeptides are effective against resistant bacterial strains due to significant antimicrobial activity. Such molecules possess the potential to be successfully utilized against secondary bacterial infections and treatment of chronic wounds. Our work explores the synthesis and characterization of a hydrogel system specifically engineered with high swelling capacity (~ 450% swelling) and optimized solubility to facilitate efficient delivery of a novel antibacterial drug for accelerated wound healing. The fabricated hydrogel features a highly porous and specialized three-dimensional polymeric network designed through cross-linking strategy. This framework enables the material to effectively absorb large volumes of wound exudate and maintain a moist interfacial environment a superior swelling ratio, allowing re-epithelialization. Furthermore, the sustained and localized release of encapsulated antibacterial agents was ensured by the solubility of the hydrogel through sustained release of the compound and controlled degradation of the hydrogel. Such mechanism of the hydrogel maintains therapeutic concentrations at the wound site over extended periods, while preventing the formation of bacterial biofilms. Significant inhibitory effects against both Gram-positive (*S. aureus*) and Gram-negative (*E. coli)* bacteria was exhibited by the hydrogel under in vitro evaluations. Evaluation of mechanical properties (~ 10 MPa stress and ~ 20 % EB) confirmed that the hydrogel retains structural integrity under physiological conditions while remaining flexible enough to conform to irregular wound geometries. With complete biodegradation upon disposal under natural environmental conditions, the developed hydrogel presents a significant approach towards a biomaterial with sustained and specialized antibacterial activity for infectious wound healing application.

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Vinylsilanes as Ethylene Surrogates: Rh(I)-Catalyzed Direct Hydroarylation of *In Situ* Generated Ethylene

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Abstract: A modular and practical approach to the Rh(I)- catalyzed hydroarylation of ethylene with arenes bearing a quinoline amide group has been developed[1]. To address the inherent challenges of ethylene hydroarylation, particularly the reliance on high ethylene pressure[2], this approach employs vinylsilane as a bench-stable, safer surrogate for the *in situ* generation of ethylene. Comprehensive mechanistic studies support a sequence involving the insertion of vinyl silane, ethylene release, and subsequent hydroarylation, highlighting the efficiency and practicality of this transformation.

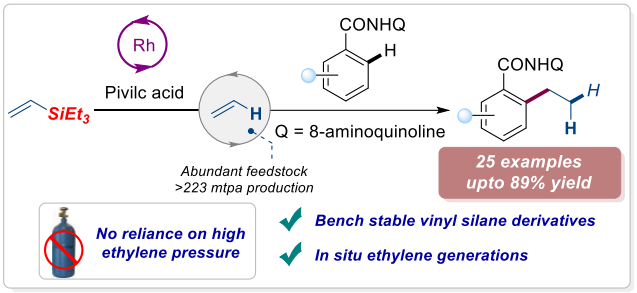

Figure 1. Rh(I)-catalyzed hydroarylation using vinylsilane as an ethylene surrogate.

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Calcination of Post-Functionalized Metal-oxo Cluster Hybrid to Bifunctional Electrocatalyst: Cooling-Driven Control of Defects and Selectivity for HER and MOR

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Abstract: Hydrogen is a clean, high-energy fuel, but conventional water splitting is limited by the sluggish and energy-intensive oxygen evolution reaction (OER). Replacing OER with the methanol oxidation reaction (MOR) greatly lowers the anodic potential and enables the co-production of value-added formate.[2] Methanol is cheap, abundant, and oxidizes at very low potentials, offering major energy savings. Developing efficient non-noble-metal catalysts is therefore crucial for advancing hybrid MOR-assisted hydrogen-generation systems. Polyoxometalates (POMs) are nanoscale metal-oxide clusters with exceptional redox activity and structural versatility, which can be further enhanced through POM–organic hybrid formation, particularly Class II covalently linked systems.[1] In this work, an aryl-sulfonium hybrid of Mo-based POM (HB) was designed to produce $Mo^{6+}/Mo^{4+}/Mo^{0}$ species and MoS_2 upon annealing, offering active sites for HER and favorable adsorption sites for MOR.[2] Post-functionalization of HB (PHB) added an additional carbon source, forming N-doped graphitic carbon that enhances conductivity. Incorporation of a nickel complex into PHB yields NiPHB, which, after calcination, introduces Ni^{2+}/Ni^{0} species known to catalyze both HER and MOR. Post-calcination, a cooling-controlled protocol was applied to NiPHB to generate NiPHBcc and NiPHBrc products, with NiPHBrc exhibiting a higher density of structural defects, thereby significantly boosting HER activity. In contrast, conventionally annealed NiPHBcc retains more Ni^{2+}, making it more selective and active toward MOR. Comparative analysis clearly shows that defect engineering, metal incorporation, and precursor modification work synergistically to tune catalytic behavior. Overall, every level of structural modification enhances performance, demonstrating the versatility of POM-hybrid design. Together, these strategies provide a powerful platform for creating highly efficient, multifunctional HER/MOR electrocatalysts.[3]

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Effect of Donor Substitution on Locally Excited and Charge Transfer States in Imidazo[4,5-c] pyridine

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Abstract: A comparative study was carried out to understand the effect of donor substitution on the photophysical behaviour of imidazo[4,5-c] pyridine derivatives. This motivated us to explore 2-(4'-N,N-dimethylaminophenyl)imidazo[4,5-c]pyridine(DMAPIP-C) and 2-(phenyl)imidazo[4,5-c]pyridine (PIP-C), where the key difference is the presence of a strong electron-donating dimethyl amino group in DMAPIP-C, while PIP-C does not have such a donor group. In this study, we examine the role of donor substitution by analysing their photophysical properties. Photophysical studies show that DMAPIP-C exhibits dual emission behaviour, consisting of locally excited (LE) emission and an additional red-shifted emission due to the formation of a twisted intramolecular charge transfer (TICT) state. The presence of the dimethyl amino group enhances intramolecular charge transfer, and this effect further increases in the presence of Zn^{2+} ions, leading to stabilisation of the charge-separated state and stronger TICT emission. In contrast, PIP-C mainly shows LE emission and does not exhibit significant TICT behaviour. Only small spectral changes are observed upon the addition of Zn^{2+} ions, indicating limited charge transfer due to the absence of a strong donor group. Overall, the study shows that donor substitution plays an important role in controlling the excited-state behaviour and emission properties. The results indicate that structural modification can effectively tune the balance between LE and TICT processes, which is useful for designing efficient fluorescent materials.

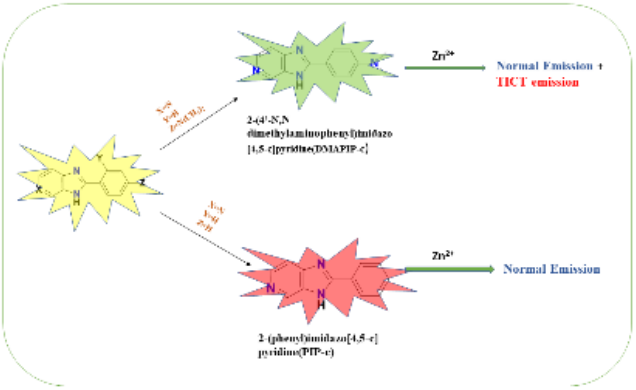

Fig 1. Comparative Emission behaviour of DMAPIP-c and PIP-c

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Fe-Doped $CuCo_2S_4$ Thiospinel as a High-Performance Oxygen Electrocatalyst for Rechargeable Zinc–Air Batteries

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Abstract: The commercial viability of rechargeable zinc–air batteries (ZABs) is hindered by their poor round-trip efficiency, dendritic growth of the anode as well as expensive cathode electrocatalysts with limited stability and durability in alkaline medium during prolonged operation. In this work, we demonstrate a facile one-step hydrothermal synthesis of Fe-doped $CuCo_2S_4$ thiospinels. Both experimental and theoretical analyses confirm that Fe incorporation into the $CuCo_2S_4$ lattice markedly enhances electrocatalytic activity.1 The optimized composition, $Fe_{0.03}CuCo_2S_4$, exhibits outstanding bifunctional activity with an oxygen reduction reaction (ORR) onset potential of 0.89 V vs RHE, a half-wave potential ($E_{1/2}$) of 0.80 V vs RHE, and an oxygen evolution reaction (OER) overpotential of 330 mV at 10 mA cm^{-2}, resulting in a low bifunctional voltage gap (ΔE) of 0.76 V. Furthermore, a prototype ZAB assembled using $Fe_{0.03}CCS$ as the air cathode delivers a peak power density of 82 mW cm^{-2} and a specific capacity of 803.4 mAh gZn^{-1}. This study highlights a promising strategy for designing efficient bifunctional electrocatalysts.

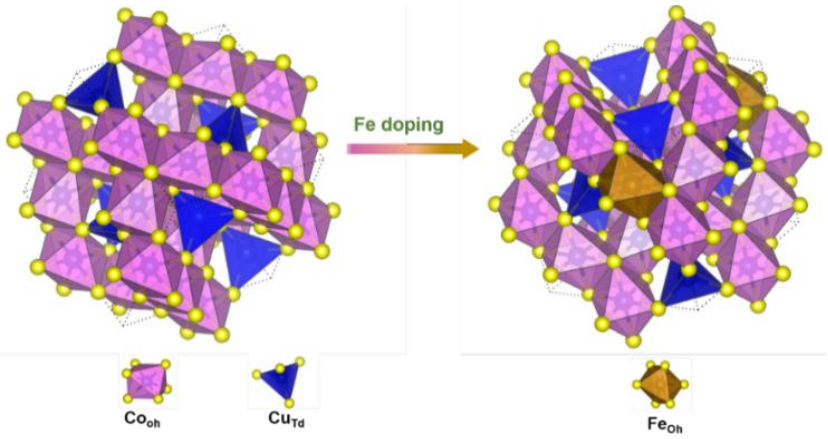

Figure 1. Schematic representation of the crystal structure.

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Pyrene based Chemosensor: Synthesis, Characterization and Application towards Metal Ion Sensing

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Abstract: In this work, two pyrene-based Schiff base ligands (L1 and L2) were synthesized via. condensation of pyrene-1-carboxaldehyde with 2-amino-4-chlorophenol and 2-aminophenol, respectively. Spectroscopy investigations reveal that L1 shows fluorescence turn on effect in case of Cu^{2+} and Fe^{3+} where as L2 is spectroscopically inactive under the same condition. The yellow colour of ligands changes orange in case of Cu^{2+} and brown in case of Fe^{3+}. Furthermore, the structural properties of the ligands (L1 and L2) determined by ESI Mass, NMR and FTIR. On the other hand, job's plot shows that L1 bound Cu^{2+} and Fe^{3+} ions at 1:1(ligand metal) ratio with detection limit 0.75µm and 0.90µm for Cu^{2+} and Fe^{3+}. However, L1 was effectively used to the building of logic gates and the quantitative detection of Cu^{2+} and Fe^{3+} ions in actual water samples. Additionally, solvent phase DFT calculations were used to determine the optoelectronic and structural characteristics of the L1 and Fe (III) and Cu (II) complexes.

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Metal-Doped Carbon Nanodots for Selective Lysosomal and Mitochondrial Imaging in Live Cells

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Abstract: Selective visualization of subcellular organelles is crucial for understanding cellular functions and disease progression. Herein, we report iron (Fe)-doped and manganese (Mn)-doped carbon nanodots (CNDs) as organelle-selective fluorescent nanoprobes for precise intracellular staining. Fe-doped CNDs exhibit preferential accumulation within lysosomes, whereas Mn-doped CNDs selectively localize within mitochondria, enabling distinct and reliable labeling of these organelles. Both nanoprobes display strong fluorescence intensity, excellent photostability, and negligible cytotoxicity, making them well-suited for high-resolution confocal imaging. Colocalization studies with commercially available organelle-specific dyes further validate their targeting specificity and intracellular distribution. The probes provide clear contrast and stable fluorescence signals, allowing detailed visualization of organelle morphology and spatial organization. This work demonstrates the potential of metal-doped CNDs as efficient and versatile fluorescent probes for organelle-specific imaging. Furthermore, it lays a foundational role for future studies aimed at exploring dynamic cellular processes and investigating cell death pathways, including ferroptosis and apoptosis, using such nanomaterial-based imaging platforms.

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Energy-Efficient Hydrogen Production via Urea Oxidation using $CoSe_2$ Nanoparticles

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Abstract: The electrochemical urea oxidation reaction (UOR) offers an energy-efficient strategy for hydrogen production while simultaneously enabling wastewater remediation. In this work, nanostructured cobalt selenide ($CoSe_2$) was synthesized and evaluated as an efficient electrocatalyst for UOR under alkaline conditions. Structural and morphological characterizations confirm phase-pure $CoSe_2$ nanoparticles. Electrochemical measurements reveal low onset potential, high catalytic activity, and excellent operational stability toward urea oxidation. The enhanced performance is attributed to the high electrical conductivity and abundant electrochemically accessible active sites of $CoSe_2$, which facilitate efficient charge transfer and reaction kinetics. These findings demonstrate the potential of $CoSe_2$ as a promising non-noble metal catalyst for wastewater-assisted hydrogen generation and provide a foundation for further performance optimization through targeted defect and compositional engineering.

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Silver-enabled Inverse electron demand thermal decarbonylative skeletal expansion: a new gateway to the synthesis of multifunctionalized quinoline

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Abstract: Herein, we have reported an efficient Lewis acid catalysed decarbonylative tandem inverse electron demand hetero Diels-Alder reaction in a very moderate temperature for the construction of quinoline derivatives from 2-(p-tolyl)-1H-inden-1-one with a variety of internal alkynes. To understand the role of the Lewis acid in the reaction, HOMO-LUMO gaps are compared for the adducts formed between the diene and Lewis acid. A detailed mechanistic investigation, utilizing density functional theory (DFT) calculations, revealed a clear preference for the inverse electron demand hetero Diels-Alder reaction pathway. The release of carbon monoxide gas has been detected through headspace gas chromatography analysis. This strategy enables the one pot synthesis of quinoline derivatives which offer substantial potential in drug discovery.

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In_2Se_3 in dispersions: Exfoliability, Stability, and Photo-electrochemical implications

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Abstract: In_2Se_3, a binary sesquichalcogenide has received considerable consideration due to its suitable band gap and optical characteristics, making it a good candidate for high-performance photodetectors. Scalability and integrability of liquid phase exfoliation (LPE) for 2D material production is unmatched and solvation medium selection strongly governs the exfoliability and stability. For exfoliability, we have devised a method involving Hansen solubility parameters (HSP) for optimum system identification. Solvent dependent stability of the dispersions is revealed by computing instability index, sedimentation velocity, and extinction decay time constants with help of LUMiSizer: dispersion analyser. One critical implication in case of In_2Se_3 is the reversible but detrimental phase transformation from alpha to beta, which generates Se vacancy cycle after cycle, thus it is crucial to identify a low-boiling point solvent if functional devices have to be fabricated over large areas with printing protocols. Presented methodology enables to choose effective solvents for large scale production which has been identified as 2-propanol. Obtained dispersions are spray printed onto functional substrates for broad band photoelectrochemical photodetection (PEC). Bane of most PEC systems is the transient losses of photo-generated charge carriers at the electrode-electrolyte interface. In this work, we employ electroless deposition of Au nanoparticles onto In_2Se_3 thin films, which in turn impedes the hole-annihilation losses leading to sharp transients in PEC current. We report as low as 5% photocurrent loss for optimal Au decoration with a responsivity of 2.3 mA/W, detectivity of 4×10^9 Jones, and ~30 ms rise and fall times. The implications of incorporation of the Au-NP on In_2Se_3 have been critically investigated by various methods like incorporating a hole scavenger and transient absorption spectrum analysis. Both methods convincingly depict role of Au in hole annihilation at the electrode-electrolyte interface leading to ameliorated transient losses. This work assists large-scale production of In_2Se_3 dispersions by providing HSP parameters for the material and identifying a suitable low-boiling point solvent which overcomes the challenges with temperature induced Se-vacancy generation. Fabricated devices have been utilised for electroless decoration of In_2Se_3 with Au enhances the PEC PD performance by suppressing the transient losses.

Esterase-responsive Fluorogenic Prodrugs of Aldose Reductase Inhibitor Epalrestat: An Innovative Strategy towards Enhanced Anticancer Activity

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Abstract: In addition to the conventional chemotherapeutic drugs, potent inhibitors of key enzymes that are differentially overexpressed in cancer cells and associated with its progression are often considered as drugs of choice for treating cancer. Aldose reductase (AR), which is primarily associated with the complications of diabetes, is known to be closely related to the development of cancer and drug resistance.[1] Epalrestat (EPA), an FDA-approved drug, is a potent inhibitor of AR and exhibits anticancer activity.[2] However, its poor pharmacokinetic properties limit its bioavailability and therapeutic benefits.[3] We report herein the first examples of the esterase-responsive turn-on fluorogenic prodrugs RM-13 and RM-28 for the sustained release of EPA to the cancer cells with turn-on fluorescence readout.[4] Prodrugs were designed to be activated by esterases, enabling simultaneous release of the active drug (EPA) and a fluorophore, as confirmed by spectroscopic and HPLC studies. The released EPA showed effective inhibition of AR in aqueous conditions, while the prodrugs demonstrated enhanced anticancer activity in HeLa cervical cancer cells. Intracellular drug release was further verified through fluorescence "turn-on" imaging. Overall, these fluorogenic prodrugs improve EPA's anticancer efficacy and therapeutic potential.

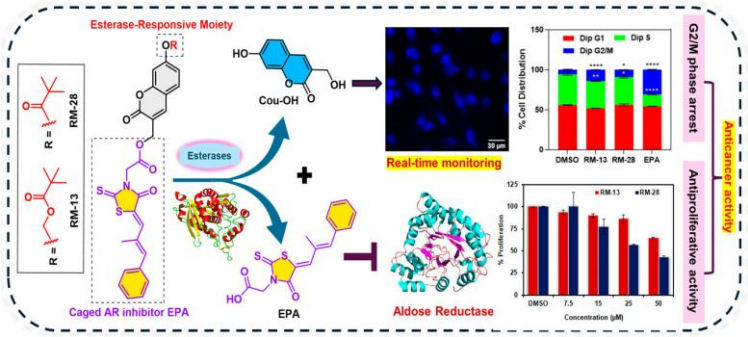

Figure 1. Graphical abstract representing the activation of RM-13 and RM-28 in the presence of esterase with concomitant turn-on fluorescence.

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Construction of Mixed Addenda Polyoxometalates by Cooperative Self-Assembly and Tuning of Their Optoelectronic Properties

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Abstract: Polyoxometalates (POMs), molecular metal oxides with tunable structures and redox properties, enable diverse catalytic applications. Sandwich-type POMs, with TM centres bridged by lacunary polyoxoanions, enhance stability and redox tunability, while mixed-addenda variants (Mo/W) enable orbital engineering. Incorporation of Mo into sandwich POMs lowers the band gap, tuning optoelectronic properties for enhanced functionality. Here, we demonstrate how a cooperative mixed-metal mixed-addenda strategy—using diverse TM centres (TMe(II)=Fe/Co/Ni/Zn; TMi(III)=Mn/Fe) and addenda (X=Zn/Co; Mo/W)—constructs novel Weakley-type sandwich POMs exemplified by $[Co_2Fe_2(H_2O)_2(CoW_9O_{34})_2]^{n-}$ and $[Zn_2Fe_2(H_2O)_2(ZnW_9O_{34})_2]^{n-}$ plus their Mo/W mixed-addenda variants. This approach drives orbital engineering through controlled d-orbital interactions between TM centres and addenda sites, enabling band-gap modulation, directed charge transfer from metal-oxo frameworks to reduced TM/Mo sites, and tailored LUMO distributions for optimised redox behaviour. To demonstrate these effects, OER studies confirm the orbital-engineered POMs' superior electrocatalytic performance for oxygen evolution in water splitting.

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Rational Design of Cu-Based Metal-Organic Framework (MOF) for Selective Electrochemical Nitrate-to-Ammonia Conversion

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The electrochemical nitrate reduction reaction (NO_3RR) has emerged as a sustainable and environmentally friendly method for the simultaneous remediation of nitrates and the synthesis of ammonia (NH_3) under ambient conditions, offering a promising alternative to the energy-intensive Haber–Bosch process. However, the slow reaction kinetics, inadequate intermediate adsorption, and competing hydrogen evolution reaction significantly restrict the catalytic efficiency and NH_3 selectivity of the currently available electrocatalysts. In this study, we have synthesized the Cu-based metal–organic framework (Cu-MOF) and employed it as an electrocatalyst in its pristine form for effective NO_3RR under ambient conditions. The synthesized Cu-MOF exhibited exceptional electrocatalytic performance for ammonia production due to the unique coordination environment of the Cu active centers, which provide a greater number of accessible active sites. The catalyst achieved a high Faradaic efficiency of 85.5% with an NH_3 yield rate of 1.25 mmol h^{-1} cm^{-2} at a low applied potential of −0.336 V vs. RHE (0.1 M Na_2SO_4 + 0.01 M KNO_3), demonstrating remarkable activity and selectivity for nitrate conversion. Furthermore, the catalyst displayed good stability for up to 21 hours, maintaining a Faradaic efficiency of 76.2%. Additionally, the effect of pH (0.1 M KOH + 0.01 M KNO_3) was also investigated, where the catalyst sustained a Faradaic efficiency of 88.5% at -0.78 vs RHE. Thus, this research underscores the potential of pristine Cu-based MOFs as highly effective and sustainable electrocatalysts for ammonia electrosynthesis and provides valuable insights into the rational design of advanced porous catalytic systems for energy conversion and environmental remediation.

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Development of a simple dipeptide - based liquid droplets as compartments and fibrils as enzyme mimics

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Abstract: Coacervates, formed by liquid–liquid phase separation (LLPS), are widely recognized as model protocells—primitive cell-like compartments that could have facilitated the emergence of life. These microdroplets create distinct physicochemical environments that promote chemical reactions by enhancing the local concentration of reactants. However, coacervates are generally made of multiple macromolecular components, and designing short peptide analogues capable of self-coacervation has proven difficult. Here, we present a minimalistic dipeptide design, made of one hydrophobic residue attached with polar residue histidine. This dipeptide can self-coacervate into micrometre-sized liquid droplets. These droplets act as microreactors. This work provides a stepping stone for new coacervate-based protocells made of simple peptide species. Furthermore, at lower concentrations and varying pH, the dipeptide assembles into fibrillar morphologies. Theses fibrillar morphologies are chosen for hydrolase activity. The presence of histidine makes them an efficient catalyst as esterase mimics. These findings not only offer insights into the origins of protocellular structures but also pave the way for innovative material designs with dual functionality—self-coacervation and catalysis. Overall, this study provides a unique route for the development of versatile materials with applications in catalysis and synthetic biology. “We designed a dipeptide with balanced hydrophobicity and hydrophilicity that forms fibril at low concentration and coacervates at higher concentration. The peptide showed catalytic activity in both fibrillar and coacervate states. The design is versatile and hence suitable for diverse applications”.

Synergistic role of the Cu+/Cu0, acidic-basic sites, and the oxygen vacancy for the hydrodeoxygenation of the lignin-derived compounds

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Abstract: The synthesis of value-added chemicals from lignin has gained much attention in recent years. However, despite the extensive use of noble metal-based catalysts and high-pressure hydrogen, the hydrodeoxygenation (HDO) of lignin derivatives is still challenging. In this work, non-noble metal-based heterogeneous catalysts derived from layered double hydroxide have been explored for HDO reaction without molecular hydrogen. A series of CuMgAl (CMA) catalysts has been studied, wherein CMA1.5 catalyst shows a high catalytic activity for HDO of vanillin with 100% conversion and 87% yield of 4-methyl-2-methoxyphenol (MMP) within 30 min at 180 °C in isopropyl alcohol. The detailed investigations show that superior catalytic activity is attributable to synergistic role of Cu^0/Cu^+ ratio, acidic–basic sites, and oxygen vacancies (O_v). Furthermore, density functional theory studies and various control reactions confirm the reaction mechanism, role of O_v, acidic and basic sites for HDO of vanillin. In addition, catalyst shows excellent activity for various other lignin derivatives, demonstrating its broad substrate scope. The catalyst also exhibits excellent productivity (49.71 $mmol_{MMP}\ g_{cat}^{-1}\ h^{-1}$), superior to earlier reports. Hence, this work can pave the way toward a green and sustainable catalytic transfer HDO of lignin derivatives to value-added chemicals within short reaction times.

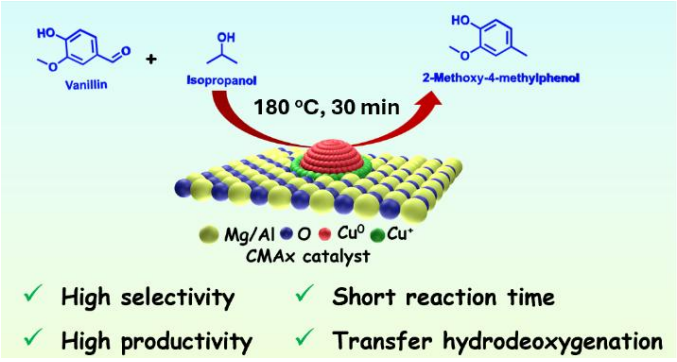

Figure 1. Catalytic hydrodeoxygenation of vanillin to MMP using CMAx catalyst.

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Regeoselective hydro-heteroarylation of 1,6-diyne via carboxamide assisted indole c(2)-h activation using cobalt catalyst

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Abstract: In this study, the novel reactivity of a cobalt (III) catalyst in the functionalization of 1,6-diynes was presented. The reaction mechanism was analysed, revealing the in-situ generation of a six-membered cobalt cycle, which subsequently underwent further functionalization with 1,6-diynes. Experimental evidence from radical quenching experiments indicated the involvement of an ionic pathway in this conversion. Furthermore, the hydrogen scrambling experiment lent further support to the proposed mechanism. Significantly, this methodology exhibited extensive versatility, accommodating a diverse array of electronically distinct substrates and reactive partners in a highly atom-efficient manner.

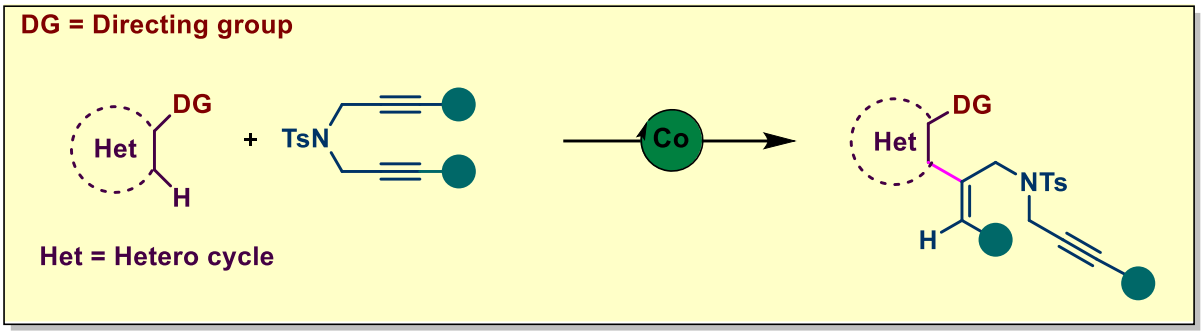

Figure 1. Synthesis of enyne through cobalt catalysed

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Differences Between Cobalt(II)-Exchanged X and Y Faujasite Zeolites and Catalytic Conversion of Alkene to Cyclic Carbonate

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Abstract: Zeolites are crystalline aluminosilicates comprising of TO_4 (T = Si or Al) units. Zeolites X and Y are faujasite zeolites with Si/Al ratios of 1.23 and 2.75, respectively. The negative charge of the framework is balanced by exchangeable cations. During ion-exchange, the incoming ion can occupy certain positions in the unit cell, which are represented using roman numerals: I, I', II, II', III, and III'(as shown in the figure below). Co^{2+}-exchanged X and Y zeolites (CoX and CoY) show distinct behaviors towards the occupancy of the Co^{2+} ion in different positions of zeolites X and Y. This difference is reflected in their interactions with solvent *N,N'*-dimethylformamide. Co^{2+} in zeolite X exists as a tetrahedral coordination in DMF, whereas in zeolite Y, the oxide of cobalt is observed. These observations were noted from UV-Vis DRS, XPS, TPR, BET, and Raman studies. The distinction also becomes apparent during the catalytic conversion of styrene to styrene-carbonate. This transformation has been attempted in the presence of a mixture of O_2 and CO_2 in DMF as a solvent at atmospheric pressure. With varying Co^{2+} loading, as catalyst, CoX and CoY exhibited opposite trends in styrene carbonate yields. A maximum yield of 35.7% for styrene carbonate was achieved with CoX with relatively higher metal loading whereas similar yield was obtained by CoY with relatively lower loading. Differences in the recyclability properties of CoX and CoY were also noted.

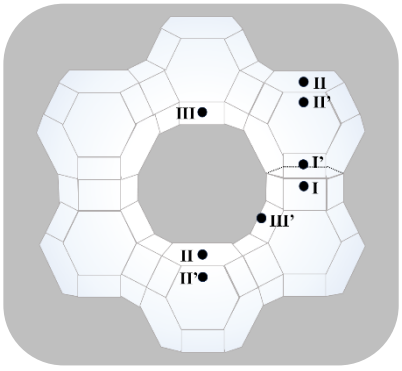

Figure 1. Structure of Faujasite zeolites and the ion-exchange positions.

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Mitigating Cuproptosis in *Solanum lycopersicum* Root Using Iron Oxide Nanoparticles

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Abstract: Copper (Cu), while essential for plant metabolism, becomes acutely cytotoxic upon excess accumulation, inducing oxidative stress and severe growth inhibition. Although cuproptosis has been well characterized in mammalian systems, whether a similar cell death pathway exists in plants remains unclear. To investigate this, we used *Solanum lycopersicum* root apex cells as a model system. Our results show that excess Cu first damages the mitochondria, disrupting their normal function and causing a sharp rise in reactive oxygen species (ROS). These elevated ROS then travel to the nucleus, where they disturb chromatin organization and alter nuclear structure. This sequence of events points to mitochondrion to nucleus is stress signalling pathway of copper toxicity in plants. Guided by this mechanistic insight, we engineered glutathione (GSH) and 3-mercaptopropionic acid (MPA)-functionalized chitosan-coated Fe_3O_4 nanoparticles as a targeted, multi-modal mitigation strategy. This nano-platform simultaneously harnesses Fe_3O_4 nanozyme ROS scavenging, GSH-mediated intracellular redox restoration, and MPA thiol-driven selective Cu^{2+} sequestration, collectively restoring cellular homeostasis and alleviating copper-induced cytotoxicity in plants.

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Synthesis of glycerol carbonate from glycerol using ZnO decorated functionalised gC_3N_4 with urea as CO_2 surrogate

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Abstract: The production of a variety of functional moieties of industrial importance from CO_2, a molecule with relatively low reactivity, is a challenging subject. According to the Global Opportunity Analysis and Industry Forecast for 2022-2031, the biodiesel market was valued at 2,781.0 million in 2021 and is anticipated to expand to 3,579.1 million by 2031, with a compound annual growth rate (CAGR) of 2.6% [1]. The refined glycerol segment dominated the market, accounting for a 77.1% share [2]. This context presents a substantial opportunity to employ glycerol as a sustainable and alternative feedstock for numerous chemical intermediates. Organic carbonates, such as glycerol carbonates, are essential commodity chemicals due to their extensive use and growing demand as chemical intermediates, particularly as polymer precursors [3]. By utilizing urea as a CO_2 surrogate, glycerol carbonate can be synthesized from glycerol, a by-product or waste from the oleochemicals industry, thereby supporting the integrated bio-refinery initiative. ZnO-gC_3N_4 catalyst materials have demonstrated high efficiency in converting glycerol to glycerol carbonate using urea. Comprehensive studies of these catalyst materials reveal that both basic and acidic sites within the catalyst system contribute to their exceptional activity. The basic and acidic sites on the same catalyst activate the glycerol and urea molecules, respectively.

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Dynamic hysteresis and transitions controlled by asymmetry in potential barrier shaping

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Abstract: The majority of the state transitions in nature and in designed systems follow nonlinear and nonequilibrium paths. Sometimes bistability induced by the nonlinearity of the dynamics of such processes has an interesting interplay with the inherent fluctuations or noise, which is characteristic of the nonequilibrium phenomena. In many such cases, external forcing, which appears as a signal, becomes an inevitable part of the dynamics, leaving significant effects on the system's response[1]. In the case of dynamic hysteresis, the external signal is particularly periodic, which generates a periodic response for the system; however, with a relaxational delay. Our study considers the role of asymmetry in the potential and how the presence of this asymmetry governs the dynamics of the system consequently affecting the transition from one state to another. We investigate the precise role of the underlying potential in regulating the fundamental processes of dynamic hysteresis. We identify that it is possible to induce symmetry breaking in dynamic hysteresis, and consequently to observe dynamic transitions under moderate conditions, which is absent for the symmetric case, if appropriate asymmetry is implemented in the design of the underlying potential. This kind of asymmetry appears through the disparate widths of the two wells of the intrinsic bistable potential governing the dynamics and the barrier separating them. It is characteristically distinct from the potential in which the two minima are energetically dissimilar. Our understanding suggests that only the intrinsic asymmetry of the former type can substantially influence the elemental dynamics of the processes to generate significant effects on the outcomes. Our study presents a novel approach to quantitatively regulate the outputs, to increase or decrease the extent of dynamic hysteresis, based on the requirements, by effectively controlling the proper asymmetry of the intrinsic potential. The results obtained numerically have been further corroborated with a semi-analytical approach considering the bistable potential.

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Diphenylimidazol-acetylcoumarin (ACDPI) a promising fluorescent donor material for organic photovoltaics: Photophysical, Solvatochromic, and Electronic structure studies

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Abstract: In this study we report the solvatochromic behavior and photophysical properties of the fluorescent probe diphenylimidazol-acetylcoumarin (ACDPI). The effects of solvent polarity, specific solute–solvent interactions, and excited-state (ES) dipole moment variations were analyzed using established solvatochromic models. The time-dependent fluorescence measurements provided deeper insight into solvent–solute interactions in relation to Catalan parameters and Stokes shift behavior. Catalan multiparametric analysis revealed that solvent dipolarity/polarizability (SdP) dominantly govern the solvatochromism. Upon increasing the solvent dipolarity and acidity the fluorescence decay time decreases, whereas higher polarizability enhanced it. The steady state and time-resolved fluorescence decay analysis suggest the intramolecular charge-transfer (ICT) process with high ES dipole moment than the ground state (GS). The quantum chemical calculations (DFT and TD-DFT) corroborates experimental observations including dipole moments, HOMO–LUMO energy levels, band gaps, and simulated absorption spectra. The low HOMO–LUMO energy gaps (3.40 eV in solvents and 3.08 eV in gas phase) and experimentally estimated band gaps (2.48–2.59 eV) suggested the suitability of probe as a promising optoelectronic material. Molecular electrostatic potential (MEP) mapping and natural bond orbital (NBO) analysis suggested potential reactive sites for photochemical interactions and stabilization of charge-transfer characteristics within the molecule, respectively. Probe shows nonlinear optical (NLO) properties. The polarizability (α) and first-order hyperpolarizability (β) values are 50.98×10^{-24} and 15.94×10^{-30} esu, respectively. Additionally, in toluene enhanced oscillator strength and a predicted power conversion efficiency (PCE), ~ 37% highlight its potential as an efficient light-harvesting and donor material for organic solar cells.

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Superabsorbent Hydrogel for Antibacterial Drug Delivery Capable of Infectious Wound Healing

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Abstract: Chronic wounds and secondary bacterial infections present significant challenges in clinical wound management, necessitating the development of advanced drugs and biomaterials that offer both protective coverage and therapeutic intervention. Antimicrobial molecules developed as substitutes of antimicrobial peptides and lipopeptides are effective against resistant bacterial strains due to significant antimicrobial activity. Such molecules possess the potential to be successfully utilized against secondary bacterial infections and treatment of chronic wounds. Our work explores the synthesis and characterization of a hydrogel system specifically engineered with high swelling capacity (~ 450% swelling) and optimized solubility to facilitate efficient delivery of a novel antibacterial drug for accelerated wound healing. The fabricated hydrogel features a highly porous and specialized three-dimensional polymeric network designed through cross-linking strategy. This framework enables the material to effectively absorb large volumes of wound exudate and maintain a moist interfacial environment a superior swelling ratio, allowing re-epithelialization. Furthermore, the sustained and localized release of encapsulated antibacterial agents was ensured by the solubility of the hydrogel through sustained release of the compound and controlled degradation of the hydrogel. Such mechanism of the hydrogel maintains therapeutic concentrations at the wound site over extended periods, while preventing the formation of bacterial biofilms. Significant inhibitory effects against both Gram-positive (*S. aureus*) and Gram-negative (*E. coli)* bacteria was exhibited by the hydrogel under in vitro evaluations. Evaluation of mechanical properties (~ 10 MPa stress and ~ 20 % EB) confirmed that the hydrogel retains structural integrity under physiological conditions while remaining flexible enough to conform to irregular wound geometries. With complete biodegradation upon disposal under natural environmental conditions, the developed hydrogel presents a significant approach towards a biomaterial with sustained and specialized antibacterial activity for infectious wound healing application.

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Organophotocatalytic synthesis of oxadiazoles: Applications in natural product diversification

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Abstract: Oxadiazoles remain pivotal structural motifs in both natural product synthesis and drug discovery. These scaffolds demonstrate a broad spectrum of pharmaceutical utility[1], including roles as anti-cancer drug (Zibotentan), anti-hypertensive drug (Nesapidil), and antibacterial agent while also serving as critical building blocks in OLED as well as functional materials science. To match the versatile utility of 1,3,4-oxadiazoles, researchers have developed[2] various synthetic strategies, most notably the oxidative cyclization of N'-benzylidenebenzohydrazide and the dehydrative cyclization of 1,2-diacylhydrazines. However, many conventional methodologies rely on transition metal catalysis or using of strong oxidizing agents. These constraints often may restrict practical application such as diversification of natural derivatives. We report an efficient and simple organophotocatalytic[3] approach for the synthesis of 2,5-disubstituted-1,3,4- oxadiazole from N′-benzylidenebenzohydrazide in MeOH in moderate to good yields. In this approach, the reaction has been caried out under mild, relatively low catalyst loading and metal free condition. Importantly, the present method has allowed derivatization of several natural products resulting in diversification of natural product based molecular library.

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Selenium nanoparticles loaded, multifunctional, self-assembled peptide gel for enhanced wound healing

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Abstract: Chronic wound healing poses a significant clinical challenge, driven by multiple pathological barriers, including bacterial colonization, persistent inflammation, impaired cellular response, and inadequate angiogenesis, all of which disrupt the natural healing cascade. Furthermore, the excessive use of antibiotics in wound management has led to the emergence of drug-resistant pathogens, highlighting the need for alternative, drug-free therapeutic approaches. To address this challenge, we have developed drug-free materials with the capability to exhibit antibacterial, antioxidant, and pro-angiogenic properties. We developed a drug-free, multifunctional biomaterial with intrinsic antibacterial, antioxidant, and pro-angiogenic properties. A self-assembled lauric acid-conjugated peptide gel was fabricated, incorporating pro-angiogenic selenium nanoparticles within its fibrous network (SePG). The SePG gel exhibited strong antioxidant activity (~91%) and potent antibacterial efficacy (~89% against *E. coli* and ~94% against *S. aureus*). *In vitro* studies showed high cytocompatibility, with enhanced cell viability (~109% in L929 and ~95% in HUVECs) and improved endothelial tube formation, confirming pro-angiogenic potential. Scratch assays revealed accelerated cell migration and improved wound closure in SePG-treated groups compared with untreated controls. Consistent with these findings, *in vivo* studies showed that SePG markedly accelerated wound healing, achieving approximately 92% wound closure within 6 days. Histological analyses further confirmed enhanced re-epithelialization and increased collagen deposition. Additionally, SePG exhibited superior hemostatic performance, with minimal blood loss (0.09 ± 0.05 mg) and a shortest hemostatic time (50.67 ± 8.5 s). Collectively, these findings suggest that SePG is a promising drug-free, bioactive platform for accelerated wound healing and rapid hemostasis, integrating antioxidant, antibacterial, and angiogenic properties.

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Sustainable CS-MWCNT doped Eutectogels synthesis via Rapid Frontal Polymerisation: High-Strength Conductive Composites

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Abstract: Frontal polymerisation (FP) offers a rapid, energy-efficient route to fabricate multifunctional eutectogels, yet integrating conductive nanofillers like multi-walled carbon nanotubes (MWCNTs) remains underexplored for electronic applications. Here, we report chitosan-functionalized MWCNTs (CS-MWCNTs) incorporated into a polymerisable deep eutectic solvent (DES) to form eutectogel composites. CS grafting onto oxidised MWCNTs via amide coupling enhances filler dispersion and interfacial hydrogen bonding within the DES matrix, [1] enabling homogeneous nanocomposites. Thermal FP, initiated at localised hotspots, propagates self-sustaining fronts (<4 min) to yield robust CS-MWCNT/eutectogels with tunable MWCNT loadings (0.5–3 wt%). The resulting composites exhibit superior mechanical strength, ionic conductivity, and adhesiveness, attributed to percolated MWCNT networks reinforced by dynamic DES crosslinking. Self-healing efficiency exceeds 90% at 60 °C, driven by reversible H-bonding. For electronics, these eutectogels serve as flexible strain sensors (gauge factor ~2.5, 500% stretchability) and Joule-heatable actuators, withstanding >1000 cycles. FP scalability and waste-derived DES compatibility position CS-MWCNT eutectogels[2] as sustainable alternatives to conventional conductive polymers, advancing soft robotics and wearable devices.

Keywords: Frontal polymerisation, eutectogels, flexible electronics, deep eutectic solvent.

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Dansyl-based aggregation-induced emission material for differential recognition of toxic hair color ingredients: towards functional device applications

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Abstract: We designed and synthesized an imino-linked dansyl-based molecule, DHNB, which exhibits interactions with the hair color ingredient p-phenylenediamine (PPD) and its oxidative trimer, Bandrowski's Base (BWB), over other analytes tested. Variable interactions, such as intra- and inter-molecular hydrogen bonding and environment-responsive conformational dynamics, were observed, leading to contrasting responses amongst the most responsive analytes. DHNB exhibits excited state intramolecular proton transfer (ESIPT)-assisted aggregation-induced emission (AIE) in MeOH:H_2O (10: 90), which is utilized for the detection of hair color ingredients. The presence of BWB quenches the fluorescence emission of DHNB in MeOH:H_2O (10 : 90) at 497 nm, whereas in the presence of PPD, the emission at 497 nm is quenched, with simultaneous appearance of a new blue shifted band at 402 nm. Importantly, the successful detection of PPD in a commercial hair color sample underscores the practical applicability of DHNB. Furthermore, variations in the charge transport properties of DHNB in MeOH:H_2O (10:90) and upon interaction with BWB/PPD were observed via current-voltage (I-V) measurements, suggesting its strong potential as an electrical sensor device.

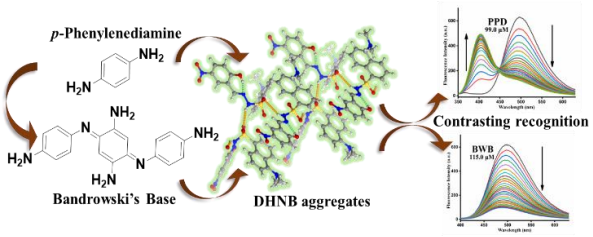

Figure 1. An AIE probe (DHNB) enables selective detection of toxic hair dye components, p-phenylenediamine (PPD) and Bandrowski's base (BWB), via ESIPT-driven contrasting fluorescence responses.

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Bifunctional Sr(II)-Based Coordination Polymer for Fluorescent Sensing of Ba(II)/ Nitroaromatic Compounds and Supercapacitor Applications

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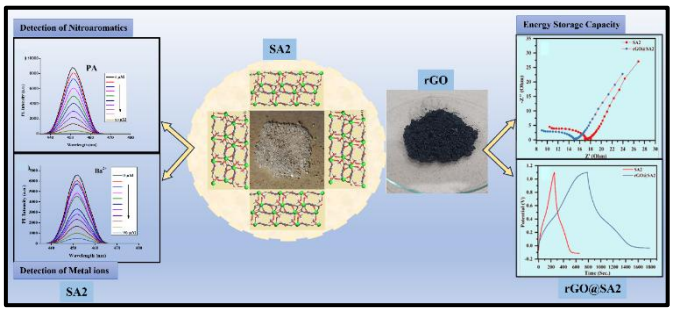
Abstract: Coordination polymers (CPs) based on main group elements are being investigated extensively for energy storage and sensing applications due to their electropositive characteristics and structural adaptability. In this study, Strontium metal ion-based CP (SA2) was synthesized using 3,5-pyridine dicarboxylic acid (PDC). SA2 was validated using single-crystal X-ray diffraction (SC-XRD). According to the topological rod net representation SA2 followed the *(6,3) lla* underlying net topology. However, to improve the electrochemical properties of SA2, a nanocomposite rGO@SA2 was fabricated by inducing reduced graphene oxide (rGO) via sonication method. The successful synthesis of SA2, rGO, and rGO@SA2 were confirmed by spectroscopy and microscopy (PXRD, FT-IR, TGA, UV-Vis, SEM, and HR-TEM, respectively). SA2 demonstrated remarkable fluorescence selectivity for picric acid (PA-95%) among 1,4-nitroaniline (NA-83%) and benzoic acid (BA-49%) and was an excellent sensor for Ba^{2+} (92%) metal ions. Furthermore, the electrochemical investigation was carried out using galvanostatic charge-discharge (GCD) and cyclic voltammetry (CV) techniques, which revealed that SA2 and rGO@SA2 had good specific capacitances of 153.57 Fg^{-1} and 383.38 Fg^{-1} at a current density of 0.5 Ag^{-1}, respectively. After 2000 cycles, rGO@SA2 retained a capacitance of 96.32%. Figure 1 depicts the graphical abstract, summarizing the scope of the current work.



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Interfacial Built-In Electric Field at p–n Junction in $Bi_2Sn_2O_7/InVO_4$ for Efficient Photocatalytic Degradation and Electrocatalytic HER

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Abstract: Herein, a heterostructure of pyrochlore-based *p*-type $Bi_2Sn_2O_7$ and *n-type* $InVO_4$ has been developed for photocatalytic generation of hydroxyl radical (*OH*·) and singlet oxygen ($^1O_2$), and for electrocatalytic hydrogen evolution reaction (HER). The enhanced photocatalytic generation of *OH*· and $^1O_2$ is confirmed by electron paramagnetic resonance (EPR) studies upon exposure to visible light at λ = 420 nm.[1] The enhanced generation of reactive oxygen species accounted for 95.8% photocatalytic degradation of tetracycline hydrochloride within 20 min (pseudo-first-order degradation rate constant of $k = 0.105$ min^{-1}), which is attributed to the interfacial built-in electric field at the p–n junction of $Bi_2Sn_2O_7/InVO_4$, as suggested by the Mott-Schottky, XPS and KPFM studies. Similarly, the efficient electrocatalytic activity of $Bi_2Sn_2O_7/InVO_4$ is revealed from a lower HER overpotential (η_{10} = 121 mV) as compared to the pristine $Bi_2Sn_2O_7$ or $InVO_4$, and it achieved 95.2% faradaic efficiency. The improved HER is attributable to the mobility of charges facilitated by the internal electric field in $Bi_2Sn_2O_7/InVO_4$, adsorption/desorption of hydrogen intermediates at the interface, improved charge kinetics (Tafel slope = 32 mV dec^{-1}), higher electrochemical surface area, and lower charge transfer resistance.[2]

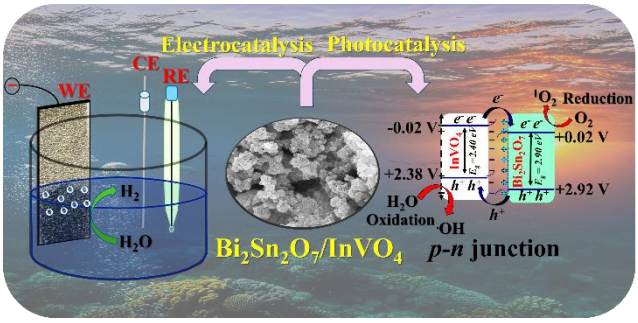

Figure 1. Representation of the Built-in Electric Field at the Interface of the p–n $Bi_2Sn_2O_7/InVO_4$ and the respective electrocatalytic alkaline HER (left) and photocatalytic ROS generation (right) for tetracycline degradation.

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Study of stochastic thermodynamics and dynamic hysteresis in autocatalytic reaction networks

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Abstract: From a bigger perspective, we aim to study the kinetic and thermodynamic aspects of chemical computation, which is a recent and very important field of research. The idea is to identify whether there are advantages of chemical computations over conventional computational processes. The analyses focus on a systematic exploration of parameter regimes and identifying the conditions that yield favorable, efficient, and robust reaction outcomes. The components of the chemical computational processes are reported to be the reaction networks involving autocatalytic steps. Therefore, we concentrate on a specific chemical reaction network represented by the Schlögl model, to start with. Here, an autocatalytic step is present that gives rise to bistability in terms of the concentration of the autocatalytic species involved in the reaction through a nonlinear feedback mechanism. The external drive is incorporated in the reaction network through the rate of pumping of another species, which is periodic in time. The lag of the system's response in terms of the concentration evolution of the autocatalytic species with respect to the external control manifests in the formation of hysteresis loops. The amplification of the system's feedback towards the external periodic drive under definite conditions is understood through the study of the hysteresis loop area. The loop area tends to vanish in the quasi-static limit, signifying the dynamic nature of the hysteresis. We noticed the turnover of the quantity with respect to the relevant control parameters of the dynamics. We suggest that our present study can be considered to be the initial steps in understanding some of the kinetic aspects related to chemical computation. Also, we emphasize that this is an early analysis of dynamic hysteresis in chemical reactions, where the concentration of the chemical species is the regulating variable. We carry out stochastic thermodynamic calculations in the form of Shannon entropy. We link this quantity to the response of the system through hysteretic behavior to interpret the connection of hysteresis and information loss in a chemical system.

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Synergistic Heterostructure of Flower-Like Iron-Cobalt-Nickel Layered Double Hydroxide and Copper Cobalt Seleno-spinel for High-Performance Screen-Printed Energy Storage and Sensors

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Abstract: A scalable strategy for the fabrication of a tri-functional microelectronic platform comprising a micro-supercapacitor, humidity sensor, and electrochemical sensor is demonstrated using a single screen-printable conductive ink. The ink was formulated from a novel FCN/CCS nanocomposite, integrating the high electrical conductivity of $CuCo_2Se_4$ with the abundant catalytically active sites of FeCoNi-LDH. This multifunctional ink enables the fabrication of devices through a simple and cost-effective screen-printing process. The resulting flexible screen-printed microsupercapacitor delivered a high areal capacitance of 573.8 mF cm^{-2}, with corresponding energy and power densities of 89.7 mWh cm^{-2} and 453.2 mW cm^{-2}, respectively. Owing to the hydrophilic nature of FeCoNi-LDH, the printed humidity sensor exhibited a wide detection range of 11–97% relative humidity, rapid response/recovery times of 78/106 s, and low hysteresis (1.67% at 85% RH). The practical applicability of the device was demonstrated by monitoring humidity variations in fresh meat degradation over two days. In addition, the electrochemical sensor showed excellent electrocatalytic activity toward methotrexate (MTX) detection in pharmaceutical and biological samples, with good repeatability (RSD = 3.53%). This work provides a low-cost, scalable route to integrate multifunctional sensing and energy-storage devices. [1]

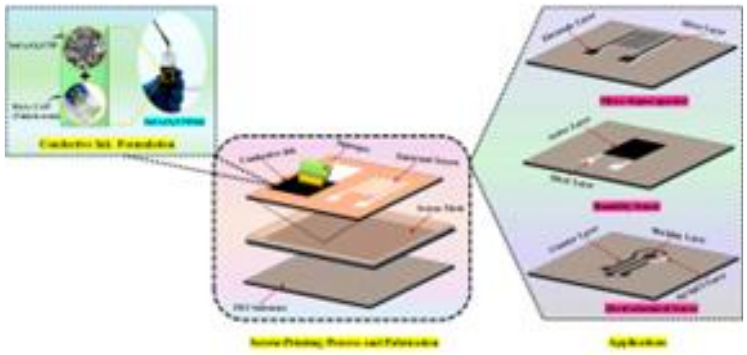

Figure 1. Schematic representation of an energy storage and sensing device

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Electrocatalytic nitrogen reduction under ambient conditions using metal boride catalysts

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Abstract: Ammonia serves a dual role as an efficient hydrogen carrier owing to its high energy density, and as an essential raw material widely utilized across fertilizer production, pharmaceutical manufacturing, and various light industrial applications. The electrochemical nitrogen reduction reaction has recently emerged as a sustainable and energy-efficient strategy for ammonia synthesis under ambient conditions. However, achieving high catalytic efficiency and selectivity remains a significant challenge. Herein, a sequence of metal boride catalysts was prepared *via* a simple one-step hydrothermal method. Their structural and morphological features were systematically characterized using standard analytical techniques. The electrocatalytic efficacy of the amorphous catalysts was assessed using cyclic voltammetry and linear sweep voltammetry in a three-electrode system, with catalyst-coated electrodes serving as the working electrode. The yield of products, Faradaic efficiency, and possible reaction mechanism will be discussed in detail, highlighting the potential of metal boride catalysts for efficient ambient ammonia synthesis.

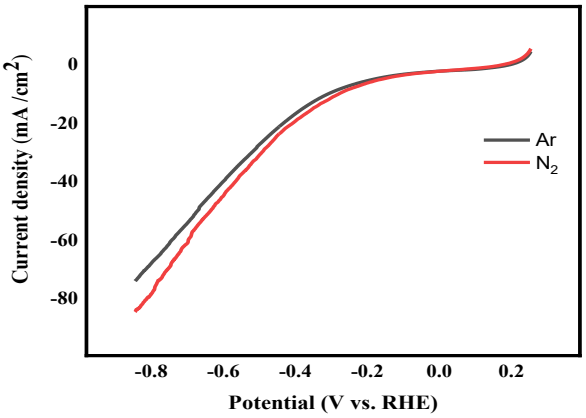

Figure 1. Linear sweep voltammetry profiles of catalyst-coated electrodes in Ar- and N_2-saturated solution comprising 1.0 M KOH and 0.1 M Na_2SO_4.

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Crowder Induced Phase Separation Modulates the Huntingtin Protein Aggregation Landscape

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Abstract: Huntington's disease (HD) is a progressive neurodegenerative disorder caused by the misfolding and aggregation of the huntingtin (HTT) protein, resulting from expansion of the polyglutamine tract in the HTT gene. Aggregation of mutant HTT is modulated by macromolecular crowding, a defining feature of the spatially heterogeneous intracellular environment. Here, we examine the influence of mixed macromolecular crowders on the aggregation of the intrinsically disordered Huntingtin exon-1 protein with a pathogenic polyglutamine length (HD39Q). Using thioflavin T (ThT) kinetics, we show that binary mixtures of polyethylene glycol (PEG8), dextran (40 and 70), and Ficoll 70 produce biphasic aggregation kinetics, reflecting distinct nucleation and growth regimes. Additionally, confocal imaging reveals that these binary mixtures give rise to phase-separated conditions, wherein crowding-induced liquid–liquid phase separation (LLPS) influences the spatial distribution of aggregates in a composition-dependent manner. Extending beyond binary systems, ternary crowder systems were also investigated to better mimic intracellular complexity, giving rise to hierarchically organized droplet architectures that further modulate aggregation pathways and protein localization. Comparative aggregation studies with model proteins (bovine serum albumin, β-lactoglobulin, and lysozyme) reveal that aggregation and partitioning depend on both the biomolecular properties and phase composition. These findings demonstrate that mixed macromolecular crowding reshapes the aggregation landscape by introducing spatiotemporal heterogeneity, thereby enhancing physiological relevance.

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Self-Assembled Triblock Copolymer Micelles as Precursors for N, S, Fe-Doped Electrocatalysts for Efficient Oxygen Reduction Reaction

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Abstract: Efficient electrocatalysts for the oxygen reduction reaction (ORR) are critical for advancing sustainable energy conversion technologies. In this study, we report the design and synthesis of iron-incorporated triblock copolymer based electrocatalysts supported on nitrogen, oxygen, and sulfur co-doped micellar systems featuring a hierarchical meso-macroporous architecture[1]. A reversible addition fragmentation chain transfer (RAFT) polymerization strategy was employed to fabricate well defined micelle forming triblock copolymer templates[2]. The synthesized polymers were systematically loaded with varying Fe-to-polymer weight ratios to investigate their influence on catalytic performance. Comprehensive structural and physicochemical characterization was carried out using ^{1}H NMR, FT-IR, TGA, XRD, and UV-Vis spectroscopy. Notably, the triblock copolymer exhibited a morphological transition from conventional spherical micelles to vesicle-like nanostructures, offering valuable insights into the tunability of polymer self-assembly for catalytic applications[3]. Electrochemical studies of Fe^{2+}-loaded systems, complemented by BET surface area analysis and XPS investigations, demonstrated that the catalyst with an optimized Fe-to-polymer ratio of 1.0:1.0 delivers superior ORR activity. The enhanced performance is attributed to its favourable surface area, hierarchical porosity, and enriched heteroatom (N and S) content, which collectively promote efficient oxygen reduction kinetics. This work highlights a versatile polymer-templating approach for the development of advanced, non-precious metal-based ORR electrocatalysts with tunable morphology and improved catalytic efficiency.

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Zeolite Encapsulated Ni-Salmphen Complex: A Novel and Promising Class of Anticancer Agent

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Abstract: Cancer, being the second leading cause of death worldwide, is a major health challenge. After the breakthrough discovery of cisplatin as a chemotherapeutic agent, despite further advances, these approaches remain largely nonspecific, result in substantial toxicity and due to the improved immune systems of cancerous cells, have led to the development of drug resistance. To overcome these types of issues, an appropriate drug delivery system can effectively enhance the efficacy. Zeolites are biocompatible drug-delivery agents and, due to their porous frameworks, can release chemotherapeutic agents in a controlled manner. In this study, we demonstrate the anticancer activity of the Ni-Salmphen metal complex encapsulated in Faujasite zeolite-Y and zeolite-X, which differ in their Si/Al ratios. Ni(II)-Salmphen-encapsulated zeolite material has been thoroughly characterized by FT-IR, UV-Vis, UV-Vis-DRS, DLS, PXRD, and FESEM. For the internalization of zeolite system, zeolite-Y and zeolite-X have been tagged with coumarin-6 dye. Fluorescence spectroscopy reveals neutral and monocationic species of the dye., Both encapsulated complexes exhibit IC_{50} values of 5-10 µg/mL against MCF-7 breast cancer cells, with significant increases in reactive oxygen species, while having minimal effect on the viability of non-cancer cells. Moreover, they appear non-toxic to non-cancer cells, showcasing high selectivity towards cancer cells. To assess the stability and degradation of the Ni-Salmphen-encapsulated systems, these systems have been incubated at a lysosomal pH of 4.5. The slight leaching of the encapsulated compounds has been analyzed using UV-Vis spectroscopy, HRMS, and nitrogen physisorption techniques. The pH studies and biological assays demonstrate that Ni(II)-Salmphen, when entrapped in Faujasite zeolites, exhibits enhanced stability, promising cytotoxic properties and selectivity.

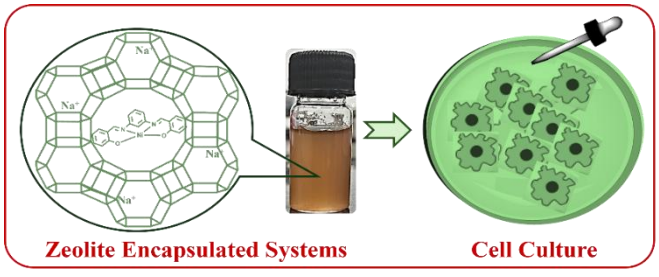

Figure 1. Ni(II)-Salmphen entrapped in Faujasite zeolites as anticancer agent for breast cancer cells.

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Three-Component Reaction through Rh(III) Catalyzed Strain Re-lease of Bicyclo[1.1.0]butanes

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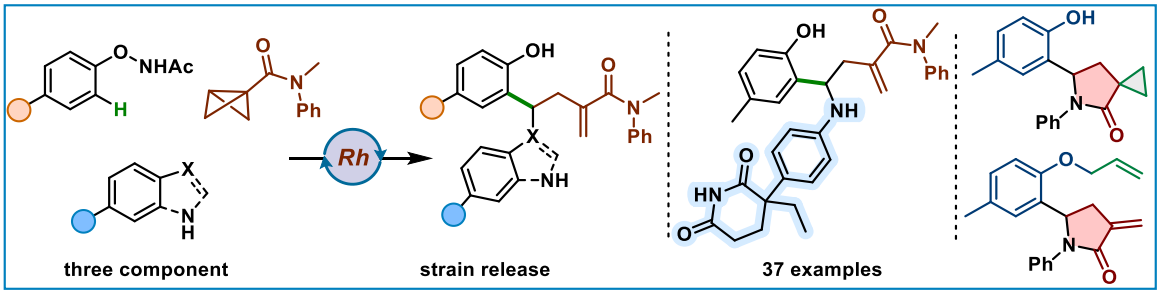
Abstract: We present a three-component reaction through Rh(III)-catalyzed strain release of bicyclo[1.1.0]butanes (BCBs) to synthesize substituted acrylamides. This protocol represents the first example of nucleophilic attack on the Rh(V) nitrenoid complex generated by the coupling of phenoxyacetamides and strained BCBs. The reaction proceeds under mild conditions and demonstrates broad compatibility with various functional groups on both phenoxyacetamides and nucleophiles, affording valuable substituted acrylamides. Furthermore, the products can be further transformed into important synthetic building blocks. Preliminary mechanistic studies support the proposed catalytic cycle.



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Growth of Lead-Free Perovskites Shell for $CsPbBr_3/Cs_2MoBr_6$ Core/Shell Nanocrystals for Enhanced Stability

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Abstract: All inorganic Colloidal lead halide perovskite nanocrystals (NCs) exhibit promising potential in photovoltaics and optoelectronics owing to their unique photophysical properties. However, their practical applications remain limited by challenges, including uncontrolled instantaneous nucleation in conventional synthesis, intrinsic structural instability, and lead toxicity risks. Shell-coating is an effective method for enhanced environmental stability while reducing toxicity by choosing non-toxic shell materials such as metal oxides, polymers, silica, etc. However, multiple perovskite NCs can be encapsulated within the shell material and a uniform shell growth of well-isolated NCs is still challenging. In this work, lead free vacancy ordered halide perovskites Cs_2MoBr_6 shells are attempted on the surface of $CsPbBr_3$ NCs by a hot injection colloidal method. The resulting core/shell nanocrystals demonstrate significantly enhanced optical performance and stability, maintaining intact lattice structures even after 90 days of ambient storage. Further, the effectiveness of the non-toxic double perovskite shell protection is demonstrated by the enhanced environmental and phase stability against UV illumination, water and heat. Using transient absorption spectroscopy, we investigated the disparity in the hot carrier thermalization pathways in the $CsPbBr_3$ and $CsPbBr_3/Cs_2MoBr_6$ core/shell NCs under the same laser fluence, which established the charge transfer from $CsPbBr_3$ to Cs_2MoBr_6. Our results will promote the further commercial development of inorganic perovskite materials in optoelectronic devices.

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Design and development of a 3D Zinc–Organic Framework with Integrated Sensing and Catalytic Functions

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Abstract: Metal–organic frameworks (MOFs) constitute an important class of functional materials owing to their tunable structures and wide applicability in sensing, gas capture and separation, and catalytic transformations.[1-3] In particular, d^{10} transition metal centers, frequently employed in the construction of emissive coordination frameworks, have also demonstrated remarkable catalytic potential when integrated with suitable functional environments.[4] In this work, a 3D zinc-based framework, designated as ZMB-MOF, was obtained under solvothermal conditions. Structural integrity and phase purity were established through elemental analysis, FT-IR spectroscopy, thermogravimetric measurements, UV–Vis spectroscopy, powder XRD, and single-crystal X-ray structure determination. The material displays a prominent emission band centered at 351 nm, accompanied by a shoulder under excitation at 298 nm. Notably, ZMB-MOF exhibits pronounced sensitivity and selectivity toward 4-NP, enabling its application as a fluorescence-based sensing platform. Furthermore, the framework demonstrates efficient catalytic activity in the Biginelli reaction, delivering high product yields at a catalyst loading of 6 mol%. These findings highlight the potential of ZMB-MOF as a multifunctional material for sensing-driven environmental monitoring and catalytic applications.

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Ligand and Temperature Controlled Stereodivergent Nickel-Catalysed Hydrophenoxylation of Ynamides

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Abstract: The controlled synthesis of both *E*- and *Z* stereoisomers remains a long-standing challenge in organic synthesis, yet it is important for accessing structurally and functionally diverse enamides. This study demonstrates the synthesis of E- and Z-hydrophenoxylated enamides using a nickel(II)-catalyst alongside phenols. The stereochemical outcome is controlled by the ligand environment and temperature. Ligands promote syn-addition via a keteniminium intermediate to afford the E-isomer, and elevated temperatures enable efficient E→Z isomerization to deliver the Z-isomer with excellent selectivity. This efficient and versatile strategy exhibits a broad substrate scope and functional group tolerance, including acids, bioactive estrone derivatives, sesamol, and related compounds.

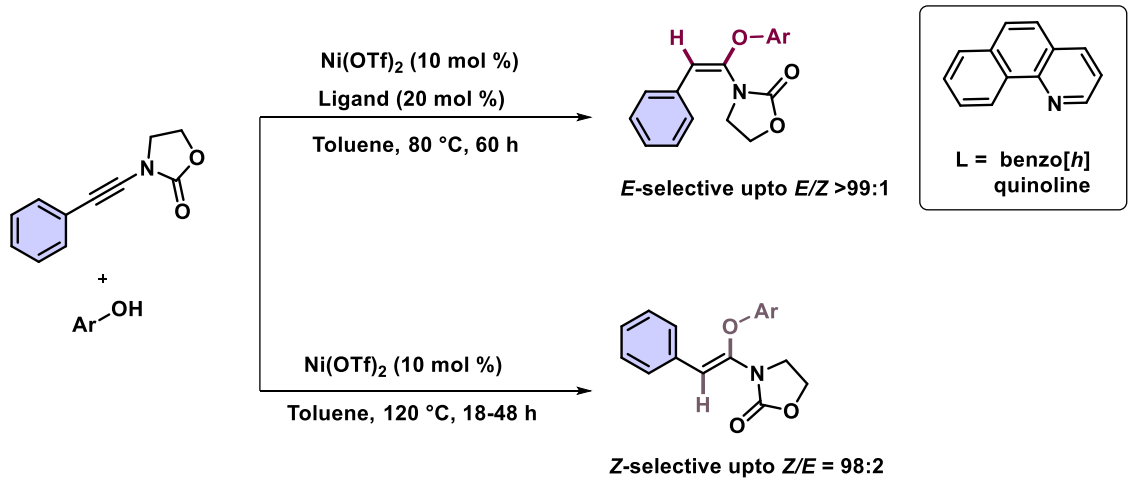

Figure 1. Nickel catalysed stereodivergent hydrophenoxylation of ynamides.

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Understanding the performance of Ni3S2/NiO Heterojunction as a Bifunctional Electrocatalysts for 3000-Hour Stable Splitting of Untreated River Water

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Abstract: The high cost and limited scalability of water electrolysis remain major barriers to green hydrogen production, largely due to poor durability of advanced electrocatalysts under practical conditions. Herein, a NiOS@ANF electrode with engineered Ni_3S_2/NiO interfaces was developed through a rapid (<2 h), scalable (16 cm^2), and energy-efficient electrochemical route as an alternative to conventional Ni foam. The optimized interfacial structure and in-situ phase reconstruction significantly enhanced electrocatalytic activity, lowering the overpotential by 434 mV for OER and 224 mV for HER compared to Ni foam. Improved performance originated from reduced charge-transfer resistance, faster kinetics, and increased active-site density. The NiOS@ANF electrolyzer maintained stable operation, whereas the conventional Ni foam cell showed 34% activity loss within 16 h. In untreated river water containing 6 M KOH, the electrode exhibited enhanced HER and OER activities after prolonged operation. Long-term testing demonstrated stable performance for 126 days with preserved morphology. Post-operando Raman, XPS, and HR-TEM analyses identified NiO and NiOOH as the dominant reconstructed active phases during HER and OER, respectively, highlighting the role of controlled phase reconstruction in achieving high activity and durability.

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Metal-Organic Framework Engineered Flexible Papertronic Supercapacitors

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Abstract: Paper-based supercapacitors represent an emerging class of flexible energy storage devices that are attracting growing interest from both academia and industry. With a unique bulk porous structure and rough absorptive surface, the paper based SCs avails reasonably good performance at a low cost.[1,2,3]. In this work, we demonstrate a flexible paper-based supercapacitor using a dual-metal NiMn-MOF/PANI composite electrode[4,5]. Combined with a PVA/KOH gel electrolyte, the fabricated NiMn-MOF/PANI paper-based device exhibited a high areal capacity of 158 mC cm^{-2} at 5 mV s^{-1} and 160 mC cm^{-2} at a current density of 0.2 mA cm^{-2}. The device also delivered a high energy density of 26.6 µWh cm^{-2} and a power density of 0.60 mW cm^{-2}, along with excellent flexibility and remarkable cyclic stability, retaining 83% of its initial capacitance after 6000 cycles. These results highlight its potential as a promising candidate for lightweight and flexible energy storage applications.

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Visible Light-Induced Decarboxylative Annulation of olefin with Amines and α-Keto-acids for substituted quinolines Synthesis

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Abstract: Efficient and sustainable approach for the synthesis of substituted quinolines have been developed *via* visible light-promoted metal-free three-component decarboxylative annulation pathway. This first protocol combines readily available feed-stock α,β-unsaturated acids, aromatic amines, and *α*-keto acids in a cascade manner to access 2,4-diarylquinolines under eco-benign conditions. In the second protocol, instead of α,β-unsaturated acids, different mono-substituted olefin moieties are utilized as coupling partners such as pinacol vinyl boronate, vinyl trimethyl silane, vinyl sulfonyl benzene, vinyl pivalate, *N*-vinyl pyrrolidine etc. to deliver 2-aryl quinoline as the major product. In the third protocol, we have chosen di-substituted olefin partner such as stilbene, cinnamonitrile, cinnamate ester, chalcone moiety as alkene source and like the previous cases we have achieved trisubstituted quinoline architecture. Moreover, mechanistic investigation reveals that the initial decarboxylative cross-coupling of olefin partners and aromatic amines forms a 2-vinyl aromatic amine intermediate. The successive condensation of *α*-keto acid with 2-vinylic aniline intermediate, 6π-electrocyclic ring closing and decarboxylative aromatization afforded the desired *N*-heterocyclic products. Broad substrates scope with reactive functional group tolerance, generation of complex chemical architecture, biologically relevant molecules and synthesis of antibacterial agents make these protocols more attractive and synthetically applicable towards the construction of complex *N*-heterocycles.

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A Novel Terephthalaldehyde-Functionalised Poly (aryl ether) Dendron: Self-Assembly and FRET Studies

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Abstract: Organic materials exhibiting Förster Resonance Energy Transfer (FRET) have been widely used for energy harvesting, colour tuning, and developing light emitting diodes, solar cells, and sensors. However, designing molecules for FRET is challenging due to poor control over molecular orientation that favours the resonance energy transfer. To overcome this limitation, a novel gelator- terephthalaldehyde functionalised poly (aryl ether) dendron (TFP) was prepared and employed as an acceptor to investigate resonance energy transfer from tryptophan donor in the gel medium. The gel has been prepared through self-assembly of TFP in DMF/H_2O mixture (1:1 v/v) with a critical gel concentration value of 3 mg/mL. The donor-acceptor system served as an efficient FRET pair in both solution and gel states. It was found that the fluorescence from the donor was completely quenched in the gel state compared to the solution state, suggesting enhanced energy transfer in the gel state.

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Influence of Sensitizer Concentration on Local Structural Disorder in $NaYF_4:Yb^{3+}/Er^{3+}$ Nanocrystals

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Abstract: Lanthanide-doped upconverting materials have emerged as a highly promising class of materials in recent years, owing to their exceptional optical characteristics such as large anti-Stokes shifts, sharp line-type emissions, long emission lifetimes, outstanding photostability and efficient near-infrared excitation. These unique features enable efficient background-free photon upconversion and endow the materials with remarkable versatility across a broad spectrum of applications, including bioimaging, medical diagnostics, colour displays, optical thermometry and advanced photonic devices. $NaYF_4$ co-doped with Yb^{3+}/Er^{3+} at an optimized composition of 79.5/20/0.5 is widely regarded as a benchmark upconversion system, as this ratio maximizes sensitizer-to-activator energy transfer while suppressing concentration quenching. Recent studies however highlight the critical role of defects and local disorder in enhancing upconversion efficiency by breaking local symmetry around rare-earth ions and partially relaxing parity-forbidden 4f–4f transitions. Alkali-metal-ion doping further amplifies these effects through lattice strain and crystal-field modulation. Since conventional diffraction techniques primarily probe long-range structural order, establishing a direct correlation between local structural disorder and optical performance becomes critically important. Here, we revisit $NaYF_4:Yb^{3+}/A^{3+}$ nanocrystals by tuning sensitizer concentration to elucidate its impact on local structure and upconversion efficiency.

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Modulating the electronic structure through phase engineering in V-doped Fe-based selenides for water splitting

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Abstract: In the grim situation of energy shortage, the development of earth-abundant, cost-effective, and durable electrocatalysts capable of replacing price-constrained noble metal-based systems is imperative for scalable green hydrogen production. Transition metal selenides have emerged as viable alternatives due to their high electrical conductivity and compositional flexibility; however, their performance is often limited by insufficient active-site density and sluggish charge-transfer kinetics. To address these limitations, heterostructure engineering and high-valent metal incorporation are effective routes to improve electrocatalytic performance by tuning the adsorption energy of intermediates, thereby reducing the activation energy barrier. Herein, V-doped $FeNiSe_4$ (V@$FeNiSe_4$, single phase) and V@$FeCoSe_4$ (heterostructure) have been synthesized *via* a single-step hydrothermal route. V@$FeNiSe_4$ shows excellent OER activity and stability even in harsh conditions, while V@$FeCoSe_4$ attributes bifunctional activity, OER in alkaline media, and hydrogen evolution reaction in acidic media. The synthesised catalysts were further comprehensively characterized, which suggests that vanadium incorporation tunes electronic interactions, thereby boosting water-splitting performance.

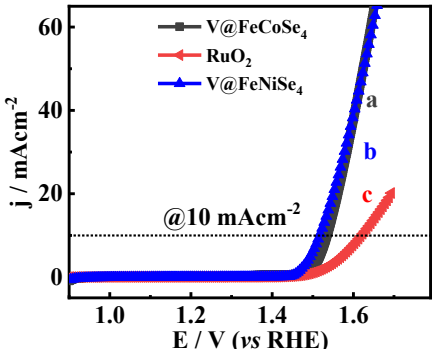

Figure 1. Linear sweep voltammetry curves of V@$FeCoSe_4$ (a), V@$FeNiSe_4$ (b), and RuO_2 (c) in alkaline media, demonstrating the efficient OER activity of the V-doped catalysts.

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Polyoxometalate- Derived BiNPs@Bi_2MoO_6 Composites for Electrocatalytic N_2 Reduction Reaction

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Ammonia plays a pivotal role in agricultural and industrial production as an important chemical feedstock. Recently, it has also been recognized as a viable carbon-free energy carrier and an efficient medium for hydrogen storage and transportation. The traditional Haber–Bosch process for ammonia synthesis operates under extreme conditions, including elevated temperatures, high pressure, and hydrogen gas. Alternatively, the electrocatalytic nitrogen reduction reaction (ENRR) provides a sustainable route to NH_3 production from N_2 and H_2O under ambient conditions, powered by renewable energy. Bi-based catalysts are promising for ENRR owing to their ability to inhibit HER and selectively adsorb N_2. Since Mo is present in natural nitrogenase enzymes involved in N_2 fixation, the combination of Bi and Mo is highly suitable for ENRR.[2] This work presents an approach of synthesizing Bi_2MoO_6-supported bismuth nanoparticles (BiNPs) from polyoxometalate-based precursors.[1] Earlier studies have shown that Bi_2MoO_6 has good catalytic properties due to its aurivillius layered structure and chemical stability. The BiNPs@Bi_2MoO_6 system benefits from the combined advantages of bismuth nanoparticles (BiNPs) and the Bi_2MoO_6 support, resulting in significant improvements in catalytic performance. The incorporation of BiNPs enhances the material's electronic properties, providing high stability, recyclability, and long-term catalytic activities. The preparation of BiNPs@Bi_2MoO_6 from POM precursors is unprecedented. Initial studies showed that the synthesized BiNPs@Bi_2MoO_6 composite is active for the electrocatalytic reduction of N_2 to NH_3 which is confirmed by indophenol test and NMR.

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Unveiling the Potential of Organic Photocatalysts in Modern Synthetic Chemistry

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Abstract: Photocatalysis has significantly advanced modern synthetic chemistry by enabling highly selective transformations under mild conditions.[1] Photocatalysts typically engage substrates through single-electron transfer (SET) or energy transfer (EnT) pathways. Herein, we report a new class of cost-effective organic photocatalysts based on 3-thioaryl-4-hydroxycoumarin scaffolds, which exploit a stabilized charge-transfer (CT) excited state to deliver both strong reducing power and efficient energy transfer capability.[2] The spatial separation of the HOMO and LUMO in these systems stabilizes the CT state, thereby enhancing both SET and EnT reactivity. This dual activation mode facilitates the reduction of redox-inert substrates to generate reactive radical intermediates, enabling a broad range of C–S, C–P, C–B, and C–C bond-forming transformations. In parallel, the EnT pathway supports processes such as E/Z olefin isomerization and [2+2] photocycloadditions.

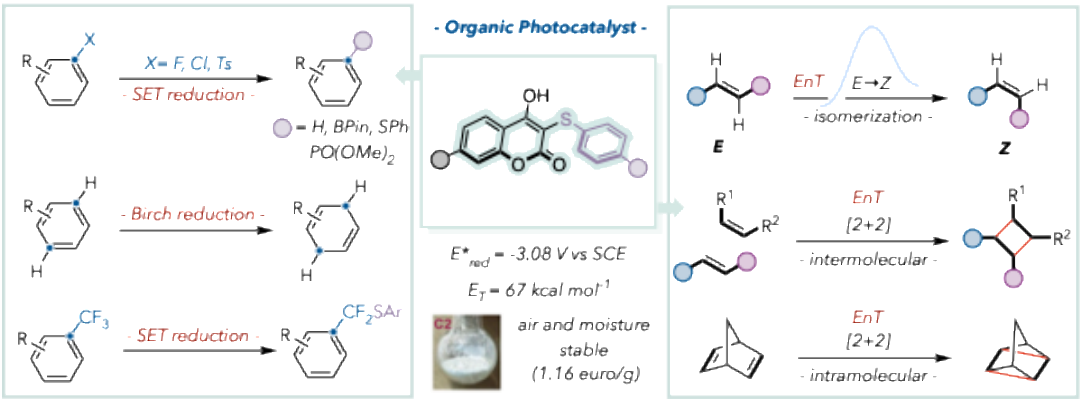

Figure 1. Development of bifunctional photocatalyst and its exploration in various photochemical processes.

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Modifying the proton transfer triggered proton transfer by substitution in the Oxadiazole-containing system

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Abstract: A new kind of proton transfer triggered proton transfer (PTTPT) was reported in 3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazole (bis-HPTA). In bis-HPTA the proton transfer in only ring triggered the proton transfer in the other ring. This motivated us to further explore the effect of structural modification and substitution and hence 2,2'-(1,2,4-oxadiazole-3,5-diyl)diphenol (HPOD) and its methoxy derivative 2-(3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl)phenol (MPOD) was synthesized. In this study, we examine the role of dual versus single proton transfer units by studying the photophysical properties along with DFT calculations. Single crystal analysis indicates that both HPOD and MPOD are of planar structures with hydrogen bonds existing between the two-proton donor-acceptor units. Although HPOD possesses two intramolecular hydrogen-bonded units, the proton transfer occurs only in one ring, but it did not trigger the proton transfer in other ring. HPOD emits tautomer emission in non-polar solvent cyclohexane whereas in other solvent it shows dual emission normal and tautomer emission, an additionally anion emission is also observed in solvents like methanol, dimethylformamide. MPOD also show ESIPT, but it is reduced ESIPT. Time resolved studies also confirm these results. In overall the studies show that the substitution of more electronegative oxygen atom reduces the efficiency of proton transfer.

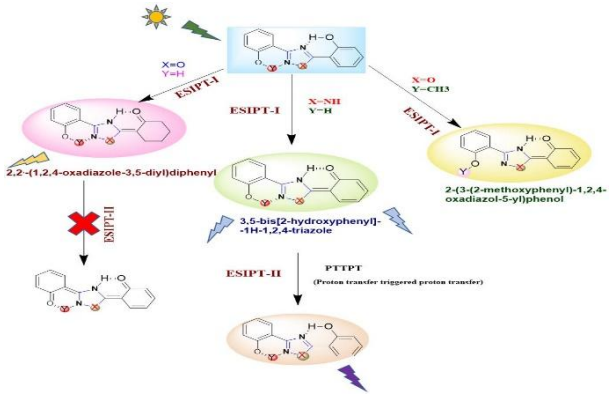

Fig 1. ESIPT process in HPOD and MPOD.

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Theoretical Investigation on Mechanism and Reaction Kinetics of OH Radicals and Cl Atoms with $CF_zH_{3-z}NCX$ (z = 0, 1, 2 and X = O, S) Compounds

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Abstract: Covalent isocyanates and isothiocyanate (R-NCO & R-NCS) are useful chemicals in synthetic chemistry and materials science.[1] They are employed in several industrial uses, such as electrophilic reagents in synthesizing polymers like polyurethane and carbamate insecticides. MIC (CH_3NCO) is the isocyanate family's most straightforward and hazardous member. Its nature is explosive and highly volatile. In this work, we have studied the kinetics and reaction mechanism of alkyl isocyanate (CH_3NCO, CH_2FNCO, and CHF_2NCO) and isothiocyanate (CH_3NCS, CH_2FNCS, and CHF_2NCS) with OH radicals and Cl atoms using DFT-based CCSD(T)/cc-pVTZ//BH&HLYP/cc-pVTZ theoretical methods.[2-4]

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Storing Visible Photon Energy in Strained Chemical Bonds

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Abstract: A "mostophore" is a molecular entity that can be converted from a low-energy form to a higher-energy, metastable form upon light irradiation and can later release the stored energy as heat when triggered.[1] These systems use photoswitchable molecules that undergo light-induced isomerization, allowing efficient capture and storage of solar energy in a renewable and emission-free manner.[2,3] As dependence on fossil fuels decreases, such molecular systems offer a promising solution for solar energy conversion and storage. In addition, there is increasing interest in stimulus-responsive energy storage materials that respond to external factors such as heat, pH, moisture, pressure, or electric fields. These materials have the potential to enable safer and more efficient batteries and smart electronic devices.[4]

In this work, we have chosen α-cyanostilbene derivatives as mostophores. Their extended π-conjugation allows efficient absorption of visible light, while strong π-π stacking facilitates [2+2] photocycloaddition. The presence of a strong electron-withdrawing group at the stilbene unit promotes efficient cycloreversion.[5] The resulting closed cycloadduct contains a strained cyclobutane ring, making it well-suited for solar energy storage and responsive to environmental stimuli.

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Harnessing Atomic-Scale Disorder to Boost Optical Thermometry in NIR Upconversion Systems

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Abstract: Near-infrared (NIR) photon upconverting (UC) crystals have recently attracted considerable attention as promising materials for contactless nanothermometry. In such systems, temperature sensing is generally based on the fluorescence intensity ratio (FIR) of the emitted photoluminescence, and therefore improving FIR remains a major challenge for achieving high-resolution temperature detection. In this work, we present a crystal-engineering strategy to enhance the temperature sensitivity of Y_2WO_6-based UC crystals by tuning the atomic-scale disorder within the host lattice. A series of Li^+-doped Y_2WO_6 crystals co-doped with Yb^{3+} and Er^{3+} were synthesized, all crystallizing in the monoclinic *P2/c* structure. Controlled incorporation of defects in the lattice generated structural disorder, which was identified through the presence of compressive microstrain. This structural modification was accompanied by a noticeable enhancement in upconversion photoluminescence intensity. To gain deeper insight into the local structural environment, pair distribution function (PDF) analysis was performed using high-energy synchrotron X-ray diffraction (λ = 0.55946 Å), allowing real-space examination of the diffraction data. In addition, X-ray absorption fine structure (XAFS) measurements were carried out to probe the local atomic arrangement. These complementary analyses revealed that the composition denoted as WO-3, which exhibited the highest absolute and relative temperature sensitivities, also possessed the greatest degree of local lattice disorder. The findings conformed the hypothesis of relaxation of the parity-forbidden selection rules, through local symmetry distortion enhances the optical transitions responsible for upconversion emission. Overall, this study highlights controlled lattice disorder as an effective strategy for improving the temperature sensitivity of NIR-UC materials for nanothermometry applications.

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A Novel Spectrophotometrically Investigated V(V)- iodochlorhydroxyquin complex and its Analytical Applications

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Abstract: A concise and innovative spectrophotometric method was developed for the trace-level determination of vanadium using iodochlorhydroxyquin (ICQ), an 8-hydroxyquinoline derivative. This approach relies on chelation, forming a green V(V)-ICQ complex under acidic conditions. The complex is formed rapidly and can be extracted into the non-aqueous organic solvent chloroform, with maximum absorbance observed between 390 and 413 nm. The metal-to-ligand [M:L] stoichiometric ratio of the complex in the chloroform phase was established as 1:2 using Job's continuous variation method and the mole ratio method. Linearity was confirmed within the vanadium (V) concentration range of 0.0–7.0 µg mL^{-1}. Key analytical parameters, including a molar absorption coefficient of 7.38 × 10^3 L mol^{-1} cm^{-1}, standard deviation (± 0.0005), Sandell's sensitivity (0.0069 µg.cm^{-2}), % RSD (0.2 %), limit of detection (0.21 µg mL^{-1}), and correlation coefficient (0.999), highlighted the method's precision, versatility, sensitivity, and cost-effectiveness. The synthesized complex was tested on various synthetic samples, including compositions analogous to standard vanadium alloys. The results demonstrated excellent performance, suggesting its potential for industrial applications.

Carbene-Metal-Acetylide Complexes with Ligand-to-Ligand Charge Transfer Luminescence and Their Applications in Photocatalysis

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Abstract: N-heterocyclic carbene (NHC) ligands gained much attention as an important class of ligands in the field of luminescent metal complexes, as they act as strong σ-donor and weak π-acceptor ligands.[1] Carbene-metal-amide (CMA, M = Cu, Ag, Au) complexes have emerged as a prominent area of research due to their high luminescence, excellent stability, and tunable emission wavelengths.[2] CMA complexes have been well explored with a diverse range of applications such as in photocatalysis, bioimaging, solar energy conversion, photodynamic therapy, and light-emitting diodes (LEDs).[3] In contrast, carbene-metal-acetylide (CMAc) complexes have attracted comparatively less attention but these complexes shows good to excellent photophysical properties. Most of the CMAc complexes are explored with Au(I),[4,5] such complexes remain largely unexplored with Cu(I) and Ag(I) and overall, these types of complexes are not explored in the context of photocatalysis. In this regard, we designed and synthesized a series of linear carbene-metal-acetylide (CMAc) complexes and studied their application in visible-light driven photocatalysis.

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Non-Epitaxial Encapsulation of Leas-based Perovskite with Lead-free Perovskite for Efficient Charge Transfer

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Abstract: Colloidal heterostructures of halide perovskite nanocrystals often suffer from uncontrolled ion migration and lattice incompatibility, limiting the formation of well-defined interfaces. Here, we report a unique core–frame heterostructure comprising $CsPbBr_3$ nanocrystal cores surrounded by $Cs_3Bi_2Br_9$ nanoplatelets. Unlike conventional epitaxial core–shell systems, the two components remain spatially separated by an ≈2 nm organic ligand layer, where attachment occurs via weak van der Waals interactions mediated by oleic acid ligands. This non-epitaxial architecture originates from competing nucleation and leading to simultaneous growth of enlarged $CsPbBr_3$ cores and anisotropic $Cs_3Bi_2Br_9$ plates. Steady-state photoluminescence of $CsPbBr_3$ is significantly quenched in the heterostructure. Ultrafast spectroscopic studies reveal that the quenching arises from photoinduced electron transfer from $CsPbBr_3$ to $Cs_3Bi_2Br_9$, despite the absence of direct lattice contact. This work establishes a new class of ligand-separated heterostructures, where morphology and interfacial spacing dictate charge transfer dynamics

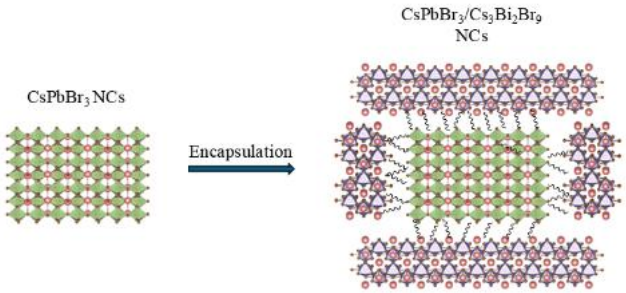

Figure 1. Atomic model of the $CsPbBr_3$ (CPB)/ $Cs_3Bi_2Br_9$ (CBB) core–frame heterostructure, highlighting the encapsulation of $CsPbBr_3$ by $Cs_3Bi_2Br_9$

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Calcium Lactate Catalyzed Tetrahydro-4*H*-benzopyran Synthesis in Green Environment

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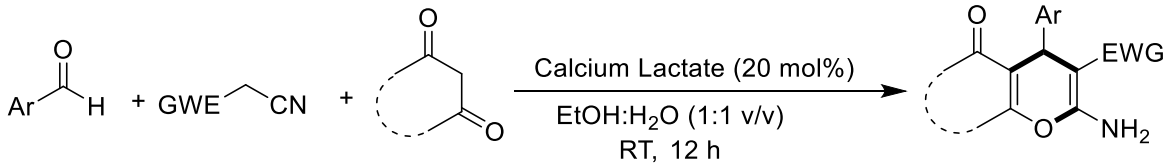
Abstract: Calcium, the fifth most abundant element in Earth's crust and the third most prevalent metal after iron and aluminium, is a readily accessible, cost-efficient, and environmentally benign alkaline earth metal.[1] The application of calcium salts like $CaCl_2$, $CaCO_3$, $Ca(OTf)_2$, $Ca(NTf_2)_2$ as a catalyst is common but our team hereby report for the first time to utilize easily available, cheap and almost negligibly toxic calcium lactate as a green catalyst. Calcium lactate is normally used as food additive, and it also coagulates milk to get cottage cheese (known as Chhena/Chhana in the Indian subcontinent).[2] It is usually applied as a calcium supplement to treat hypocalcemia (calcium deficiencies)[3] and as a coagulant for removing suspended particles from water.[4] We already used calcium lactate for 2-amino-4*H*-chromene synthesis in our previous works,[5,6] in the present work we tested its efficacy for accelerating the tetrahydro-4*H*-benzopyran synthesis via MCR strategy of aromatic aldehydes, malononitriles or its surrogates and cyclic 1,3-dicarbonyls (Scheme 1). This is a simple, eco-friendly, green method for synthesizing biological relevant benzopyrans via a one-pot, three component reactions in green solvent at room temperature.



Scheme 1. Calcium lactate catalyzed tetrahydro-4*H*-benzo[*b*]pyrans synthesis.

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Large-Scale Fabrication of Ambient Pressure-Dried Bilayer Aerogel with Exceptional EMI Shielding and Minimal Reflection

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Abstract: Aerogels are widely recognized for their lightweight structure, high porosity, and excellent functional tunability. However, conventional fabrication methods such as freeze-drying and hydrothermal processing often face significant limitations in large-scale production due to their high cost, time-consuming nature, and poor control over shape engineering. To address these challenges, we have successfully developed a scalable and low-cost approach for aerogel fabrication through ambient pressure (natural) drying. This method eliminates the need for complex equipment and allows seamless integration of structures without any junctions or cracks.[1,2] In this work, a bilayered aerogel composite consisting of MXene graphene-based materials and a MXene layer was fabricated under natural drying conditions. The 3D interconnected porous network of the MXene graphene-based nanocomposite provides moderate electrical conductivity, enabling optimized impedance matching, balanced dielectric permittivity, and strong electromagnetic (EM) wave attenuation through conduction loss, interfacial polarization, and multiple scattering effects. The back MXene layer, with its high electrical conductivity, functions as a back reflector to block EM wave transmission, enhancing the overall shielding performance. Owing to the synergistic effect of the bilayer structure, the aerogel composite demonstrates a remarkable total shielding effectiveness of 50 dB across the X-band (8–12 GHz) at a thickness of only 2.5 mm, with an absorption contribution exceeding 80%. This study highlights a promising route for large-scale, cost-effective fabrication of high-performance aerogel-based materials for next-generation electromagnetic interference (EMI) shielding applications.

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Metal-Free α-Sulfonylation of β-Ketothioamides: Access to α-Sulfonyl-β-Ketoamides

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Abstract: Herein, we report a metal and additive-free unprecedented reactivity of β-ketothioamides with sulfonyl chlorides for the synthesis of previously unreported 2-sulfonyl-3-oxo-N,3-diarylpropanamides via in situ thioamide to amide conversion followed by dehydrohalogenative C−S cross-coupling at room temperature under an open air for the first time. The protocol demonstrates not only its operational simplicity, efficiency, mild condition, and scalability, but also easy to get the diverse a-sulfonyl-β-ketoamides in good to high yields. Additionally, the DFT and photophysical studies supported the proposed mechanism, and revealed unique excitation-dependent emission coupled with ESPT for the synthesized sulfones.

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Dual-Mode Fluorescent Sensors for Rapid Detection of Hydrogen Sulphide: Applications in Food Spoilage Monitoring

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Abstract: Food safety is a major concern, with the WHO reporting 4,20,000 deaths every year due to the consumption of contaminated food[1]. Food spoilage is the major factor for this. Hence, there is a necessity for rapid detection methods. Hydrogen Sulphide is a key biomarker of food spoilage, and it also serves as a neurotransmitter[2]. Hence, we report the synthesis of a series of fluorescent sensors for detecting and quantifying sulphide. The developed sensors exhibit great selectivity over other sulphur-containing analytes. It exhibits dual-mode sensing via fluorescence via enhancement in fluorescence intensity under a UV lamp, and also distinct visible colour changes. We introduced structural variations by modifying the substituents, such as including an electron-donating group and a withdrawing group, into the sensors to see the effect on fluorescence. The sensors showed high sensitivity with low detection limits in the ppm range. These findings highlight the potential of the proposed systems for rapid, visual and real-time monitoring of food spoilage.

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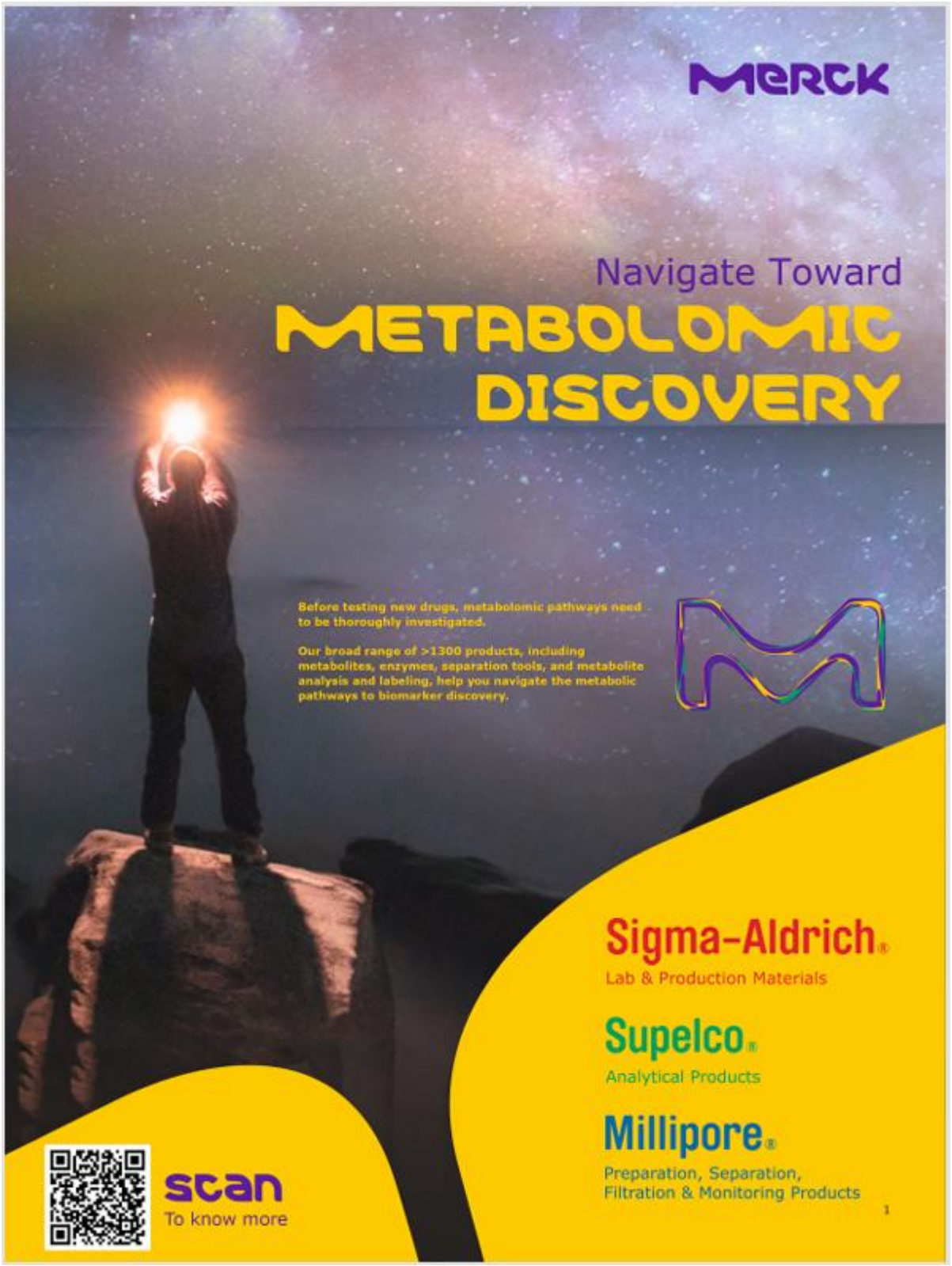
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