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International Conference on

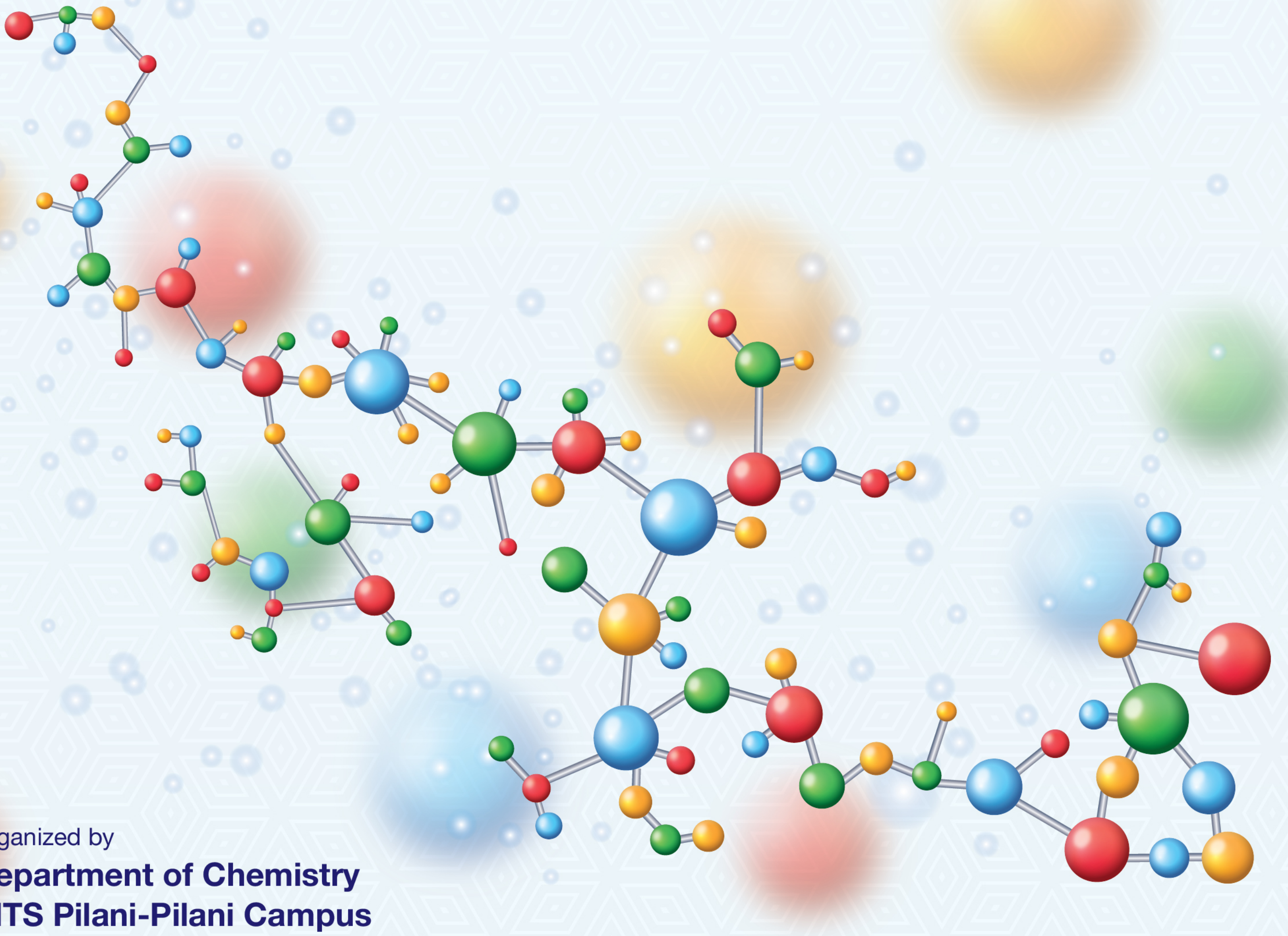
NANO- AND FUNCTIONAL MATERIALS (NFM-2026)

Materials for a Sustainable Future

17-18 APRIL 2026

BOOK OF

Abstracts



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Department of Chemistry
BITS Pilani-Pilani Campus

International Conference on Nano- and Functional Materials (NFM-2026):

Materials for a Sustainable Future

17-18 April 2026

Book of Abstracts

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BITS Pilani

Department of Chemistry, Pilani Campus

Contents

Messages v

About the Department xii

Materials Research at BITS Pilani xiv

Organizing Committee xvi

Conference Advisory Board xvii

Local Functional Teams xviii

Scientific Program xix

Oral Presentation Schedule xxi

Our Sponsors xxii

Abstracts of Technical Sessions

1 **Plenary Lectures** 01

2 **Keynote Lectures** 05

3 **Invited Lectures** 11

4 **Oral Presentation** 29

5 **Poster Presentations** 43

Notes 107

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Prof V Ramgopal Rao, Ph.D.,
Fellow of IEEE, TWAS, INAE, INSA, IASc, NASI
Vice-Chancellor & Senior Professor

Former Director (2016-2021), IIT Delhi
J. C. Bose National Fellow

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Message

It gives me great pleasure to know that the Department of Chemistry, BITS Pilani, is organizing the International Conference on Nano and Functional Materials, NFM 2026, on 17 to 18 April 2026, with the theme Materials for Sustainable Future. Nano and functional materials are central to many of the technologies that will shape a more sustainable future, spanning energy, healthcare, electronics, catalysis, and agriculture.

This conference brings together an important interdisciplinary community of researchers, faculty members, and students to exchange ideas and build meaningful collaborations in a rapidly evolving area of science and engineering. Such platforms are important for connecting fundamental research with emerging technological needs.

I convey my best wishes to the organizing team, speakers, participants, and students for the success of NFM 2026. I am sure the conference will lead to valuable discussions and new research directions.

Warm regards,

Ramgopal Rao

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Birla Institute of Technology and Science, Pilani
Pilani Campus

Prof. Sudhirkumar Barai, Ph.D.
Director & Senior Professor

Message from Director's Desk

It is my great honor to warmly welcome everyone, on behalf of Birla Institute of Technology and Science Pilani, Pilani Campus, to this prestigious gathering of academicians, researchers, and young scholars from India and around the world attending the **International Conference on Nano- and Functional Materials (NFM-2026): Materials for a Sustainable Future,** organized by the Department of Chemistry on April 17–18, 2026.

The Department of Chemistry, one of the Institute's oldest and most vibrant departments, has consistently contributed to excellence in teaching and research. Recently, faculty members have made significant progress across various research fields, earning notable academic awards and securing competitive funding from government agencies and industry.

I am pleased to see that the conference has drawn approximately 100 participants. The discussions cover a wide range of topics in chemical sciences, materials science, and related interdisciplinary areas, all aligned with the global goal of sustainable development. I am confident that the exchange of ideas, interdisciplinary collaboration, and scholarly debates will spark innovation, inspire new viewpoints, and make valuable contributions to solving future challenges.

I extend my best wishes to all delegates, both domestic and international, for their meaningful contributions and presentations.

I also sincerely appreciate the efforts of the faculty members and research scholars of the Department of Chemistry in organizing this important academic event.

I wish the conference great success and hope it will be intellectually stimulating and professionally beneficial for everyone involved.

Sudhirkumar Barai

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Birla Institute of Technology and Science, Pilani
Pilani Campus

Prof. Inamur Rehman Laskar, Ph.D.
Professor and Head, Department of Chemistry

Message

It is a great opportunity for me to say a few words about the 3rd edition of the International Conference on Nano & Functional Materials (NMF-2026), which is being organized by our department on 17–18 April 2026.

Materials play a vital role in our daily lives, and scientists across the world are continuously developing advanced materials to improve the quality of human life. From a scientific perspective, understanding the nature of materials and guiding them toward translational research requires expertise from multiple disciplines.

In 2014, a few colleagues from the Department of Chemistry initiated discussions with researchers from other disciplines within our institute. This collaborative effort led to the conception of a platform where various aspects of materials could be presented, discussed, and explored in depth.

This year marks the third time our department is organizing this conference, reflecting its growing importance and success. I am confident that the deliberations on diverse aspects of materials and their applications will deeply engage all participants.

I sincerely hope that the conference concludes with great success and leaves a lasting impact on everyone involved.

(Inamur Rahaman Laskar)

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Birla Institute of Technology and Science, Pilani
Pilani Campus

Prof. Bibhas Ranjan Sarkar, Ph.D.
Assistant Professor
Department of Chemistry, Pilani Campus

Message from Convener

On behalf of the organizing committee of the conference, we extend our heartiest welcome to all the delegates of the Interanation Conference on Nano- and Functional Materials (NFM-2026): Materials for Sustainable Future, being organized by the Department of Chemistry, Birla Institute of Technology and Science, Pilani, during 17-18 April, 2026.

The conference is themed on Materials for Sustainable Future is a major focus of global academic and industrial research, keeping in mind the responsible use of resources for the generations to come. The endeavors in this area are largely observed to be centered around design and development of new materials having myriad of applications in different sectors such as energy, commodity chemicals, fine and specialty chemicals and many more, which impact our everyday life. The event will open up cross-disciplinary discussions from eminent speakers with varied expertise. The young researchers and participants are expected to obtain crucial training and exposure to interdisciplinary lines of thought and enrich themselves herefrom. The event will host about 19 scientific lectures by eminent scientists/ academicians and 70 posters, 12 oral presentations by budding researchers.

I would like to take this opportunity to express our sincere thanks to Prof. V. Ramgopal Rao, our Hon'ble Vice-Chancellor, whose enthusiasm and support has motivated us strongly. We are indebted to Prof. Sudhirkumar Barai, Director, BITS Pilani, Pilani Campus, for extending his unconditional support in organizing this event. We also sincerely thank Prof. N. V. M. Rao, the Dean of Administration, all Deans and Associate Deans, Chief Warden, Unit Chiefs, and other institute office-bearers for their kind help and cooperation at every stage. I would also thank the sponsors for contributing to the noble cause of the Conference.

(Convener, NFM 2026)

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About the Department

One of oldest & ever-evolving department having a vision to excel in teaching & research, recently reinforced with enthusiastic young faculty members. Active research in the frontier areas of both fundamental and applied chemistry has been appreciated nationally & globally for several decades. The department continues to grow and attain new paradigms in chemistry education in the country. Prof. Inamur Rehman Laskar is the current Head of the Department.

FACULTY PROFILE / WOMEN SCIENTISTS

Prof. Ram Kinkar Roy
Physical Chemistry

Prof. Dalip Kumar
Organic Chemistry

Prof. Anil Kumar
Organic Chemistry

Prof. Inamur R. Laskar
Inorganic Chemistry

Prof. Ajay Kumar Sah
Inorganic Chemistry

Prof. Saumi Ray
Physical Chemistry

Prof. Bharti Khungar
Inorganic Chemistry

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Organic Chemsitry

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Inorganic Chemistry

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Dr. Amrita Chakraborty
Physical Chemistry
Women Scientist

Materials research at BITS Pilani, Pilani Campus

An interdisciplinary group of faculty members from different departments of the Pilani campus are actively doing research in the highly evolving area of materials and their applications. The approaches and focus are different depending on the areas of individual specializations. The team includes Prof. J. Panwar (Biosciences), Prof. I. R. Laskar, Dr. S. Pande, Dr. R. Sakhuja, Dr. B. R. Sarkar, Dr. M. Basu (All in Chemistry), Dr. R. K. Gupta, Dr. S. Gangopadhyay (both in Physics), Dr. D. Chitkara, Dr. A. Roy (both in Pharmacy), Dr. S. Belgamwar, Dr. RadhaR. Mishra, Dr. Tribeni Roy (Mechanical Engg.), Dr. B. Roy, Dr. S. Chatterjee, Dr. S. Ghosh (Chemical Engg.), Dr. A. Hazra (in Electrical Engg.),. The group had organized NFM-2014 in November 2014 as a national conference to initiate communication and cross-disciplinary interactions which had considerably contributed to the growth and visibility of the University among the research peer-groups. The members have recently been awarded several research funding in respective areas from various national funding agencies.

The group is visioning quantum development in research, collaborations keeping with the societal requirement of technology development. The materials group extends warm welcome to all the delegates.

An International Conference on Nano- and Functional Materials, (NFM-2017) was organized by Department of Chemistry, BITS Pilani, Pilani Campus, during November 16-18, 2017. More than one hundred participants attended the three-day conference that witnessed 48 talks, 16 student oral presentation, and 110 posters exploring variety of research fields bonding with nano- and material science.

Organizing committee

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Prof. G. Sunder, Director, *Off-Campus*

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Prof. Ram K. Roy

Chairman

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Convener

Prof. Bibhas Ranjan Sarkar

Co-conveners

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Committee	**Coordinator**	**Members**
Travel and Accommodation	Prof. Satyajit Patra	Prof. Avik Pati Prof. Subhashis Gangopadhyay
Inaugaration	Prof. Saumi Ray	Prof. Surojit Pande
Registration/ Reception	Prof. Avik Pati	Dr. Amrita Chakraborty
Faculty talks (Day 1 and 2)	Prof. Prashant U Manohar	Prof. Anish Rao Prof. Arnab Hazra Prof. Ram K Roy
Catering and Food	Prof. Bibhas R Sarkar	Prof. Surojit Pande Prof. Inamur R. Laskar
Poster Sessions	Prof. Paritosh Shukla	Prof. Dalip Kumar Prof. Ajay K Sah Prof. Radha R Mishra Prof. Shamik Chakraborty
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Oral Presentaion	Prof. Anil Kumar	Prof. Pritam Jana
Treasurer	Prof. Avik Pati	Prof. Anish Rao

Scientific Programme

International Conference on Nano- and Functional Materials (NFM) 2026: Materials for a Sustainable Future

17th -18th April 2026, *Venue: 6110, J C Choudhry NAB Auditorium, BITS Pilani*

DAY 1		
April 17th, 2026 (Friday)		
08:00 AM - 09:00 AM	**Registration**	
Inaugural Ceremony		
09:00 AM - 09:10 AM	Welcome and Invocation	
09:10 AM - 09:15 AM	About the Conference	**Prof. Bibhas R. Sarkar** *Convener, NFM-2026*
09:15 AM - 09:20 AM	About the Department	**Prof. Inamur R. Laskar**, *HoD Chemistry, Chairman NFM-2026*
09:20 AM – 09:35 AM	Welcome Address	**Prof. V. Ramgopal Rao**, *Vice-Chancellor, BITS Pilani*
09:36 AM – 09:45 AM	Address by Chief Guest	**Prof. Ashok K. Ganguli**, *Director, IISER Berhampur*
09:45AM – 09:47 AM	Vote of thanks	**Prof. Mrinmoyee Basu,** *Co-Convener, NFM-2026*
Group Photograph and High Tea (9.50-10.10 AM)		
Session I	**Session Chair: Prof. Anshuman Dalvi, Professor, BITS Pilani**	
10:10 AM – 11:00 AM	**Plenary Lecture** *(Inaugural Talk)*	**Prof. Ashok. K. Ganguli**, *Director, IISER Berhampur, India* **Title:** Design of functional nanostructures for energy and biomedical applications
11:00 AM – 11:30 AM	**Invited Lecture**	**Prof. Dilip K. Maiti,** *University of Calcutta, India* **Title:** Synthesis and Fabrication of Organic Nanomaterials for Sensors, Devices and Other Innovative Applications
11:30 AM - 11:50 AM	**Tea/ Coffee Break**	
Session II	**Session Chair: Prof. Saumi Ray, Professor, BITS Pilani**	
11:50 AM - 12:40 PM	**Plenary Lecture**	**Prof. Saurav Goel**, *London South Bank University, UK* **Title:** Sustainable Frontiers in Precision Manufacturing and Engineered Surfaces
12:40 PM - 01:10 PM	**Invited Lecture**	**Prof. Shubhangi B. Umbarkar**, *CSIR-NCL, Pune, India* **Title:** Green Catalytic Delignification Process for Microcrystalline Cellulose from Sugarcane bagasse
13:10 PM - 14:30 PM	**Lunch Break @ Institute Cafeteria**	
Session III	**Session Chair: Prof., Bharti Khungar, Professor, BITS Pilani**	
14:30 PM -15:00 PM	**Invited Lecture**	**Prof. Sugata Ray,** *IACS Kolkata, India* **Title:** The impact of x-rays with high brilliance on the oxidation state of arsenic ions and consequently on the nucleation of arsenic bearing phases within aqueous medium
15:00 PM - 15:30 PM	**Invited Lecture**	**Prof. Mrinal Pal,** CSIR-*CGCRI, Kolkata, India* **Title:** The scent of health: Semiconductor nanocomposites-based gas sensor towards human healthcare
15:30 PM - 16:00 PM	**Invited Lecture**	**Prof. Asish Pal,** *INST-Mohali, India* **Title:** Supramolecular Engineering Strategy: from Chiroptical Amplification to Tunable Properties in Chiral Polymers
16:00 PM - 16:20 PM	**Tea/ Coffee Break**	
Session IV	**Session Chair: Prof. Dalip Kumar, Senior Professor, BITS Pilani**	
16:20 PM – 16:50 PM	**Invited Lecture**	**Prof. Biswarup Chakraborty,** *IIT Delhi, India* **Title**: Mechanistic investigation of the electro-/photo-chemical synthesis of ammonia
16:50 PM - 17:30 PM	**Keynote Lecture**	**Prof. Yosi Sacham,** *Tel Aviv University, Israel* **Title:** Synthetic Biology-based Functional Plant Sensors for Sustainable Precision Agriculture
Session V	**Poster Presentation and Evaluation** **Session Chair: Prof. Arnab Hazra, Prof. Subhashis Gangopadhyay, and Prof. Radha R. Mishra**	
17:30 PM - 19:00 PM	**Poster session**	***@ Rotunda - All Posters in All Themes***
19:00 PM- 20:00 PM	**Cultural Program @ Pooja Ground**	
20:00 PM - Onwards	**Conference Gala Dinner @ Pooja Ground**	

DAY 2		
April 18th, 2026 (Saturday)		
Session VI	**Session Chair: Prof. Anil Kumar, Professor, BITS Pilani**	
09:30 AM - 10:00 AM	**Invited Lecture**	**Prof. Sameer Sapra**, *IIT Delhi, India* **Title:** Optoelectronics, Electrocatalysis and Charge Storage using Transition Metal Dichalcogenide based Nano-heterostructures
10:00 AM - 10:30 AM	**Invited Lecture**	**Prof. Kamalendra Awasthi**, *MNIT Jaipur, India* **Title:** Engineering Polymer Hybrid Nanomaterials Toward Selective and Sensitive Gas Detection
10:30 AM - 11:10 AM	**Keynote Lecture**	**Prof. Youhong Tang,** *Flinders University, Australia* **Title:** Vortex fluidic mediated aggregation induced emission luminogens and beyond
11:10 AM - 11:30 AM	**Tea/ Coffee Break**	
Session VII	**Session Chair: Prof. Ajay K Sah, Professor, BITS Pilani**	
11:30 AM - 12:00 PM	**Invited Lecture**	**Prof. Sasanka Deka,** *University of Delhi, India* **Title:** Synergistic Interactions of Single Atoms with Semiconductors for Maximized Photocatalytic Hydrogen Generation and H2O2 Production
12:00 AM - 12:30 PM	**Invited Lecture**	**Prof. Bidisa Das,** *TCG Crest, Kolkata, India* **Title:** OER Activity of Fe-Oxyhydroxide Nanostructures from Solution to Surfaces: A DFT Study
12:30 PM - 13:00 PM	**Invited Lecture**	**Prof. Kaushik Ghosh,** *INST-Mohali, India* **Title:** Multifunctional 2D Material-Based Sensors and Energy Harvesting Systems
13:00 PM - 14:20 PM	**Lunch Break @ Institute Cafeteria**	
Session VIII	**Session Chair: Prof. Indresh Kumar and Prof. Prashant U. Manohar, BITS Pilani**	
14:20 PM - 15:20 PM	**Oral Presentations**	
	Room # 6109 **Room # 6110**	**Oral presentation # 1 - 6** **Oral presentation # 7 - 13**
15:20 PM - 15:50 PM	**Invited Lecture**	**Prof. Rahul Prajesh,** *CSIR-CEERI, Pilani, India* **Title:** Functional Materials to Sensor Systems: Devices, Platforms, and Applications
15:50 PM - 16:20 PM	**Invited Lecture**	**Prof. Parvej Alam,** *The Chinese University of Hong Kong, P R China* **Title:** Enhancing Organic Long-Persistent Luminescence via Trace Doping and Triplet-Triplet Energy Transfer
16.20 pm – 16.50 pm	**Invited Lecture**	**Prof. Hema Kuntrapakam,** *IIT-Jodhpur, India* **Title:** Balancing Molecular Freedom: Confinement and Constraints in Supramolecular Materials Design
16:50 PM - 17:30 PM	**Keynote Lecture**	**Prof. Kausik Mukhopadhyay,** *University of Central Florida, USA* **Title:** Injectable Siloxane-based Rapid Treatment for Augmented Hemostasis
17:30 PM - 17:45 PM	**Tea/ Coffee Break**	
Valedictory Ceremony		
17:45 PM - 17:55 PM	**Summary of Events – Prof. Paritosh Shukla, BITS Pilani**	
17:55 PM - 18:25 PM	**Closing Remarks**	**Prof. N. V. Muralidhar Rao,** *Dean of Administrations, Pilani Campus*
18:25 PM - 18:30 PM	**Prize Distribution**	**Announcement and Distribution of Awards**
18:30 PM - Onwards	**Campus Tour**	
20:00 PM - Onwards	**Dinner at VFAST Lawns**	

List of Oral Presentaions

OP1: Dr. Bikash Jana **Title:** Nanoscale Design Principles for Solar-to-Fuel Conversion: Insights from Carbon Dot Photocatalysts	**OP7: Anita Khichar** **Title:** Investigating WSe_2-PMMA Nanofibers for emerging memory and synaptic characteristics
OP2: Parmeshthi Parikh **Title:** Design and Synthesis of Amphiphilic Glucoconjugates: Reactivity Toward Terbium Sensitization and Chiroptical Properties	**OP8: Prashant Choubey** **Title:** Type-II WO_3/NiOOH nanoflakes enable efficient and selective low-bias photoelectrochemical saline water-splitting reaction
OP3: Ajeet Singh **Title:** Natural Sunlight Harvesting Benzothiadiazole-based Molecular Photocatalyst for H_2O_2 Production: A Recyclable Homogeneous Biphasic System	**OP9: Astha Gupta** **Title:** Stabilizing Ru Single Atom Catalyst Through Electronic Metal-Support Interaction with $NiCo_2O_4$ Support for Overall Water Splitting and Urea Electrolysis
OP4: Bharat Kaushik **Title:** Development of Iridium-based Metal Complex for Low-Cost Detection of Creatinine and Human Serum Albumin (HSA) from Human urine	**OP10: Gopu J** **Title:** Lightweight copper nanowire-hollow glass microsphere loaded melamine formaldehyde composite for electromagnetic shielding application
OP5: Priyanka Bhardwaj **Title:** Sulfonamide-based COFs as Efficient Additives in Polyethylene Oxide for Improved Ionic Conductivity	**OP11: Sakshi Maan** **Title:** Benzimidazole Derived Optical Luminogens: From switchable mechanochromism to the detection of biomarkers
OP6: VAISHNU SK **Title:** Structure–Property Relationships in PBSA/PHBH Biopolymer Blends: A Molecular Dynamics Study for Sustainable Packaging Application	**OP12: Sameer Rai** **Title:** Interplay of Sn-Induced Electronic Perturbation and Surface Defects in Bi_2MoO_6 for Improved N_2 Photofixation

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Plenary Lecture

Plenary Lecture 01

Design of functional nanostructures for energy and biomedical applications

Ashok K. Ganguli

Department of Chemistry, Indian Institute of Technology Delhi
New Delhi 110016, India
Department of Chemical Sciences, Indian Institute of Science Education & Research,
Berhampur, Odisha 760003, India

Abstract: Designing nanostructures with varied size, shape and function has been a key focus in our research[1,2]. Among various nanomaterials, semiconductor nanoheterostructures have been designed to efficiently harness solar energy and utilize the charge carriers for visible-light photocatalysis and water splitting[3 - 5].

Upconversion materials have attracted considerable research interest for their application in bioimaging due to their unique optical properties. Rare-earth doped $NaBiF_4$ based upconversion nanomaterials have been designed for bioimaging[6] of cells and for near-Infrared activated photodynamic therapy[7]and as nanoscintillators[8]. Rare-earth doped MOF's have been designed as luminescent non-contact thermometers in environments where conventional probes are impractical[9].

Surface - modified spiky silica nanoparticles with MOFs (Metal-Organic Frameworks) like ZIF-8 with a spiky surface demonstrate high doxorubicin loading capacity[10]. MgO@silica core-shell nanoparticles with rough surface morphologies exhibited a significantly higher drug encapsulation efficiency (~97%) for the anticancer drug Doxorubicin (Dox) and superior anticancer efficacy[11].

Reference:

1. A K Ganguli, A Ganguly and S. Vaidya, Chem. Soc. Rev (2010)
2. I.Majumdar et al, *J. Phys. Chem C* **130**, 538(2026).
3. S. Kumar, K. Ojha and A. K. Ganguli. Adv. Mater. Interfaces, **4**, 1600981(2017)
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11. M. K. Sharma et al, New J Chem., **48**, 5760 (2024)
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Plenary Lecture 02

Sustainable Frontiers in Precision Manufacturing and Engineered Surfaces

Saurav Goel*

*London South Bank University

*Email: *goels@lsbu.ac.uk*

Abstract: Precision manufacturing (PM) pushes the boundaries of traditional machining, molding, and forming by incorporating advanced techniques such as scanning lithography, diamond machining, and laser machining. These approaches leverage diamond tools and cutting-edge metrology to tackle "Beyond Moore" fabrication challenges. The emergence of hybrid manufacturing methods, which integrate intelligent techniques such as laser and vibration assistance although addressing many limitations of conventional machining but remains a costly proposition. The talk will introduce a novel, accessible alternative to these methods while exploring the new frontiers of PM, including its application in fabricating next-generation antimicrobial surfaces. The discussion will also emphasize the role of advanced computational techniques in understanding organic-inorganic interactions and highlight how Nature-inspired sustainable design and material development. Furthermore, breakthroughs in AI-driven approaches for creating environmentally friendly and sustainable materials will be showcased.

Keynote Lectures

Keynote Lecture 01

Synthetic Biology-based Functional Plant Sensors for Sustainable Precision Agriculture

Yosi Shacham

Scojen Institute of Synthetic Biology, Reichman University, Director,
Prof. Emeritus, Tel Aviv University
Email: *shacham.yosi@gmail.com*

Abstract: Synthetic biology-based functional plant sensors are emerging as a transformative, sustainable approach to precision agriculture, enabling crops to directly report their health, nutritional status, and environmental stressors in real-time. In this talk, we will describe a novel approach for designing genetic circuits that enable the engineering of "smart" crops that can generate detectable signals when facing issues such as drought, nutrient deficiency, or pest attacks, thereby enabling precise, on-demand agricultural inputs.

We will present novel synthetic-biology-based sensors that use gene expression to up- or down-regulate other genes. We will present circuit modeling of such sensors, assuming both DNA and RNA regulation, and discuss integration issues of such sensors with CMOS VLSI circuits.

Keynote Lecture 02

Vortex fluidic mediated aggregation induced emission luminogens and beyond

Youhong Tang*

*Flinders University, Australia
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Abstract: Aggregation-induced emission (AIE) is a unique and abnormal fluorescence phenomenon that has attracted increasing research interest over the past decades. Since its discovery in 2001, many AIE-active molecules with different structure, functional groups and optical properties have been reported. These AIE-active molecules can be further utilized to fabricate various functional materials, which have exhibited great potential for different applications [1]. The recently developed vortex fluidic device (VFD) is a relatively inexpensive research tool for controlling chemical reactivity and selectivity, materials synthesis and probing the structure of self-organized systems, offering a range of benefits over conventional processing [2]. Here, a few case studies will be talked about to demonstrate the innovation of combining AIE and VFD together to form AIE functional material [3-5].

This significant strategy in functionalised materials with AIE features has the potential for developing more efficient techniques for characterizing advanced nanomaterials and understanding biological processes and detection methodologies.

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Keynote Lecture 03

Injectable Siloxane-based Rapid Treatment for Augmented Hemostasis

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Abstract: There is an urgent need to develop effective hemostatic treatments that can stop blood loss while being easy to use at the point of care [1]. Traditional methods, such as gauze and tourniquets, have shown limited effectiveness; as a result, the development of new hemostatic materials has advanced greatly over the past decade. Although recent efforts have successfully engineered new hemostats, creating effective, biocompatible, fast-acting hemostatic material that is simple to apply and remove, cost-effective, and practical remains challenging. The goal is to provide a means for rapid bleeding control from trauma wounds that surpasses current options within a few minutes [2]. Here, we introduce a unique hemostatic bandage system, SILFOAM, designed for its efficacy across different blood flow rates using a non-invasive model, providing an easy, quick, and affordable way to test hemostats prior to in vivo studies [3]. The formulation of our bandage involves two parts, A and B, both consisting of a homogeneous mixture of siloxane A, a silicone-curing catalyst, inorganic oxides, and a non-ionic surfactant. Part B similarly contains a homogeneous mixture of siloxane B, an activator, silica, and a surfactant [4]. When combined, these components react in situ to form a self-conforming, flexible, sponge-like foam that adheres to and surrounds the wound, acting as a barrier by generating autogenous pressure to stop bleeding. Upon interaction, the activator molecules rapidly decompose, producing oxygen or carbon dioxide gas, serving as a blowing agent that foams the siloxane into a sponge-like structure in less than a minute. Various inorganic oxides have been tested at different concentrations to identify the optimal composition for expansion and temperature, reducing the risk of embolism. Additional studies on mechanical durability, thermal properties, surface adhesion, hydrophobicity, rheology, closed porosity through imaging, spatiotemporal analysis, and other in vitro assays will also be shared. Bleeding effectiveness for this material and other hemostats was evaluated using a noninvasive torso hemorrhage model (manikin) equipped with an electronic bleeding controller. We are currently developing a new version using calcium oxide to improve biocompatibility and enable bioactive Ca^{2+} release, along with incorporating TRAP-6, a synthetic peptide that activates platelets, to accelerate clotting through targeted biochemical signaling. By combining physical tamponade with biochemical platelet activation, these efforts aim to overcome key limitations of current trauma dressings. These innovative strategies for creating hemostatic dressings with gas-generating blowing agents offer a practical approach to a biocompatible, effective bandage system capable of treating various wounds, including pressure sores, ulcers, and stubborn open wounds.

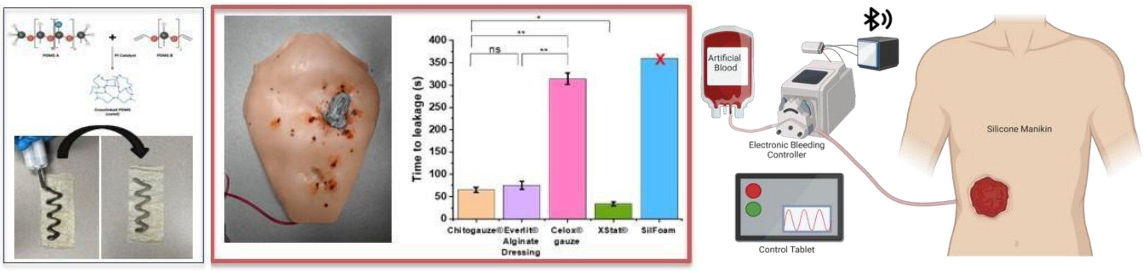

Figure 1 – Inorganic Oxides and Peptide-integrated Siloxane Hemostats

Keywords*:* Polymer, Wound-healing, Hemostasis, Noninvasive, Antibacterial, Peptide

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Invited Lectures

Invited Lecture 01

Synthesis and Fabrication of Organic Nanomaterials for Sensors, Devices and Other Innovative Applications

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Abstract: Organic nanomaterial-products are lighter, more flexible, biodegradable, ease for fabricating devices, less expensive, non-magnetic and easily be purified. Semiconducting, electronic and optoelectronic properties can easily be modified through changing size, shape, chemical structure, morphology and installation of a wide range of functional groups, which in turn generates innovative semiconducting, conducting, photoluminescence, storage, display and sensing performances to achieve highly efficient devices. Consequently, organic nanomaterials open up the door to many exciting and advanced new applications that would be impossible using inorganic materials. Thus, design and synthesis of new organic compounds, their fabricated unidirectional materials and development of new electronic property are desirable for achieving organic electronics-based high-tech devices of ultimate sensitivity and day-to-day usable innovative component. We have designed, synthesized and fabricated several types of organic nanomaterials and found them as a valuable nanomaterials for sensing device for lethal gaseous phosgene, detecting health pollutant cyanide in water, detecting poisonous metal ions, luminescent material for inkless writing and self-erasing application, nanofiber-based materials for crossbar devices to achieve organic resistive random access memory (RRAM) and write-once-read-many-times (WORM) memory devices for non-editable database, archival memory, electronic voting, and radio frequency identification (RFID), solar cell, fruit protection and anti-ovarian cancer applications.[1]

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Invited Lecture 02

OER Activity of Fe Oxyhydroxide Nanostructures from Solution to Surfaces: A DFT Study

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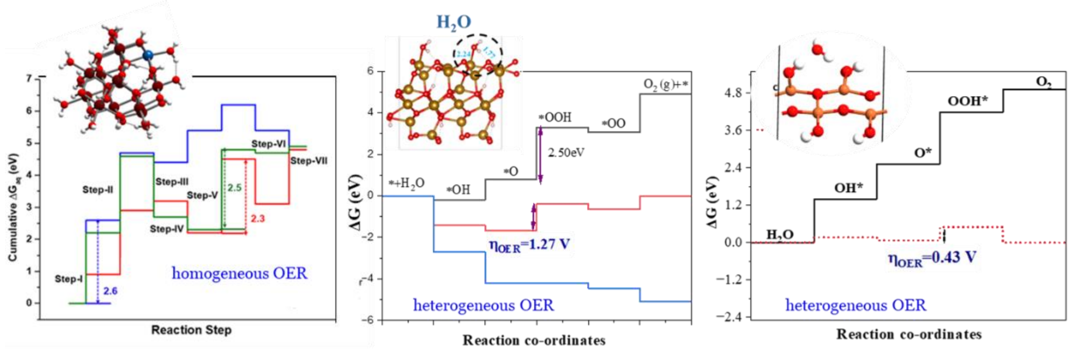
Abstract: Nanostructured minerals such as Fe oxyhydroxides (FeOOH), which are responsible for the geochemical cycling and mobility of numerous nutrients and contaminants in the environment, are also potential "earth-abundant" catalytic materials. The formation of FeOOH minerals involve nucleation of multinuclear Fe oxyhydroxide clusters in aquatic environments that form during early-stage polymerization.[1–3] We have used these nanostructures as model clusters to theoretically study various chemical processes occurring in the environment, such as the surface adsorption of contaminant ions and catalysis using Density Functional Theory (DFT) [4,5]. Accurate predictions of these processes require microscopic insights into the underlying reactions, beginning with an understanding of the hydrolytic and subsequent polymerization steps of Fe(III) ions in aqueous solutions. Consequently, we theoretically investigated the formation of dimeric Fe oxyhydroxide clusters in an aqueous medium starting from hydrated monomeric ions and examined the mechanistic pathways [6]. We then studied Fe oxyhydroxides for catalytic applications, specifically for the Oxygen Evolution Reaction (OER) starting from small soluble clusters in a homogeneous medium to solid surfaces under a heterogeneous environment. Previous experimental studies have reported that lab-synthesized solid Fe oxyhydroxides exhibit inferior electrocatalytic performance compared to *in-situ* synthesized electrocatalysts for OER, primarily due to their poor conductivity. To address this, we first explored Fe oxyhydroxide nanoclusters that may form *in situ* in aqueous media and studied their stepwise reaction mechanisms and associated free energies.[5] We systematically compared the catalytic performance of pure and transition-metal-doped Fe oxyhydroxide clusters.

Building on the understanding of OER activity of FeOOH clusters in homogeneous medium, we investigated the OER activities of FeOOH surfaces. We specifically considered two polymorphs, Ferrihydrite and Lepidocrocite; and explored the low-index surfaces as heterogeneous catalysts for OER. Our results indicate that, while Ferrihydrite is less electrocatalytically active, the layered Lepidocrocite surface shows much superior OER activity, showing an overpotential of 0.43 V [7] which we analysed through detailed electronic structure investigations.

This comprehensive understanding of abundantly available Fe oxyhydroxide minerals, spanning multiple length scales in homogeneous and heterogenous media, provides insights into their structural tunability and highlights their potential for strategic application as efficient OER catalysts.



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Invited Lecture 03

Balancing Molecular Freedom: Confinement and Constraints in Supramolecular Materials Design

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Abstract: Biological systems regulate function by carefully balancing molecular freedom. Rather than eliminating motion, they selectively restrict conformational and spatial degrees of freedom in a controlled manner to pre-organize interactions, bias energy landscapes, and guide selective outcomes. Confinement and constraint, therefore, operate as complementary strategies for directing molecular behaviour. 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.[4] Across crystalline lattices, coordination cages, and peptide-based assemblies, my research explores how balancing molecular freedom through confinement and constraint provides a general strategy for supramolecular materials design.

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Invited Lecture 04

Supramolecular Engineering Strategy: from Chiroptical Amplification to Tuneable Properties in Chiral Polymers

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Abstract: The ever-evolving interest in conjugated polymers towards sustainable energy storage, optical devices and sensing stems from their tunable optoelectronic property and high environmental stability over conventional inorganic materials. In that regard, polydiacetylenes are a fascinating class of conjugated polymers known for sensing and recognition owing to their stimuli-responsive ene-yne backbone.[1] Inducing chirality in polydiacetylenes provides an additional handle for tunable chiroptical behavior in thin-films and solutions.[2] Although polydiacetylene research has made significant contributions towards colorimetric sensing, the role of chirality-driven structure-property relationship in polydiacetylene self-assembly has not been explored toward flexible optoelectronics.

Chiral polymers consistently maintain a competitive edge over their achiral counterparts due to their effective utilization of asymmetry, allowing them to mimic natural systems across various domains. The uniform and ordered macroscopic structures of chiral π-conjugated polymers, capable of adapting their morphologies, offer a wide array of opportunities in chiral photonics with applications in electronics, spintronics and sensing. The recent surge in the development of chiral conjugated polymers and organic-inorganic hybrid systems[3-4] across diverse research fields such as plasmonics, chiroptics, and magneto-optics has attracted significant attention, positioning it as an emerging and crucial area with the potential to drive advancements in metamaterial applications.

We explore the role of chiral group interactions and molecular packing in a photoswitchable and photopolymerizable diacetylene system to control the ordering in polydiacetylene monolayers via azobenzene photoisomerization.[5-6] Also, we report the development of novel chiral conjugated polymers based on thiophene systems, utilizing peptides as versatile chiral precursors. To introduce a photocontrol element, azobenzene moieties were incorporated, enabling photoisomerization-based manipulation. The lecture highlights the interplay between molecular design and emergent optical properties in chiral conjugated polymers.

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Invited Lecture 05

Synergistic Interactions of Single Atoms with Semiconductors for Maximized Photocatalytic Hydrogen Generation and H_2O_2 Production

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Abstract: Single-atom catalysts (SACs) are a type of catalyst in which individual metal atoms are dispersed on a support material, rather than being present in clusters or nanoparticle (NP) cocatalysts, thus considered a bridge between homogeneous and heterogeneous catalysis.[1,2] Here, we present recent advancements of our group in the development of SAC for green hydrogen generation, oxygen reduction reaction for H_2O_2 production, and nitrate reduction for NH_3 production.[3,4] We introduced a simple, eco-friendly one-step hydrothermal method for synthesizing atomically dispersed Pd single-atom catalysts on $CuCo_2S_4$ semiconductor nanosheets, Pt SAs on g-$C_3N_{4.6}$ semiconductor, and Ni SAC on SnS_2 nanosheets. The structure of the SACs is investigated by aberration-corrected transmission electron microscopy and X-ray absorption fine structure (XAFS) spectroscopy. The novel synthesis process ensures strong coordination between the Pd SAs and S ions on the $CuCo_2S_4$ nanosheet surface, reducing overall charge transfer resistance and making them ideal for photogenerated electron capture based on an asymmetric charge density distribution. Similarly, we observed Pt-N and Ni-S_4 coordination in the other SACs. The SACs can facilitate the reduction of O_2 to H_2O_2, NO_3^- to NH_4^+, and H^+ to H_2 with high recycling stability.[3,4]

Keywords: single-atom catalyst; photocatalysis; H_2 evolution; nitrate reduction; oxygen reduction.

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Invited Lecture 06

Green Catalytic Delignification Process for Microcrystalline Cellulose from Sugarcane bagasse

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Abstract: India is second largest producer of sugarcane in the world after Brazil with around 18% of the world production. Bagasse is a large volume byproduct of the sugar industry which is used for energy generation in boilers. For conversion of bagasse into fermentable sugars, pretreatment is essential for removal of lignin and breaking lignocellulosic structure. The typically followed thermochemical methods involve steam explosion, alkali pretreatment, acid pretreatment, ammonia fiber expansion and organosolv. Cellulose is a major constituent of the biomass waste. Microcrystalline cellulose and nano-cellulose are very high value and low volume products which finds application in large variety of sectors. Typically Kraft process is used for separating cellulose from lignocellulosic materials. It is highly energy intensive and uses large excess of alkali and sulphur compounds generating large amount of effluent. Though this is existing commercial process, the more environmental friendly process is highly desired. **CSIR-NCL** has developed catalytic process for delignification of sugarcane bagasse under very mild conditions without generating any effluent. The end product of the delignification process is microcrystalline cellulose (MCC) which is a high value product with applications in various sectors. MCC is a pure partially depolymerized cellulose synthesized from α-cellulose precursor is used as a texturizer, an anti-caking agent, a fat substitute, an emulsifier, an extender, and a bulking agent in food production. The most common form is used in vitamin supplements or tablets. The MCC can be synthesized by different processes such as reactive extrusion, enzyme mediated, mechanical grinding, ultrasonication, steam explosion and acid hydrolysis. The later process can be done using mineral acids such as H_2SO_4, HCl and HBr as well as ionic liquids. The role of these reagents is to destroy the amorphous regions leaving the crystalline domains. In NCL process the MCC is obtained in single step with no effluent generated.

The process developed by NCL have following advantages:

- ☐ Hydrogen peroxide as oxidant
- ☐ Homogeneous catalyst
- ☐ No NaOH/Na_2S required as in Kraft process
- ☐ No harsh reaction conditions needed
- ☐ Low cost catalyst
- ☐ No acid/base, hence no special MOC for reactor
- ☐ Water used in the process can be recovered & reused
- ☐ Experiment on 1 kg bagasse scale carried out
- ☐ No effluent generated – ZLD process

Invited Lecture 07

Mechanistic investigation of the electro-/photo-chemical synthesis of ammonia

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Abstract: Photo(electro)catalytic nitrate reduction reaction (NO_3RR) to produce green ammonia is not only a sustainable solution to bypass the energy-intensive Haber-Bosch process but also thermodynamically challenging due to the requirement of sequential multielectron ($8e^-$) and proton ($9H^+$) transfers. The selective reduction of nitrate to ammonia proceeds via the formation of multiple reaction intermediates like $[NO_2]^-$, [NO], and $[NH_2OH]$. The rate-determining step of NO_3RR is the formation of $[NO_2]^-$, and the selectivity toward NH_3 (over NO_2, NH_2OH, N_2) formation is controlled by the optimum adsorption of the $[NO_2]^-$ intermediate to the catalyst surface. In our recent studies, metal-oxide nanoparticles such as FeO(OH), Mo_7 cluster-protected SnO_2, and CeO_2 nanoparticles were chosen as photo- and/or electro-catalysts to perform selective NO_3RR to produce NH_3.[1-2] Detailed spectro-electrochemical and electro-kinetics studies were conducted to understand the electrochemical rate constant. Labelling and in-situ spectroscopic studies were conducted to track some reactive intermediates of NO_3RR to validate the reaction mechanism (Figure 1). In my talk, I will briefly present these recent findings.

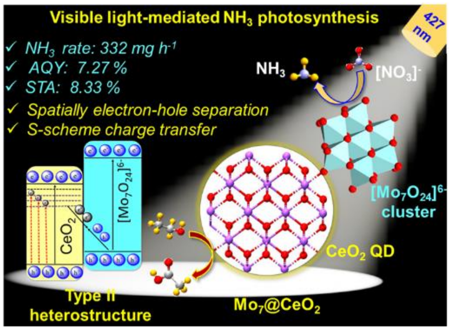

Figure 1. Visible-Light-Driven Ammonia Photosynthesis through S-scheme charge transfer pathway

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Invited Lecture 08

Multifunctional 2D Material-Based Sensors and Energy Harvesting Systems

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Abstract: Over 15 years after the first report of 2D material, Graphene and 2D material remain an active field of research considering their large surface area, excellent electrical and thermal conductivity, and abundance of catalytic sites in the field of electronic, photonic, sensing and energy harvesting. Although the layered structures demonstrate many beneficial attributes in this field, doping, functionalization, and patterning of these materials further open up a large area of research for enhancing sensitivity and active sites. Despite their potential, the challenge lies in fully harnessing these properties to develop multifunctional devices that can address complex real-world problems. One such challenge is the growing demand for advanced sensors for healthcare and environmental monitoring as well as efficient energy conversion systems towards sustainable energy solutions.

Our research has been centred on advancing the application of 2D materials and graphene-based systems, with a focus on creating integrated solutions for sensing, energy harvesting, and environmental monitoring. We explore how various stimuli influence their electrical properties, discovering that chemical vapor deposition-grown SnSe flakes exhibit negative photoconductivity. This phenomenon is attributed to the adsorption and desorption of water and oxygen molecules at the edge active sites of SnSe. By etching the flakes along their most active planes, further enhancing their photodetection capabilities (Figure 1a). Additionally, its sensitivity to humidity has been harnessed to create a highly responsive humidity sensor, which can be utilized for monitoring human respiration—an important application in medical diagnostics.[1] To further enhance the utility of these materials, we have functionalized them with specific dopants, enabling their application in energy harvesting. SnSe, after functionalization, is used as an electrocatalyst in electrochemical hydrogen generation, showing improved catalytic performance with an overpotential decrease by several hundred millivolts. Furthermore, an on-chip microcell configuration facilitates the study of light and electric field effects on the catalytic properties and identifying the active catalytic sites. Parallelly, we developed self-powered ultrafast sensors using nitrogen-doped graphene anchored with cobalt nanoclusters (Co-N-Gr) which exhibits triboelectric nanogenerators (TENGs) not only provide exceptional sensitivity for detecting NO_x levels in human respiration but also offer the ability to differentiate respiratory conditions, such as acute exacerbations of chronic obstructive pulmonary disease (AECOPD) (Figure 1b).[2] This work laid the foundation for exploring the broader potential of Co-N-Gr towards energy harvesting. The hydrophilicity and enhanced charge transfer capabilities of the such doped carbonaceous system allowed us to achieve a significant increase in power generation by 108 times, particularly in environments with varying pH levels and the presence of acidic contaminants. This seamless transition from sensing to energy harvesting highlights the

versatility of 2D materials as multifunctional materials capable of integrating environmental monitoring, healthcare with sustainable energy solutions.

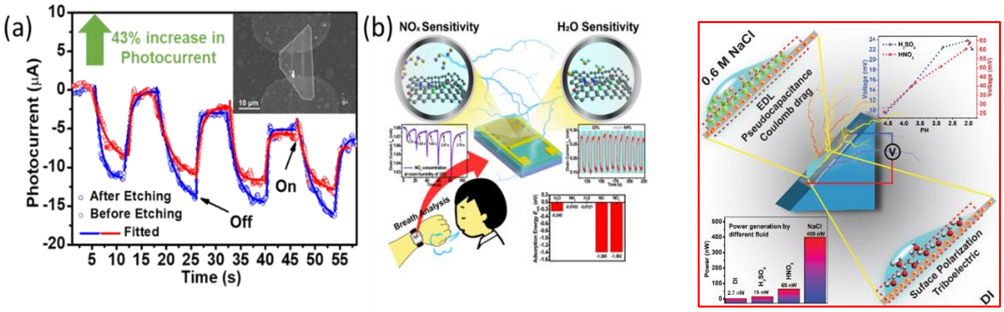

Figure 1. (a) SnSe flakes show increased photocurrent after being etched along the most active plane directions; (b) Co-N-Gr template being used for detecting NO_x levels and human respiration monitoring (c) Co-N-Gr template for hydro-voltaic power generation.

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Invited Lecture 09

Functional Materials to Sensor Systems: Devices, Platforms, and Applications

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Abstract: Advances in nano and functional materials have significantly expanded the capabilities of modern sensing technologies, enabling the development of highly sensitive, selective, and application-specific sensor systems. This talk presents a comprehensive overview of the journey from functional materials to integrated sensor systems, highlighting the interplay between material properties, device design, and system-level implementation. The discussion begins with the role of functional materials such as metal oxides, thin-film platinum, and emerging nanostructured materials in enabling diverse sensing mechanisms, including resistive, thermal, and optical transduction. Building on these material platforms, various microfabricated devices are demonstrated, including metal oxide-based gas sensors, platinum-based temperature sensors (RTDs), MEMS-based infrared emitters, and thermal flow sensors. Emphasis is placed on design strategies that leverage material properties to improve performance, stability, and scalability.

The talk further explores the transition from individual devices to integrated sensing platforms, covering microheater design, packaging, signal conditioning, and system-level calibration. Case studies covering environmental monitoring, industrial sensing, and emerging applications are presented to illustrate the practical realization of these technologies. Finally, key challenges and future directions in the field are discussed, including material reliability, system integration, and the need for application-driven sensor design. The work highlights how a unified approach that bridges materials science and engineering can enable the development of next-generation sensor systems tailored for real-world applications.

Invited Lecture 10

Enhancing Organic Long-Persistent Luminescence via Trace Doping and Triplet-Triplet Energy Transfer

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Abstract: Organic long-persistent luminescence (OLPL) materials have attracted significant attention for their unique afterglow properties and applications across biomedical imaging and optoelectronics. Our research has achieved a major breakthrough by using trace-doping strategies to extend OLPL duration to up to 7 hours.[1,2] This process, influenced by the "Sergeant and Soldier" effect, alters crystal packing and significantly enhances OLPL efficiency.

Notably, we have visualized the exciton transition process in these hybrid materials under various excitation conditions. Spectroscopic analysis revealed that the improved performance stems from triplet-triplet energy transfer (TTET) of abundant triplet excitons from the host, rather than enhanced intersystem crossing between the guest and host. This insight into the TTET mechanism opens new possibilities for tuning luminescent properties in room-temperature phosphorescence.[3] These findings have broad applications in advanced optoelectronics, lighting technologies, and next-generation biomedical imaging.

Keywords: Organic long-persistent luminescence materials, trace-doping strategy, triplet-triplet energy transfer, room-temperature phosphorescence.

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Invited Lecture 11

The impact of x-rays with high brilliance on the oxidation state of arsenic ions and consequently on the nucleation of arsenic bearing phases within aqueous medium

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Abstract: The speciation of arsenic (As) in aqueous environments, particularly the relative concentration ratio of highly toxic and mobile arsenite (As(III)-bearing) anion and comparatively less toxic and less mobile As(V)-bearing arsenate anion in the system, as well as their interconversion, if at all, is a critical issue related to environment and health. Confining these toxic species within stable crystalline cages of naturally occurring solids and minerals, made up of arsenic and other common elements, such as iron, is being considered as an important decontamination strategy in recent times. Evidently, designing such an environmental management plan warrants several in-situ x-ray spectroscopic studies on the aqueous solution, containing arsenic and other common ions, but the present work warns against a barely noted photo-oxidation phenomenon of As(III) to As(V) within Fe-As aqueous solutions at certain pH ranges, that takes place under the influence of high flux synchrotron x-ray irradiation. Our x-ray absorption spectroscopy (XAS) experiments on the Fe and As K-edges with the purpose of monitoring the in-situ nucleation of Fe(III)-As(III) clusters and growth, as a function of pH, revealed this unforeseen photo-oxidation as the pH of the solutions was raised above 3.2. Our combined experimental and density functional theory-based studies proved that the accelerated photo-oxidation is primarily driven by reactive free radicals, notably the hydroxyl radical (•OH), generated through the radiolysis of water by the high energy x-ray beam of very high brilliance, and this photo-oxidation consequently drives significant structural reorganization, where Fe(III)-As(III) tooeleite-like clusters get converted to As(V)-adsorbed ferrihydrite-like moieties.

Invited Lecture 12

The scent of health: Semiconductor nanocomposites-based gas sensor towards human healthcare

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Abstract: Sensors are omnipresent and became an indispensible part of our society. Besides conventional use, gas sensor based breath analyzer has attracted increasing interest among the scientist, technocrats and clinical communities. Breath analysis is a non-invasive technique which can provide information and monitoring of various diseases. There exists a huge market for gas sensors which is ever increasing due to it's conventional as well as new application possibilities including non-invasive breath analysis for monitoring diseases.

Oxides such as SnO_2, ZnO, TiO_2, WO_2, MoO_3 etc. are being explore for gas sensing application. However, due to limitations like high operating temperature, low selectivity and stability of oxide based sensors, now a day's researcher are also trying to replace the metal oxide with much stable materials. Other than metal oxide, metal chalcogenides and some novel complex oxide composites are now being well considered due to low cost, easy fabrication and good stability. Also, use of nanomaterials has been shown to allow gas sensors to work at lower temperature, with better sensitivity, selectivity and long-term stability than sensors based on bulk materials.

Human exhale breath is composed of several gasses and hundreds of volatile organic compounds (VOCs). An accurate detection of specific gas /VOCs in exhaled breath, known as biomarkers, can provide essential information for the diagnosis of those diseases. The compounds of interest (VOCs) are generally found at ppb /sub-ppm level in healthy human breath which can increase several times in the breath of patients. However, the ability to prepare novel nanomaterial having high sensitivity, good resolution at sub-ppm /ppb level and insensitive toward moisture is required for development of breath analyzer, is currently not achievable. This presentation will cover all the aspects starting from preparation of novel nanocomposites to fabrication and performance of prototype device in detail.

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Invited Lecture 13

Engineering Polymer Hybrid Nanomaterials toward Selective and Sensitive Gas Detection

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Abstract: Advancements in gas sensing technologies demand materials with exceptional sensitivity, selectivity, and stability under ambient environments. This study presents the engineering of polymer hybrid nanomaterials based on polyaniline (PANI) and polypyrrole (PPy) for selective and sensitive gas detection. Functional nanostructures including metal oxides, carbon-based nanomaterials, and conducting polymers were systematically integrated within optimized polymer matrices, yielding hybrids with synergistic enhancements in charge transport, surface reactivity, and molecular adsorption. The engineered nanocomposites exhibited rapid response and recovery, remarkable repeatability, and high selectivity toward low concentrations of ammonia (NH_3), nitrogen dioxide (NO_2), and volatile organic compounds (VOCs). These results underscore the potential of PANI and PPy hybrid architectures as high-performance active layers for next-generation gas sensors, combining the benefits of polymer flexibility, process simplicity, and nanostructure-induced sensitivity.

Invited Lecture 14

Optoelectronics, Electrocatalysis and Charge Storage using Transition Metal Dichalcogenide based Nano-heterostructures

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Abstract: Transition metal dichalcogenides (TMD) have emerged as an important class of materials for several applications. Their two-dimensional nature renders them useful in many applications ranging from optoelectronics to batteries, spintronics and catalysis. In this talk, I will discuss the possibilities of formation of nano-heterostructures based on $MoSe_2$ – a 2D TMD and their applications for optoelectronics and catalysis, in particular water splitting. Interestingly, the TMDs can also be used as a Selenium source to passivate lead halide perovskites rendering them highly stable. Further, the TMDs have been shown to exhibit charge separation and therefore are useful for applications in photodetectors and catalysis, in particular electrocatalysis for reactions such as the hydrogen evolution reaction or the oxygen evolution reaction. Due to the layered nature of the TMDs these can accommodate ions between the layers and therefore are very advantageous for use as capacitor or battery applications. I will discuss a few of these possibilities.

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Oral Presentations

OP 01

Nanoscale Design Principles for Solar-to-Fuel Conversion: Insights from Carbon Dot Photocatalysts

Daniel Langford, Yana Reva, Yifan Bo, Kirill Gubanov, Mingjian Wu, Ayşe Günay-Gürer, Lukas A. Mai, Ryan W. Crisp, Iryna Engelmann, Erdmann Spiecker, Rainer H. Fink, Axel Kahnt, **Bikash Jana***, Dirk M. Guldi*

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Abstract: Photoactive processes—especially photocatalysis—fundamentally rely on efficient energy transfer and charge carrier dynamics, where the separation and migration of electron–hole pairs determine overall activity and selectivity. In this lecture, I will discuss the pressing importance of photocatalytic hydrogen generation, CO_2 reduction, and nitrogen fixation as sustainable pathways for addressing global energy and environmental challenges. Particular attention will be given to harnessing low-intensity sunlight, a condition especially relevant in pollution-affected regions across India, where conventional photovoltaic systems often perform poorly. The central focus of the lecture will be photocatalytic hydrogen generation enabled by carbon nanodots.[1] Their favorable band alignment, active photocatalytic centers, and tunable surface functionalities collectively facilitate proton-coupled electron transfer processes.[2] I will highlight how these nanodots surpass analogous molecular photocatalysts in optical stability and robustness, effectively mitigating deactivation pathways common in molecular systems. The mechanistic discussion will encompass exciton generation, interfacial charge transfer, and strategies to suppress recombination losses. Overall, the lecture aims to interlink nanoscale material design with the underlying photophysical principles that govern solar-to-fuel energy conversion.

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OP 02

Design and Synthesis of Amphiphilic Glucoconjugates: Reactivity Toward Terbium Sensitization and Chiroptical Properties

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Abstract: We describe the synthesis of amphiphilic 4,6-*O*-ethylidene-β-D-glucopyranosylamine-derived ligands and their corresponding terbium complexes. The complexes exhibit characteristic green luminescence attributed to Tb-centred transitions [$^5D_4 \rightarrow {}^7F_j$ (j = 6–3)] with emission bands observed at 485, 545, 580, and 620 nm.[1] The use of enantiomerically pure D-glucose in ligand design enables investigation of circularly polarized luminescence (CPL) properties.[2] The terbium complexes display comparable dissymmetry factors (g_{lum}) on the order of ~5×10^{-2} across the series, along with moderate quantum yields in the range of 1–5%. Structural elucidation was achieved by synthesising an analogous diamagnetic yttrium(III) complex. Comparative FTIR analysis of the Tb^{3+} and Y^{3+} complexes, together with NMR spectroscopy, provided insight into their coordination environments and structural features.

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OP 03

Natural Sunlight Harvesting Benzothiadiazole-based Molecular Photocatalyst for H_2O_2 Production: A Recyclable Homogeneous Biphasic System

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Abstract: Photocatalytic hydrogen peroxide (H_2O_2) synthesis offers a sustainable route for solar-to-chemical energy conversion to address the increasing global energy demand. However, developing an efficient and sustainable photocatalytic system for H_2O_2 synthesis remains a critical bottleneck. Herein, we report a unique toluene-water two-phase system for highly efficient H_2O_2 synthesis employing benzothiadiazole-based small organic photocatalyst, Py-BT-Th. Py-BT-Th shows a high H_2O_2 production rate of 107.18 mmol g^{-1} h^{-1} with turnover frequency of ~ 32 h^{-1} under natural sunlight irradiation in the toluene-water biphasic system using triethylamine as a sacrificial agent. The biphasic system promotes H_2O_2 mass transport, leading to rapid kinetics across the toluene-water interface. Experimental studies reveal that the superior photocatalytic performance of the catalyst Py-BT-Th is attributed to its donor-acceptor type molecular architecture, which promotes efficient exciton separation, high molar absorptivity ($\varepsilon = 12.27 \times 10^3$ M^{-1} cm^{-1}), long exciton lifetime (12.9 ns) and broad light-harvesting capacity. Scavenger and in-situ EPR spectroscopic studies confirm that Py-BT-Th produces H_2O_2 following a dual mechanistic route: (1) indirect two-step one-electron ORR *via* an electron transfer pathway, (2) singlet oxygen generation *via* an energy transfer pathway. In both the routes, $^{\bullet}O_2^-$ is the key intermediate that ultimately gets converted into hydrogen peroxide, in association with the oxidation of triethylamine by photogenerated holes. Overall, this work disentangles the dilemma associated with small organic photocatalysts for H_2O_2 synthesis through a recyclable toluene-water biphasic system.

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OP 04

Development of Iridium-based Metal Complex for Low-Cost Detection of Creatinine and Human Serum Albumin (HSA) from Human urine

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Abstract: The fluorescent assay is an important technique for detecting and quantifying analytes because of its high sensitivity and selectivity, fast response time, on-site detection, and portable, easy-to-handle devices.[1] We have developed binuclear iridium(III) phosphorescent complexes, M3[2] and M1, which detect creatinine and Human Serum Albumin (HSA), respectively, via a sharp emission colour change. The probe responds in powder form or as a thin film fabricated for creatinine on low-cost filter paper, and in solution phase for HSA. A real-world application is demonstrated by sensing creatinine and HSA in human urine samples. The components in urine are tested separately using probes, which are highly selective for creatinine and HSA. The tests were performed on animal models and on human urine samples collected from patients at different stages of CKD, and the results are highly encouraging. This luminescent-based detection technique has been translated into a small, portable prototype device. The device has been used to test patients' urine samples, and the results have been well validated against existing pathology techniques.

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OP 05

Sulfonamide-based COFs as Efficient Additives in Polyethylene Oxide for Improved Ionic Conductivity

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Abstract: Two novel amorphous covalent organic frameworks (COFs) functionalized with sulfonamide groups were successfully synthesized and incorporated into a poly(ethylene oxide) (PEO) matrix to develop advanced composite polymer electrolytes (CPEs). The resulting CPEs exhibit significantly enhanced physicochemical and electrochemical properties compared to pristine PEO. Notably, the optimized system delivers a high ionic conductivity of **8.7×10^{-3} S cm^{-1}** at 50 °C temperature, along with an electrochemical stability window up to 1.39 V and excellent thermal stability up to 300 °C. Electrochemical measurements reveal a specific capacitance of **186 F g^{-1}**, a coulombic efficiency of 99% at 1 V, and a high ionic transference number of 0.998, indicating dominant ionic conduction. The improved performance is attributed to strong interactions between Li^+ ions and sulfonamide ($-SO_2NH-$) functionalities, which promote effective lithium salt dissociation and enhance ion mobility. Differential scanning calorimetry confirms the predominance of an amorphous phase during operation, facilitating ion transport. The synergistic effect between the COF additives and the PEO matrix plays a key role in achieving superior conductivity and stability. This study demonstrates the potential of sulfonamide-based COFs as efficient additives for high-performance polymer electrolytes.

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OP 06

Structure-Property Relationships in PBSA/PHBH Biopolymer Blends: A Molecular Dynamics Study for Sustainable Packaging Application

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Abstract: Blending biodegradable polymers offers a scalable route to engineer materials with tailored mechanical performance for sustainable packaging. However, the properties of such blends are strongly governed by their phase morphology and interfacial interactions, which remain challenging to characterize experimentally at the molecular scale. In this work, molecular dynamics (MD) simulations are employed to elucidate the microstructure and mechanical behaviour of blends of poly(butylene succinate-co-butylene adipate) (PBSA) and poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBH) across a range of compositions. These aliphatic polyesters are attractive candidates for environmentally friendly packaging due to their biodegradability and favourable mechanical properties. The simulations reveal that PBSA/PHBH blends are predominantly immiscible, forming distinct droplet–matrix morphologies depending on composition. Notably, partial miscibility of PBSA in PHBH-rich systems is observed, consistent with reported experimental trends. Quantitative analysis further shows that the interfacial area between polymer domains plays a critical role in governing the mechanical response of the blends. In particular, the Young’s modulus exhibits a clear dependence on composition, increasing with higher PHBH content. These results demonstrate the ability of MD simulations to capture realistic blend morphologies and provide direct insight into structure–property relationships in biodegradable polymer systems. The findings offer valuable guidance for the rational design of high-performance, sustainable packaging materials through controlled manipulation of blend composition and interfacial characteristics.

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OP 07

Investigating WSe_2-PMMA Nanofibers for emerging memory and synaptic characteristics

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Abstract: In this study, we synthesized WSe_2 nanoflowers and fabricated WSe_2-PMMA nanofibers to investigate resistive switching (RS) and emulate synaptic characteristics. The electrospun WSe_2-PMMA nanofibers functioned as the active layer for both applications, with Ag serving as the top electrode and ITO as the bottom electrode. A PMMA solution was prepared in DMF, to which 10 mg of WSe_2 powder was added and stirred for 12 hours before being electrospun onto an ITO-coated PET substrate. This process was followed by annealing at 85 °C for 3 hours to ensure uniformity and stability. The device structure comprised Ag/WSe_2-PMMA nanofiber/ITO. The device's non-volatile memory properties were confirmed by its consistent bipolar resistive switching behavior, featuring an ON/OFF current ratio of approximately 10^2 and exceptional data retention exceeding 10^3 seconds. Multilayer resistive switching was effectively demonstrated by controlling the compliance current (Icc) during the SET procedure. Additionally, the synaptic characteristics were analyzed for potentiation, depression, and learning and forgetting over five cycles. The device's multi-bit storage capacity was demonstrated by achieving distinct and reproducible resistance states at three different compliance currents (0.1, 0.01, and 0.001 mA), underscoring its multi-bit storage capability. The nanofiber morphology confines ion migration paths, thereby controlling the formation and rupture of conducting filaments.

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OP 08

Type-II WO_3/NiOOH nanoflakes enable efficient and selective low-bias photoelectrochemical saline water-splitting reaction

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Abstract: WO_3, an n-type semiconductor composed of earth abundant elements, has attracted significant attention due to its favorable valence band position and high stability in both neutral and highly acidic conditions. However, its photoelectrochemical performance is limited by high surface charge carrier recombination. To address this issue the γ-NiOOH is employed as the cocatalyst on the surface of WO_3 to extract holes reaching the surface of WO_3 and to enhance the water oxidation kinetics of the system. The optimized heterostructure exhibits a substantial enhancement in photocurrent density (2.23 mA/cm^2) compared to pristine WO_3 (1.53 mA/cm^2) at +1.2 V vs. Ag/AgCl, accompanied by a cathodic shift of ~400 mV in onset potential. This significant improvement is attributed to enhanced charge separation and efficient hole transfer mediated by γ-NiOOH, which promotes oxygen evolution reaction (OER) kinetics at the interface. Despite the improved PEC performance, post-stability studies reveal dynamic structural and chemical evolution of the cocatalyst under highly corrosive saline water conditions. During a 5 h photostability test, NiOOH undergoes partial delamination within the first hour, followed by surface reconstruction and partial transformation into $Ni(OH)_2$ over prolonged operation. The transformed cocatalyst retains the initial PEC performance after initial decrement during PEC operation. Post-stability X-ray photoelectron spectroscopy (XPS) is performed after 1 h and 5 h of operation, revealing significant modifications in the electronic structure, including Fermi level upshifting associated with the formation of mid-gap states, likely arising from oxygen vacancies. The heterostructure exhibits excellent efficiency and selectivity towards water oxidation in corrosive saline water conditions, which enhances the long-term durability of the photoelectrode.

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OP 09

Stabilizing Ru Single Atom Catalyst Through Electronic Metal-Support Interaction with $NiCo_2O_4$ Support for Overall Water Splitting and Urea Electrolysis

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Abstract: Developing effective bifunctional electrocatalysts in water-splitting becomes crucial in order to avert a massive energy crisis in the near future.[1] Noble metals show an irreplaceable activity toward electrocatalytic water-splitting reactions but their high cost prevent their large-scale application.[2] Single atom catalyst manifests themselves as a new frontier in heterogenous catalysis owing to their efficiency of maximum atom utilization.[3,4] However, their tendency to get aggregate leads to the poor stability, which limits their application.[5] Herein, we overcome this challenge by stabilising a noble metal single atom catalyst through anchoring it on a metal oxide support, where a strong electronic metal-support interaction prevents their aggregation. Specifically, we have synthesized Ru single atoms anchored on the $NiCo_2O_4$ support by using the ultra-low amount of Ru. XAS and HAADF-STEM analysis confirms the presence of isolated Ru single atoms on the support. These isolated Ru atoms have a high density of unoccupied orbitals, which is favourable for electrocatalytic activity. The synthesized Ru single atom catalyst on $NiCo_2O_4$ shows superior activity for overall water splitting with a cell potential of 1.57 V to generate a current density of 10 mA/cm^2 and showing durability of 60 h. Density functional calculation reveals that supported single Ru atoms optimized the binding energies of the intermediate of both HER and OER.

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OP 10

Lightweight copper nanowire-hollow glass microsphere loaded melamine formaldehyde composite for electromagnetic shielding application

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Abstract: Electromagnetic interference (EMI) shielding materials are vital for device applications as they prevent EM disturbances and ensure reliable device performance. This work investigates the enhancement of EMI shielding performance of melamine formaldehyde (MF) resin through the incorporation of copper nanowire (CuNWs) decorated hollow glass microspheres (HGMs). A hybrid filler system was developed by anchoring CuNWs onto the surface of HGMs using 3-aminopropyltriethoxysilane (APTES) as a coupling agent. The APTES modified HGM surface provides active amine functionalities that facilitate the uniform decoration and stabilization of conductive CuNWs over the dielectric microspheres. The resulting CuNWs decorated HGM hybrid fillers were subsequently dispersed within the MF matrix, leading to a composite with a well distributed conductive network while maintaining lightweight characteristics. The synthesized composites were systematically characterized using scanning electron microscopy (SEM) to confirm surface morphology and successful CuNWs attachment, X-ray diffraction (XRD) for phase identification, Fourier transform infrared spectroscopy (FTIR) to verify chemical interactions, and electrical conductivity measurements to evaluate the formation of conductive pathways. The results indicate that the incorporation of CuNWs decorated HGMs significantly improves the electrical conductivity of the MF matrix compared to the pristine polymer. EMI shielding performance was evaluated in the X-band frequency range (8.2-12.4 GHz), where the composite exhibited a shielding effectiveness of approximately 30 dB at 15 wt% filler loading. The shielding mechanism is primarily governed by absorption-dominated processes, supported by the formation of a conductive CuNWs network and enhanced interfacial polarization. Additionally, the hollow and porous nature of HGMs promotes multiple internal reflections of incident electromagnetic waves, effectively increasing the attenuation path length and enhancing energy dissipation within the material. The synergistic interaction between conductive CuNWs and dielectric HGMs contributes to improved impedance matching and reduced reflection losses. Furthermore, the incorporation of HGMs enables the development of lightweight composites with improved thermal resistance, making them suitable for practical EMI shielding applications. The developed CuNWs decorated HGM/MF composites demonstrate a promising balance between electrical performance, weight reduction, and thermal stability, offering potential for advanced shielding materials in electronic and aerospace applications.

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OP 11

Benzimidazole Derived Optical Luminogens: From switchable mechanochromism to the detection of biomarkers

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Abstract: Molecules with solid-state luminescence and mechanochromic properties have attracted interest due to their potential applications in optoelectronic materials such as organic light-emitting diodes (OLEDs) and organic field-effect transistors (OFETs)[1]. Herein, we have synthesised BIDCPV, which exhibits Aggregation-Induced Emissive (AIE) Properties with switchable mechanochromism. Given these AIE properties, we next designed the hydroxy series of BIDCPV to examine optical changes during substitution. Having the Hydroxy substitution, along with the AIE properties, in the ortho isomer, the excited-state intermolecular proton transfer property is observed, exhibiting the dual fluorescence enhancement. To further demonstrate its efficacy, we next utilised the following derivative and synthesised the est-o-BIDCPV for the detection of overexpressed cellular esterase[2].

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OP 12

Interplay of Sn-Induced Electronic Perturbation and Surface Defects in Bi_2MoO_6 for Improved N_2 Photofixation

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Abstract: Photocatalytic ammonia (NH_3) generation has emerged as a promising green alternative to the Haber– Bosch process; nevertheless, its progress is restricted by inefficient performance and limited understanding of how N_2 is activated.[1,2] In this context, tuning the electronic structure of catalysts through elemental doping has emerged as an effective strategy to enhance ammonia production.[3,4] In this work, Sn-doped Bi_2MoO_6 is investigated as a model photocatalyst, supported by density functional theory calculations and experimental analyses, which reveal that Sn incorporation effectively tunes the electronic structure and generates catalytically active sites, thereby enhancing photocatalytic nitrogen reduction reaction (PNRR) performance. At the optimised composition (10% Sn-Bi_2MoO_6), characterised by a preferentially exposed (131) facet and a high concentration of oxygen vacancies, the catalyst achieves an NH_3 production rate of 2.07 $mmol.g^{-1}.h^{-1}$ under solar irradiation with a solar-to-ammonia conversion efficiency of ~1.4%, approximately 10.9 times higher than Bi_2MoO_6. The enriched oxygen vacancy sites significantly enhance N_2 adsorption and activation, enabling efficient N≡N bond cleavage through proton-coupled pathways. Mechanistic insights obtained from infrared spectroscopy further elucidate the reaction intermediates and dynamic processes involved. Notably, under natural sunlight in the designed prototype system, 10% Sn-Bi_2MoO_6 delivers an NH_3 evolution rate of ~450 $\mu mol.g^{-1}.h^{-1}$. The present results reveal that synergistic electronic modulation at the atomic scale and defect engineering are pivotal for improving PNRR efficiency, offering a promising route toward decentralized NH_3 production.

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Poster Presentations

PP-01

Enhanced Visible-Light Driven Dye Degradation Using g-C_3N_4/CNT Heterostructure Photocatalyst

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Abstract: The development of efficient photocatalysts for wastewater treatment remains an important research priority due to increasing environmental pollution from industrial dyes. In this work, a heterostructured photocatalyst based on graphitic carbon nitride (g- C_3N_4) and carbon nanotubes (CNTs) was successfully synthesized using a simple in situ thermal polymerization. The formation of an interconnected conductive network between g-C_3N_4 and CNTs was confirmed through structural and morphological characterization techniques like XRD, SEM, TEM. The photocatalytic activity of the prepared heterostructure was evaluated for the degradation of organic dye pollutants under visible light irradiation. Compared to pristine g-C_3N_4, the composite demonstrated significantly enhanced degradation efficiency. This improvement is mainly attributed to the increased surface area, better charge carrier separation, and the excellent electron transport capability of CNTs. Furthermore, the heterostructure exhibited good stability and reusability over multiple degradation cycles, indicating its potential for practical environmental remediation applications. Adsorption and degradation were done. These findings suggest that coupling g-C_3N_4 with conductive carbon nanomaterials provides better charge transport mechanism and suppresses recombination resulting in an effective strategy to design high-performance photocatalysts for dye-contaminated wastewater treatment.

PP-02

Variation of stabilization energy with the solvent polarity: a density functional reactivity theory (DFRT) based approach

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Abstract: Surface engineering dictates the fate and functionality of nanomedicines, where achieving ultra-stability with biocompatibility remains a formidable challenge. While polyethylene glycol (PEG) has long been the gold-standard ligand for imparting stability and stealth, issues such as accelerated blood clearance, anti-PEG immunogenicity, and non-biodegradability demand sustainable surrogates. Addressing this, we developed Exscalar gold nanoparticles (Ex@AuNPs) an ultra-stable, monodispersed, and PEG- rivalling nanoplatform synthesized through a one-step bioextraction from fish scales, yielding oligopeptylated coatings that serve as a natural molecular armor. These oligopeptides form robust stabilizing agent, endowing Ex@AuNPs with exceptional colloidal integrity against centrifugation, freeze–thawing, lyophilization, high ionic strength, organic solvents, and diverse biological fluids, while retaining non-hemolytic and cytocompatible profiles.

Extending beyond physicochemical stability, proteomic and bioinformatic analyses revealed that Ex@AuNPs interact selectively with plasma proteins—adsorbing only 67 corona constituents versus
131 for PEG-AuNPs—favoring immunoglobulins, complement C1q/C4A, and fibrinogen with isoelectric points between 5–7, signifying a refined and less opsonized biomolecular identity. Cellular assays delineated energy-dependent uptake via clathrin and scavenger-mediated endocytosis, while ultramicrotome-assisted HR-TEM remarkably confirmed nuclear translocation, an uncommon feature among non-viral nanocarriers.

Collectively, this triadic investigation spanning synthetic sustainability, molecular proteomics, and subcellular mapping—unveils the molecular armor that confers Ex@AuNPs their PEG-comparable stability, biocompatibility, and unique nuclear trafficking aptitude. These findings position Exscalar AuNPs as a next-generation oligopeptide-engineered nanoplatform, redefining sustainable nanomedicine by integrating biodegradability, biocompatibility, and precision intracellular delivery for advanced theragnostic applications.

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PP-03

The Hidden Pull: Ocular Fluidic Corona Signatures Towards the Invisible "Nanomagnets"

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Abstract: The integration of nanotechnology into ophthalmology represents a promising frontier for the development of precision diagnostics and therapeutics aimed at enhancing ocular health. While the systemic interactions of iron oxide nanoparticles (IONPs) with blood plasma have been extensively studied, their bio-nano interactions within the ocular environment, particularly in tear fluid, remain largely unexplored. In this study, we comprehensively investigated the physicochemical behaviour and proteomic corona profile of IONPs upon exposure to human tear fluid. Dynamic light scattering revealed a modest increase in hydrodynamic diameter from ~115 nm to ~139 nm, accompanied by reduction in the zeta potential from −36 mV to −29 mV, indicating positive protein adsorption. Proteomic profiling v*ia* liquid chromatography–mass spectrometry (LC-MS/MS) identified that 57 out of 91 native tear proteins selectively adsorbed onto the IONPs. Bioinformatic analysis revealed an enriched corona composed of annexins, keratins, immunoglobulins, ezrin, peripherin, cystatin-A, glyceraldehyde-3-phosphate dehydrogenase, and pyrin, proteins implicated in cytoskeletal dynamics, immune defense, tissue integrity, nucleotide binding, inflammation regulation, and signal transduction. These findings provide the first in-depth molecular snapshot of the ocular nano–bio interface, emphasizing the critical influence of tear fluid composition on nanoparticle behaviour. Our results highlight how tear-specific protein corona formation redefines the physicochemical identity of superparamagnetic IONPs within the ocular environment. These findings provide a foundational framework for considering how corona-modified magnetic nanoparticles may behave in future magnetically guided ocular therapeutic strategies.

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PP-04

Environment Regulated Self-Assembly of TPE–Peptide Amphiphile for Tunable AIE and CPL Responses

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Abstract: Fine-tuning supramolecular assembly pathways has been extensively utilized to control the morphology and functional attributes of self-assembled systems; however, its application in the development of circularly polarized luminescent (CPL) materials with adjustable properties remains relatively limited. Realizing such control requires careful manipulation of supramolecular polymerization, governed by intrinsic molecular features such as minor structural variations as well as extrinsic factors like pH, solvent composition and temperature, all of which influence the assembly pathways and resulting chiroptical properties. In this regard, peptides serve as excellent building blocks owing to their inherent chirality, tunable structures and strong responsiveness to changes in their surrounding microenvironment. We developed a tetraphenylethylene-conjugated peptide amphiphile, TPE–VFFARR, to couple aggregation-induced emission (AIE) with peptide-driven self-assembly. The system was studied in HFIP and DMSO under varying pH and ionic strength, where pH-dependent morphology changes highlight the role of guanidinium-mediated electrostatic interactions of arginine. Reduced protonation weakens repulsion, promoting tighter π–π stacking of TPE and enhanced emission. Incorporation of PEG 350 as a macromolecular crowder further modulates assembly via excluded volume effects and restriction of intramolecular rotations, amplifying AIE. Under sodium phosphate buffer (pH 9) and at pH 14 in 10% DMSO, where arginine is largely deprotonated, reduced electrostatic repulsion combined with hydrophobic collapse and crowding-induced confinement drives the formation of ordered emissive aggregates exhibiting CPL. These results demonstrate that electrostatics, solvent interactions, and crowding collectively govern packing and emission anisotropy, providing a basis for designing CPL-active soft materials for optoelectronic applications.

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PP-05

From Nanofibers to Nanotoroids: Visible Light Regulates Topological Switching in Fluoroazobenzene-tethered Peptide Assembly

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Abstract: Azobenzene-tethered peptides represent a versatile platform for designing dynamic self-assembling systems, driven by their photo responsive properties. These simplified molecular photo switches are potent aids to manoeuvre and elucidate self-assembly compared to the large complex proteins or biological systems. Herein, we report a stimuli-responsive fluorinated azobenzene ligand appended onto a self- assembling amyloidogenic peptide, which can be isomerized reversibly by light in the visible range, with each isomer having different geometric and photophysical properties. Here, the introduction of electron- withdrawing Fluorine atoms ortho to the azo unit, serves to red-shift photoisomerization wavelengths, improve photoconversion efficiency and importantly stabilize specific isomers. Effect of selective photo switching towards self-assembly chemistry and photophysical properties has also been investigated. This dynamic behaviour on exposure to specific wavelengths of light, profoundly influence the self-assembly pathways, resulting in tuneable supramolecular structures. Thus, visible light activation has provided a non- invasive method offering real-time control over structural transitions and hierarchies in assembly. Our findings reveal that the pathway complexity arises from a balance between azobenzene conformational states and the inherent aggregation tendencies of the peptide backbone.

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PP-06

Sustainable Fabrication and Photocatalytic Performance of 2% Cu-doped TiO_2 Nanocomposite for Dye Degradation

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Abstract: The use of nanocomposites in the degradation of toxic and carcinogenic industrial dyes has been recognized as an emerging technology that is considered to be more promising and environmentally friendly. Pure TiO_2 is widely recognized as a photocatalyst. However, it is primarily active under ultraviolet (UV) radiation. The problem is that UV is only 5% of the total solar spectrum. Therefore, its efficiency is limited. This research reports that 2% Copper (Cu)-doped Titanium dioxide (TiO_2) nanocomposites were synthesized through the hydrothermal method calcined at 120°C in which Titanium dioxide powder was used as the precursor. Copper sulfate was used as the precursor to dope Copper. The comprehension characterization of the nanocomposites using RAMAN, EDS, FESEM, XRD and UV-Vis spectroscopy confirmed the successful doping of Copper into Titanium dioxide demonstrating precise control of nanostructure, elemental composition and surface morphology. The efficiency of the synthesized nanocomposites as photocatalysts was examined through the degradation of Rhodamine B dye in aqueous solution under moderate sunlight. The results revealed the highly efficient degradation of dye within 12 minutes under magnetic stirring.

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PP-7

Synthesis and Characterization of 1D Cu_xO-ZnO Mixed Oxide Thin Films

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Abstract: This study reports the scalable synthesis of mixed CuO-ZnO (CZO) nanowires via controlled thermal oxidation of sputtered thin films. The integration of ZnO slows the oxidation kinetics of Cu, stabilizing the Cu_2O phase and promoting the growth of dense, well-aligned 1D nanostructures. Characterization confirms a synergistic tri-phase composition (Cu_2O, CuO, and ZnO) that facilitates the formation of interfacial p-n heterojunctions. These CZO sensors achieve a 57% response to 50 ppm methanol at a significantly reduced operating temperature of 75°C. With a detection limit of 0.5 ppm, they outperform pristine CuO in both sensitivity and power efficiency. Enhanced performance is attributed to optimized charge separation and carrier transport at the p-n interfaces. The sensors demonstrate excellent reproducibility and long-term operational stability over two months. These findings position CZO 1D nanostructures as a high- performance platform for next-generation VOC sensing.

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PP-08

Synergistic Simultaneous Degradation of Tetracycline and Methylene Blue via Au and Ag-Decorated ZnO Under Visible Light

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Abstract: Pristine and noble metal-decorated ZnO nanostructures were synthesized via a simple chemical reduction approach using hydrazine hydrate to deposit silver (Ag) and gold (Au) nanoparticles. Comprehensive characterization—including PXRD, FESEM, HRTEM, XPS, FTIR, Raman, BET, and UV-Vis spectroscopy—revealed high-surface-area nanostructures with enhanced optical properties. Photocatalytic evaluation under visible-light irradiation demonstrated that Au- and Ag-decorated ZnO exhibited significantly higher degradation efficiencies compared to bare ZnO. This enhancement is attributed to improved charge-carrier separation and localized surface plasmon resonance (LSPR) effects. Notably, the catalysts displayed excellent reusability over multiple cycles. Most importantly, the as-synthesized nanocomposites showed an outstanding capacity to simultaneously co-degrade two structurally and chemically dissimilar pollutants: methylene blue (MB, a textile dye) and tetracycline (TC, a pharmaceutical antibiotic). At pH 7, Au-ZnO achieved 95% degradation of TC (2×10^{-3} M) and 80% degradation of MB (1.0×10^{-5} M) within 120 min using only 20 mg of catalyst. This study demonstrates the potential of a single photocatalytic platform for the simultaneous removal of diverse organic contaminants, suggesting that noble metal-modified ZnO is a promising multifunctional catalyst for treating complex industrial wastewater.

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PP-09

Effect of Clay-Induced Confinement on morphology and mechanical properties of poly(3-hexylthiophene) P3HT : A Molecular Dynamics Study

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Abstract: Conducting polymers are widely used in flexible and printed electronics with applications such as neuromorphic systems, solar cells, and field effect transistors. The device performance is strongly influenced by the nanoscale morphology and molecular orientation of polymer chains, which is highly sensitive to the surrounding environment. The incorporation of clay nanomaterials can induce local ordering within the polymer matrix by influencing how the polymer backbone and alkyl side chains arrange near the interface.

In the current study, we have used molecular dynamics (MD) simulations to systematically study how varying the polymer-to-clay weight fraction creates a nanoscale confinement which affects the morphology and mechanical properties of the p-type conducting polymer, poly(3-hexylthiophene) (P3HT). We capture the transition of P3HT from bulk- like behavior to behaviour in strongly confined structures formed by clay nanomaterials. The nanoscale confinement regulates polymer packing, backbone orientation, and interfacial interactions. Confinement between the inorganic fillers creates a pronounced chain alignment which shows enhanced lamellar and π–π stacking domains. Further, this confinement induced structural reorganization directly influences the mechanical properties, leading to an increased stiffness in confined P3HT-clay films. Such confinement-induced structural changes directly influence the stacking and orientation of the polymer chains, thereby affecting the potential charge transport pathways within the system. Overall, this study shows the importance of nanoscale confinement as an effective strategy to control morphology and mechanical properties of P3HT films, providing insights for the design of high-performance polymer-based devices.

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PP-10

Enhanced Photoelectrochemical Water-splitting Reaction by Nano-dendritic $BiVO_4$ Photoanode Coupled with Nanoparticles of β-FeOOH

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Abstract: Renewable energy has received much attention recently as energy demands and environmental issues continue to climb. CO_2 from coal, oil, and natural gas causes climate change. Photoelectrochemical (PEC) water splitting constitutes a prospective methodology for utilizing solar energy, facilitating its conversion into storable hydrogen (H_2). H_2 production via PEC water splitting is recognized as a clean, green energy source due to its high calorific value, cleanliness, and renewability. Among various semiconductors used for visible light-induced water oxidation, bismuth vanadate ($BiVO_4$) stands out as one of the most promising candidates due to its suitable band gap of approximately 2.4-2.6 eV and favorable band alignments that enable excellent light absorption. Although it has great potential, the material faces significant challenges due to high recombination rates of photoinduced holes and electrons, as well as sluggish kinetics in the oxygen evolution reaction (OER). Additionally, it is susceptible to photo-corrosion, which hampers its long-term stability, an essential requirement for practical applications. In this work, we have successfully synthesized $BiVO_4$ photoanodes using the electrodeposition technique. We further enhanced their performance by modifying with an iron oxyhydroxide (β-FeOOH) co-catalyst, which is obtained via a pH-controlled dip-coating method. A saturation photocurrent density of 2.73 mA cm^{-2} at +1.4 V versus RHE under AM 1.5 G illumination is observed, which shows a 1.8-fold enhancement over pristine $BiVO_4$.

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PP-11

Rapid On-Site Detection of Hypochlorite: A Novel Phenothiazine-Based Fluorescent Probe for Environmental Water Monitoring and Paper-Based Sensing

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Abstract: Herein, we report the rational design and efficient synthesis of a novel phenothiazine-derived fluorescent probe, 10-ethyl-3-((2-(quinolin-2-yl)hydrazineylidene)methyl)-10H-phenothiazine (**PTZ-QH**), achieved under mild and straightforward reaction conditions. The molecular structure of **PTZ-QH** and its key intermediates was unequivocally established through FT-IR, ^{1}H and ^{13}C NMR spectroscopy, high-resolution mass spectrometry, and single crystal X-ray diffraction techniques. Photophysical investigations revealed that **PTZ-QH**, upon excitation at 386 nm in DMSO: H_2O (9:1, v/v), exhibits a strong emission band centered at 507 nm. The probe responds rapidly, achieving detectable signal changes within 30 s, and exhibits excellent sensitivity with a low detection limit of 16 nM. Stern–Volmer analysis revealed a well-defined linear quenching profile, with a quenching constant (K_{SV}) of 1.09×10^5 M^{-1}, indicating an efficient quenching process. Moreover, **PTZ-QH** maintains stable sensing performance over a physiologically relevant pH range of 5.0–9.0, with negligible interference from competing ions. To gain deeper mechanistic insight, DFT calculations were performed, which substantiated the proposed sensing mechanism and clarified the electronic structural changes responsible for fluorescence quenching upon interaction with ClO^- ions. Importantly, the practical applicability of the probe was validated through the fabrication of cellulose-based test strips, enabling convenient, real-time, and on-site detection of hypochlorite in aqueous samples.

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PP-12

Recent Advances in Supramolecular Sensors for the Selective Detection of Group IIIA Metal Ions with ester linker

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Abstract: Group IIIA metals, including aluminum (Al), gallium (Ga), indium (In), and thallium (Tl), are four key components that have similar electronic properties in the aqueous state. The similar properties of Group IIIA metal ions make it difficult to detect them. Due to their convenience and efficiency, supramolecular optical chemosensors have become popular for the detection of metal ions. Researchers have developed selective probes, highlighting the following four key points related to their functionality: (i) Optical and ratiometric chemosensors for Group IIIA metals, focusing on the selective detection of Group IIIA metal ions (Al^{3+}, Ga^{3+}, In^{3+}, Tl^{3+}, and Tl^{+}), individually and in combinations; (ii) Application including test strips, smartphone-assisted RGB analysis, environmental sample analysis, and bioimaging involving HeLa cells, MCF-7 cell lines, and Zebrafish larvae; (iii) As part of the design process for these probes, Schiff base types of amines are used, as well as hydrazide, carbohydrazide, thiosemicarbazone, Salen, and Salamo types of amines. The review also highlights the challenges associated with the detection of Group IIIA metal ions, with few probes available for detecting Ga^{3+} and Tl^{3+} ions, providing opportunities for researchers to develop new supramolecular sensors in future research.

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PP-13

Hierarchical Nanorods Based on ZnO Core-Nickel Selenide Shell as a Cocatalyst for Enhanced Photoelectrochemical Water Splitting

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Abstract: The photoelectrochemical water splitting (PEC-WS) offers a clean and sustainable route for solar-to-hydrogen energy conversion. Among the metal oxides, Zinc oxide (ZnO) nanorods (NRs) have attracted significant attention as a photoanode due to their high electron mobility, environmental friendliness, cost-effective synthesis, and ease of fabrication. However, the wide bandgap of ZnO (3.2 eV) limits its solar spectrum utilization, and the high recombination rate of photogenerated charge carriers restricts its overall PEC-WS efficiency1. To address these challenges, the ZnO@NiSex core-shell nanorods are developed, where the nickel selenide (NiSex)$_2$ shell acts as an efficient cocatalyst to overcome these limitations. Vertically aligned ZnO NRs were synthesized via a hydrothermal route and subsequently coated with NiSex via the electrodeposition technique. With the help of XRD, FESEM, TEM, and XPS analysis, heterostructure formation is understood and demonstrated, showing the formation of highly crystalline ZnO NRs uniformly coated with a thin layer of NiSex shell. UV-Visible studies reveal enhanced visible light harvesting ability, while PEC studies indicate suppressed charge recombination due to the effective ZnO@NiSex interface. Under AM 1.5G illumination, ZnO@NiSex photoanode exhibits a photocurrent density of 1mA cm^{-2} at 0.6 V vs RHE, nearly five times higher than pristine ZnO NRs. Chronoamperometry ZnO@NiSex under the chopped light displays a rapid and stable photoresponse, and a transient decay time was calculated to be 31 seconds. Photoelectrochemical impedance spectroscopy (PEIS) showed reduced charge carrier lifetimes and interfacial kinetics. Applied bias photo-to-current efficiency (ABPE) improved from 0.18 % (ZnO) to 0.72 % for ZnO@NiSex. The enhanced PEC activity is attributed to the synergistic band alignment and catalytic interface between the ZnO and NiSex, facilitating charge separation and accelerated water oxidation kinetics. This work demonstrates a scalable and cost-effective approach to hybrid photoanode design by integrating nanoscale cocatalyst engineering with semiconductor nanostructure. This offers a promising platform for solar-driven hydrogen generation.

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PP-14

Mn^{2+} doping in In_2S_3 Increases Photoanodic Activity for Photoelectrochemical Water-splitting

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Abstract: The photoelectrochemical (PEC) water-splitting process emerges as a significant pathway for solving global energy demands for hydrogen (H_2) generation.[1-4] Here, a visible light-active semiconductor, indium sulfide (In_2S_3), is explored. The interconnected nanosheets of In_2S_3 can generate a photocurrent density of 3.18 mA/cm^2 at 1.2 V vs. RHE in Na_2SO_4. To improve the PEC activity of In_2S_3, Mn^{2+} is incorporated into In_2S_3 through an in-situ hydrothermal method. Mn-In_2S_3 exhibits a photocurrent density of 4.49 mA/cm^2 at 1.2 V vs. RHE. It demonstrates a separation efficiency of 51.2 %, 1.58 times higher than In_2S_3 (32.4 %) at 1.2 V vs. RHE. Mn-doping facilitates the charge transportation, keeping excitons apart, suppressing their recombination. Mott-Schottky analysis indicates 3.2 times carrier density enhancement in Mn-In_2S_3. For practical applicability, the PEC performance of In_2S_3 and Mn-In_2S_3 is also determined in 3.5 wt% saline water. The Mn-In_2S_3 shows the photocurrent density of 5.23 mA/cm^2 at 1.2 V vs. RHE, ~1.5 fold higher than the bare In_2S_3 (3.40 mA/cm^2). Doping with Mn^{2+} effectively alters the band edge positions of In_2S_3, further supported by ultraviolet photoelectron spectroscopy (UPS) analysis, which indicates upward and downward shifting of the valence and conduction bands, respectively, resulting in narrowing of the band gap.

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PP-15

8-Hydroxyquinoline Azine-based ESIPT and TICT Active Fluorescence Molecular Rotors for Viscosity Detection in Fluid Beverages

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Abstract: Herein, we investigated the synthesis, characterization, and properties of fluorescence probes derived from azine-conjugated derivatives, specifically 2-(((9H-fluoren-9-ylidene)hydrazineylidene)methyl)quinolin-8-ol(FN-HQ) and 2(((diphenylmethylene)hydrazineylidene)methyl)quinolin-8-ol (BP-HQ). These probes were synthesized by reacting 8-hydroxyquinoline aldehyde with benzophenone and fluorenone, along with benzophenone hydrazides. All the intermediate hydrazine and probes were structurally characterized using FTIR, NMR, and HRMS analysis. The study demonstrated visible light absorbance and emission characteristics. The AIE studies show that FN-HQ and BP-HQ are of an ACQ nature in DMSO and water media. The fluorescence studies show a strong linear relationship between the emission intensity and the viscosity of the solvent system for both the probes FN-HQ and BP-HQ, with a viscosity FH coefficient of 1.3487 and 1.068, respectively. Further, DFT-based computational calculations were utilized to optimize ground-state and excited-state geometry, resulting in UV-Vis absorbance spectral characteristics that closely correlated with the observed spectral response. Finally, probes FN-HQ and BP-HQ were demonstrated for real-time fruit juice deuteration process monitoring

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PP-16

Recent Advancement on Fluorescence Polymer Hydrogels For Sustainable Applications

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Abstract: There is a great deal of interest in fluorescent polymer hydrogels (FPHs) for a variety of emerging applications, such as visualized sensing, smart displays, camouflage skins, soft actuators/robots, since they combine the benefits of classic fluorescent polymers and hydrogels. Due to their excellent optical properties, FPHs with good flexibility and biocompatibility have attracted more and more attention. A review of fluorescent gel preparation methods and applications is presented in this article. The preparation methods of self-assembly and polymerization of the fluorescent gel are also discussed. Moreover, examples of supramolecular fluorescent hydrogels and organo-gels are also included to provide a comprehensive overview of the development in the field. It is also discussed what the future holds for FPHs, including challenges and opportunities.

PP-17

Supramolecular Complexation of Customized Tricationic Porphyrins with Sulfobutylether-β-cyclodextrin

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Abstract: Porphyrins are macrocyclic compounds composed of four pyrrole rings, known for their high molar absorption coefficients, strong fluorescence, large Stokes shifts, and excellent thermal stability, making them efficient photosensitizers for photodynamic therapy (PDT).[1] However, aggregation-induced quenching often diminishes their PDT performance. Non-covalent interactions with supramolecular hosts can significantly enhance photodynamic efficiency by modulating their physicochemical and photophysical properties.[2] Previous studies have demonstrated improved photosensitizing behavior upon host–guest complexation.[3] In this work, we investigate the effect of host–guest interactions on the photophysical properties of tricationic porphyrins. Upon host binding, the initially broad fluorescence emission resolves into two distinct bands at 655 and 721 nm, indicating inclusion complex formation. Complexation leads to enhanced fluorescence quantum yield (Φ_f) and singlet oxygen quantum yield (Φ_Δ), along with improved photostability under light irradiation. Time-resolved fluorescence studies further support this interaction. The free form exhibits a bi-exponential decay with an average lifetime of 6.6 ns, which increases to 10 ns upon complexation. Additionally, an increase in rotational correlation time provides further evidence of encapsulation. Collectively, these results confirm successful inclusion, while detailed mechanistic insights and spectral features will be discussed further.

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PP-18

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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PP-19

Precise molecular design of a twisted pyrene-thiophene-based mechanofluorochromic probe with a large Stokes shift, and a feasibility study toward security ink and rewritable paper

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Abstract: Mechanofluorochromic materials change their fluorescence emission in response to an external force applied. This field of materials is gaining attention for its applications in mechanical force sensing, structural health monitoring, and anticounterfeiting.[1] Due to the exciting applications, this field demands new molecular designs and a clear understanding of the relationship between structure and properties. Pyrene is a high electron-rich planar polyatomic system enriched with optical properties. We present a new pyrene-based twisted molecular framework, which exhibits good MFC properties.[2] Pyrene-based twisted donor–acceptor (D–A) dyes (PySS and PySP) have been synthesised and characterised. These molecules exhibit excellent solvatochromic properties, with substantial shifts in emission wavelength (PySS: 147 nm; PySP: 130 nm). The lowest transition state contains a significant contribution from ICT characteristics, as evidenced by spectral analysis and computational calculations. By grinding, PySS and PySP display MFC features with red shifts of 50 nm and 54 nm, respectively. Interestingly, PySS shows a gradual shift from green (510 nm) to orange (578 nm) emission as pressure is increased with a hydraulic press (0 to 12.5 tons). Furthermore, we have explored the mechanism and its applications, including data encryption and decryption and security inks.

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PP-20

EOM-CCSDT some pilot applications

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Abstract: The nitric oxide anion (NO^{-}) represents a prototypical open-shell system with pronounced near-degeneracy and electron correlation effects, making it an ideal candidate for testing advanced electronic structure methods. In this work, we present a pilot study of the energetics and bonding of NO^{-} using the spin-flip (SF) and double electron attachment (DEA) variants of the Equation-of-Motion Coupled-Cluster method including full single, double, and triple excitations (EOM-CCSDT).The EOM-SF-CCSDT method employs a high-spin triplet reference state of the neutral NO system and generates the target low-spin states of NO- through spin-flip excitations (Δ M_s = -1. The inclusion of triple excitations ensures a balanced and highly accurate treatment of both static and dynamic correlation effects. This approach is particularly advantageous for systems with strong diradical character, as it avoids artificial symmetry breaking and provides a physically consistent description of near-degenerate electronic states.In contrast, the EOM-DEA-CCSDT method starts from a well-defined closed-shell reference and accesses the electronic states of NO- via the attachment of two electrons. By explicitly incorporating triple excitations, the DEA framework captures higher-order correlation effects associated with simultaneous two-electron attachment and orbital relaxation. This makes EOM-DEA-CCSDT especially suitable for describing anionic systems with complex electron correlation patterns.We perform a detailed analysis of the relative energetics of low-lying electronic states of NO^{-},comparing the performance of EOM-SF-CCSDT and EOM-DEA-CCSDT methods. The computed excitation energies and state ordering are examined to assess the reliability and consistency of both approaches at the CCSDT level. Particular attention is given to the role of triple excitations in refining energy separations and improving the description of closely spaced states.In addition, we analyze the nature of the wavefunctions in terms of leading amplitudes and dominant configuration contributions. The inclusion of triple excitations is found to play a significant role in capturing subtle correlation effects beyond the doubles level, providing deeper insight into the electronic structure and differences between the SF and DEA formalisms.To further understand the bonding characteristics, we investigate the frontier molecular orbitals and their occupation patterns. The interplay between the Π and Π* orbitals governs the bonding nature and stability of NO^{-}. Changes in electron density upon electron attachment are analyzed to elucidate bond order variations and spin density localization. The use of EOM-CCSDT methods leads to a more refined and accurate description of these features.Overall, this study demonstrates that EOM-SF-CCSDT and EOM-DEA-CCSDT provide complementary and reliable descriptions of the electronic structure, energetics, and bonding in NO-. These pilot applications highlight the importance of higher-order correlation effects and establish a foundation for applying these methods to more complex open-shell and anionic systems.

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PP-21

Structural and Dynamical Properties of Water in NaCl Electrolytes Confined between Graphene Surfaces

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Abstract: Understanding the behavior of water and electrolyte solutions under nanoscale confinement has become increasingly important in fields such as nanofluidics, desalination, and energy storage, where interfacial effects dominate fluid transport. A detailed understanding of the structural and dynamical behavior of confined water and electrolyte solutions is essential for the design and optimization of graphene-based membranes and nanochannel systems.

To gain deeper insights, equilibrium and non-equilibrium molecular dynamic simulations are performed on pure water confined between parallel graphene sheets,[1] and an aqueous NaCl electrolyte solution under identical confinement conditions. These simulation techniques provide a robust framework for examining microscopic structural arrangements and transport properties under both equilibrium and externally driven conditions. The structural characteristics of the confined systems were analyzed using radial distribution functions (RDFs) and compared with bulk water systems.[2] The results indicate that nanoscale confinement significantly alters the local structure of water molecules near graphene interfaces. In particular, the presence of Na^+ and Cl^- ions leads to a noticeable reduction in the peak intensity of the water–water RDF, reflecting disruption of the hydrogen-bond network and a decrease in structural ordering. Compared to pure water under identical confinement, the electrolyte system exhibits a more disordered molecular arrangement due to ion–water interactions. The dynamical properties were further examined through the mean-squared displacement (MSD). The MSD analysis shows that the electrolyte system exhibits reduced molecular mobility relative to pure confined water, primarily due to the combined effects of spatial restriction and ionic interactions. Additional structural insights were obtained from the static structure factor, which complements RDF analysis by probing ordering in reciprocal space. The results reveal that the incorporation of ions modifies both intermediate- and long-range correlations among water molecules. Variations in peak positions and intensities highlight significant changes in spatial organization arising from the interplay between confinement and ionic effects.

Overall, the combined analysis of RDF, MSD, and static structure factor provides a comprehensive understanding of the interplay between nanoscale confinement and ionic effects in governing the structural and dynamical behavior of aqueous electrolyte systems near graphene surfaces.

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PP-22

α-MnO$_2$ nanorods for light-driven device applications

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Abstract: α-MnO$_2$ nanorods were synthesized via a one-pot hydrothermal method and confirmed to be phase-pure with mixed Mn^{3+}/Mn^{4+} states through XRD, XPS, FESEM, FTIR, UV–Vis, and UPS analyses. An in-plane ITO/α-MnO$_2$ photodetector was fabricated to evaluate its optoelectronic performance. The device exhibits a strong and stable photoresponse under visible illumination. Under 532 nm excitation, a 34% enhancement in photocurrent is observed, driven by efficient charge-carrier separation facilitated by favourable band alignment and defect-mediated transport. At room temperature, the photodetector delivers a responsivity of 8.66 mA W^{-1} and an EQE of 2.018%, with reproducible response and recovery times of 76.5 s and 77.5 s, respectively. Remarkably, temperature-activated transport leads to a responsivity of 240.29 mA W^{-1} and an increased EQE of 56.2% at 160 °C, with a substantially reduced response time of ∼12 s. This enhancement highlights the pivotal roles of defect-state modulation and mobility improvement in governing the photoactivity of α-MnO$_2$. Overall, α-MnO$_2$ nanorods emerge as a robust, low-cost platform for high-temperature photodetection, illustrating how defect chemistry and temperature-activated transport can be engineered to achieve high-performance optoelectronic behaviour. This work provides a compelling pathway toward next-generation MnO$_2$-based photodetectors and energy-harvesting technologies.

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PP-23

Expeditious Route to Azepino-Fused Porphyrins with Superior Photosensitizing Efficiency.

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Abstract: π-extension of porphyrinoids and other aromatic molecules *via* intramolecular C-N coupling has been of keen interest to many researchers as the C-N bond fusion forces the porphyrin core and the aryl substituents to be co-planar, which promotes enhanced electronic communication between both fragments.[1] These π-extended molecules demonstrate changes in their optical as well as electronic properties. previous literatures demonstrated the use of metal oxidants [2] and the rhodium-catalyzed [3] annulation reactions and hypervalent iodine promoted intramolecular oxidative cyclization.[4] Based on the previous reports we developed a facile and rapid protocol to access azepino-fused porphyrins via iodine (III)-mediated oxidative intramolecular cyclization of β-imidazole or benzimidazole substituted porphyrins. the reaction involve the benign hypervalent iodine reagent offering a mild, scalable and sustainable route towards the formation of intramolecular C-N bonds.The synthesized compounds were found to show red shifted intense Soret bands centered between 440-460 nm and two weak bands ranging from 570 to 720 nm (Q-bands). Among the synthesized compounds, the free-base imidazoazepino-fused porphyrin was found to be an efficient $^1O_2$ producer with a higher singlet oxygen quantum yield ($\Phi_\Delta \sim 0.78$ in DMF) as compared to H_2TPP ($\Phi_\Delta = 0.64$ in DMF). It was observed that the protonated form of imidazoazepino-fused free base porphyrin exhibits a significant red shift of ~24 nm in Soret and ~150 nm in Q-Bands with a pK_a value of ~3.58, demonstrating that imidazole fusion enhances the basicity of the porphyrin system. This tunable optical behaviour highlights its potential in pH responsive photonics and PDT (Photodynamic Therapy.

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PP-24

ZnO/MoSx Heterostructure as a Noble Metal Free SERS Substrate for the Detection of MB in Lower Concentration Level

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Abstract: Surface-enhanced Raman scattering (SERS) is a sensitive spectroscopic technique that amplifies Raman signals of molecules adsorbed on rough metal surfaces or nanostructures. In order to choose a promising SERS substrate material, transition metal chalcogenide-based semiconductors have been proved as efficient materials due to their thermal stability, biocompatibility along with tunable optical and electronic properties. However, the enhancement factor (EF) obtained from semiconductor SERS substrate are quite low in compare with metal nanoparticle. To deal with that, formation of heterostructure of semiconductors has been proved as potential substrate for SERS due to high interlayer interaction, efficient photo induced charge transfer (PICT) transition, and large-scale electron-hole pair separation. In this context, we synthesized ZnO/MoS_x heterostructure and used it as a SERS substrate for sensing of methylene blue. To synthesize ZnO/MoS_x, first ZnO was synthesized using seed mediated electrodeposition followed by calcination and then MoS_x was fabricated on ZnO via electrodeposition. The as-prepared ZnO/MoS_x was characterized using XRD, XPS, Raman etc. to confirm the formation. ZnO/MoS_x was used as SERS substrate to detect MB with an ultralow concentration of 10^{-10} M with an enhancement factor of 10^6. The substrate is also very stable even up to 4 months and very robust in nature. The peak intensity at photoluminescence (PL) spectra of ZnO was decreased when MoS_x was fabricated on it indicating less electron-hole pair recombination in ZnO/MoS_x heterostructure. Thus, the improved SERS performance of the ZnO/MoS_x substrate is attributed to the efficient electron-hole pair separation at the heterostructure interface resulting facile PICT between the substrate and the analyte.

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PP-25

Pt single atoms anchored on CoOOH enable efficient bifunctional electrocatalysis for overall water-splitting reaction

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Abstract: Transition metal oxyhydroxides have emerged as promising electrocatalyst platforms for sustainable water splitting owing to their earth abundance, rich redox chemistry, and structural adaptability under alkaline electrochemical conditions. Cobalt oxyhydroxide (CoOOH) has attracted significant attention because of its layered architecture, high density of redox-active cobalt centres, excellent wettability, and favourable charge-transport characteristics. These intrinsic features make CoOOH particularly attractive for oxygen evolution reaction (OER) catalysis, where the Co^{+2}/Co^{+3} redox transitions facilitate efficient adsorption and transformation of oxygen-containing intermediates.[1] However, despite its promising catalytic attributes, pristine CoOOH suffers from sluggish reaction kinetics and limited intrinsic activity, particularly toward the hydrogen evolution reaction (HER), due to non-optimal hydrogen adsorption energetics and insufficient active site conductivity. These limitations restrict its applicability as a bifunctional electrocatalyst for overall water splitting. To address these challenges, atomically dispersed platinum sites have been anchored onto the CoOOH surface to develop a highly efficient bifunctional catalytic interface.[2-3] The incorporation of Pt single atoms maximizes noble metal utilization efficiency and also induces substantial electronic structure modulation of the CoOOH support through strong metal-support interaction. The optimized Pt/CoOOH single-atom heterostructure exhibits significantly enhanced electrocatalytic activity toward both hydrogen and oxygen evolution compared to pristine CoOOH. The improved bifunctional performance is evidenced by reduced overpotentials and accelerated reaction kinetics for both HER and OER, enabling efficient overall water splitting at low potential. The superior catalytic behaviour is attributed to the synergistic interaction between isolated Pt atoms and adjacent cobalt-oxygen coordination environments, which promotes charge redistribution, facilitates rapid electron transfer, and generates highly active dual-function catalytic sites. Furthermore, the strong anchoring of Pt single atoms on the CoOOH surface effectively suppresses noble metal agglomeration, leading to excellent structural stability during prolonged electrolysis. This work demonstrates an effective atomic-scale strategy for designing low-platinum bifunctional electrocatalysts and provides valuable insights into the development of high-performance materials for overall alkaline water splitting and sustainable hydrogen production.

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PP-26

Self-assembly of Polymer-Grafted Nanocubes

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Abstract: Understanding Polymer-grafted nanoparticles are widely employed as building blocks to produce complex materials with controlled structure and characteristics. The way anisotropic particles self assemble is greatly influenced by their shape, surface characteristics, and interactions between grafted polymer chains. This work uses molecular dynamics simulations to understand how polymer chains attached to particle surfaces affect structural organization and ordering in the system[1]. Changing the grafting density controls how closely nanoparticles interact, which affects how they arrange into ordered structures. We used the radial distribution function (RDF) to study the spacing between particles. By comparing the RDF peaks with known crystal structures, we observed that for different system sizes the arrangement shows BCC-like features, mixed structures, and in some cases FCC-like ordering to some extent. This indicates that the packing behavior depends on grafting density and system size, leading to variation in the degree of structural order. Gauss map representation is used to understand how neighboring particles are oriented with respect to each other. The Gauss map shows how local structural environments are distributed in different directions and helps identify symmetry in the system. When particles are oriented face-to-face, the Gauss map shows a symmetric pattern, whereas for other orientations the distribution appears more isotropic. We have also performed metadynamics simulations to understand which regions of the configurational space are explored by the system during molecular dynamics simulations. For this purpose, the PLUMED[2] software is used to construct free energy surface (FES) maps, which provide insight into the stability of different structural states and the extent of sampling across relevant collective variables. From the FES maps, we observe distinct minima corresponding to stable structural arrangements, while shallow regions indicate possible transitions between different configurations, showing that the system explores multiple structural states during the simulation. The findings demonstrate that polymer grafting is crucial for regulating structural organization and interparticle interactions. The system exhibits fluctuation in packing and degree of order as grafting density varies. Polymer-grafted nanocube systems' positional and orientational ordering can be fully understood by combining RDF and Gauss map analysis. Overall, this study helps explain how surface-grafted polymers influence nanoparticle self assembly and provides useful guidance for designing materials with desired structural properties. Such systems have potential applications in nanocomposites, coatings, and functional soft materials.

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PP-27

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 suitable for environmental and analytical applications.[2]

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PP-28

Engineering Reliable Resistive Switching in hBN-TiO_2 Heterostructures via Controlled Silver Filament Dynamics

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Abstract: Memristors have attracted significant attention for memory and neuromorphic computing, but a persistent problem holds them back; they're unreliable. In silver electrode-based devices, the filaments that carry current form randomly each cycle, leading to unpredictable switching voltages and poor endurance. No two cycles look quite the same, and that inconsistency is a serious obstacle for real applications. The root cause is simple; silver ions migrating through TiO_2 have no guidance. They spread laterally, nucleate wherever conditions happen to favour it, and sometimes grow so aggressively that the filament can't be cleanly dissolved on reset. Over time, the device degrades. We approached this problem by asking whether the right interface could discipline that ion migration. Our device is built on a Ti/Au/TiO_2/hBN/Ti/Ag stack, where an atomically thin hexagonal boron nitride layer sits between TiO_2 and the Ag top electrode. Hexagonal Boron Nitride(hBN) is chemically stable, mechanically robust, and crucially it forces ions to travel through defect-governed pathways rather than freely through the oxide. This transforms filament formation from a random event into a spatially confined, repeatable process. The results reflect this directly. Devices show tighter set and reset voltage distributions, more consistent resistance states cycle to cycle, and better endurance compared to TiO_2-only devices. The hBN layer prevents filaments from overgrowing and getting irreversibly stuck, which is the primary failure mode in conventional oxide memristors. Retention also improves, with resistance states remaining stable over time with minimal drift. This work shows that inserting a 2D material layer at the right interface can meaningfully fix one of the oldest problems in memristor research. The TiO_2/hBN heterostructure is a practical, scalable platform for building Ag-based memristors reliable enough for both memory and neuromorphic applications.

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PP- 29

Tuning Co (II)-MOF Catalysts with Nitrogen Ligands for Effective CO_2 Transformation to Cyclic Carbonates

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Abstract: The mixed linker strategy incorporating nitrogen-containing ligands was used to synthesize CoMOFs. Imine based ((1E,1’E)N,N’-(1,4-phenylene)bis(1-(pyridine-4-yl)methanamide) (L1) in conjunction with carboxylate- based linkers, such as 4,4’-dicarboxylic acid (H_2L3) resulted in a three dimensional pin-wheel metal-organic framework CoMOF-1 ([$Co_3(L1)(L3)_3$.2DMF]) while an amide based N,N’-bis(pyridine-4-yl)pyridine-2,6-dicarboxamide (L2) and 2,6 naphthalenedicarboxylic acid (H_2L4), resulted in a staircase threefold interpenetrated two-dimensional network CoMOF-2 ([$Co_2(L2)_2(L4)_2$].2DMSO.DMF). The three-dimensional framework in CoMOF-1 has microporous channels which showed enhanced capability for CO_2 adsorption, quantified as 41.14 cm3/g at 273 K, whereas 2D interpenetrated network of CoMOF-2 showed lower porosity thus resulted in reduction of CO_2 adsorption. CoMOF-1 is subsequently employed as a catalyst in the conversion of CO_2 to cyclic carbonates at mild reaction conditions (0.34 mol% catalyst and 0.34 mol% co- catalyst at 24 h, 80 °C, and 1 atm CO_2). Despite the reduced CO_2 uptake by CoMOF-2, it is utilized as a catalyst for the chemical fixation of CO_2 via cycloaddition, resulting in the effective conversion of CO_2 under mild conditions (0.5 mol% catalyst and 0.5 mol% co-catalyst at 24h, 80°C and 1 atm CO_2). Through thermal programmed desorption (TPD) and Brunauer-Emmett-Teller (BET) analyses pertaining to NH_3 and CO_2 gases, the role of basic sites was elucidated for both CoMOF-1 and CoMOF-2. The chemical stability and recyclability of CoMOF-1 and CoMOF-2 were demonstrated over a series of four cycles.

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PP-30

Trace-Level Dopamine Detection Using Phosphorous Doped C_3N_4 via Photocurrent Suppression Mechanism

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Abstract: Dopamine (DA) is a key neurotransmitter involved in regulating mood, cognition, and motor functions, and its abnormal levels are associated with several neurological disorders such as Parkinson's disease, depression, and schizophrenia. Therefore, the development of sensitive and reliable methods for dopamine detection important. In this work, a photoelectrochemical (PEC) sensing platform based on phosphorus-doped carbon nitride (P-C_3N_4) is developed for the detection of dopamine.

The P-C_3N_4 thin film was synthesized via thermal polymerization and employed as a visible light active photoelectrode. Phosphorus doping plays a crucial role in modulating the electronic structure of P-C_3N_4, leading to enhanced light absorption and improved separation of photogenerated charge carriers. As a result, the modified electrode exhibits a stable and enhanced photocurrent response under illumination. Upon the introduction of dopamine, a systematic decrease in photocurrent is observed. This behaviour is attributed to the oxidation of dopamine to polydopamine (PDA), which acts as an electron scavenger and forms a surface layer that hinders the transfer of photogenerated electrons to the electrode. This photocurrent suppression mechanism enables sensitive detection of dopamine. The sensor demonstrates a wide detection range from 0.01 nM to 100 nM. A pronounced response is observed in the low concentration region (0.01-5 nM), indicating high sensitivity, while a quasi-linear response is obtained in the higher concentration range (5-100 nM), allowing reliable quantitative analysis. This behaviour reflects the transition from abundant active sites at low concentrations to partial surface saturation at higher concentrations.

Overall, this study highlights phosphorus-doped P-C_3N_4 as a simple, cost-effective, and metal-free photoactive material for PEC dopamine sensing. The developed platform combines high sensitivity at trace levels with a practical working range, demonstrating its potential for applications in biochemical sensing and early disease diagnostics.

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PP-31

Development of a Photocathode for Efficient PEC Water Splitting and CO_2 Reduction: Nanoparticles of $CuBi_2O_4$

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Abstarct: Among narrow-bandgap p-type semiconductors, $CuBi_2O_4$ (CBO) has received potential interest as a photocathode for photoelectrochemical (PEC) water-splitting due to its acceptable band gap of ~1.8 eV, positive onset potential, and reasonable stability in aqueous media.[1-2] Here, a novel, solution-based two-step method is developed for the synthesis of CBO with different nanoparticle (NP) sizes. An electrodeposition process, followed by calcination, is explored for the synthesis of CBO NPs.[3] To synthesise CBO NPs of various sizes (~215 nm to 120 nm), different Cu(II) precursors are explored. Further, the as-synthesized CBOs are characterized by X-ray diffraction (XRD) and Raman Spectroscopy, and their PEC performance is evaluated as cathodes in the water-splitting reaction. From the PEC performance, it is clear that CBO of the smallest particle size can generate the highest photocurrent density, -1.27 mA/cm^2 under an applied potential of 0.2 V vs. RHE, which is nearly three times higher compared to the CBO having a NP size of ~215 nm. The enhanced PEC activity is mainly attributed to the increase in the surface-to-volume ratio of CBO. It is observed that with decreasing nanoparticle size, the carrier density increases. There is observable variation in charge transportation with NP size; as a result, charge-transfer efficiency also varies. Finally, the optimized photocathode shows considerable stability in Na_2SO_4 medium, generating unaltered photocurrent density over 1-hour study. In addition to water-splitting, CBOs also exhibit efficient activity towards CO_2 photoreduction.

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PP-32

Co(II)-Exchanged X and Y Faujasite Zeolites for CO_2 Utilisation: A Comparative Study for Oxidative Carboxylation of Alkene to Cyclic Carbonate

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Abstract: Carbon capture and utilisation (CCU) processes offer a greener alternative for synthesising a wide range of products that are traditionally produced using hazardous reagents and generate toxic waste. CO_2 can act as a C1 source and is a desirable building block for larger molecules. The cycloaddition reaction between CO_2 and epoxides yields cyclic carbonates, which have a wide range of applications. Olefins provide an alternative starting point for their synthesis. The process involves initial oxidation of alkenes, followed by in situ cycloaddition of CO_2 in a one-pot system without isolating the intermediate epoxide. Cobalt(II)-exchanged X and Y zeolites with varying metal loadings were employed to convert CO_2 to cyclic carbonates starting from alkenes. The transformation was carried out using O_2 as an oxidant in a mixture of O_2 and CO_2 under atmospheric pressure, without any radical initiator or sacrificial co-reductant. The reaction was performed following the orthogonal strategy, in which all reagents were added at the beginning, and the reaction proceeded without any intervention or change in conditions thereafter. A maximum of 35.7% yield of the cyclic carbonate was achieved. Studies revealed a stark difference among both the zeolites, primarily arising from a difference in their ion exchange behaviours. The Co^{2+} in zeolite X exists as a tetrahedral moiety whereas in zeolite Y it gets converted to oxide under reaction conditions. This was noted from various characterization techniques including UV-Vis DRS, XPS, and Raman Spectroscopy. Their catalytic and recyclability properties differed as a result of this variation.

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PP-33

A water-soluble tricationic pyrazinium-based fluorescent chemosensor for turn-off detection of TNP: Integration of photophysical performance with practical usability

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Abstract: A water-soluble tricationic pyrazinium-based fluorescent chemosensor, 1,1',1" -(benzene-1,3,5-triyltris(methylene))tris(3,5-diphenylpyrazin-1-ium)bromide (BTPPyz) exhibited aggregation-caused quenching (ACQ) behavior, confirmed by solvent-dependent fluorescence and dynamic light scattering (DLS) studies. BTPPyz was subsequently applied for the selective and sensitive detection of 2,4,6-trinitrophenol (TNP) at low concentrations. BTPPyz showed significant fluorescence quenching with a Stern–Volmer constant of 1.15×10^5 $M^{-1}$and a detection limit of 14.14 nM. Job's plot, HRMS, and ^1H NMR confirmed binding stoichiometry. The quenching behavior was attributed to a synergistic effect of ground-state charge-transfer (GSC) formation and Förster resonance energy transfer (FRET), supported by UV–vis and fluorescence spectroscopy, time-correlated single-photon counting (TCSPC), scanning electron microscopy (SEM), and DFT calculations. The spectrofluorimetric determination of TNP in environmental water was performed under optimized conditions, and the accuracy was evaluated with HPLC and spike/recovery test. BTPPyz performed efficiently in water and soil samples spiked with TNP, achieving a great recovery rate. Furthermore, BTPPyz was successfully integrated into paper strips and polymeric films, facilitating swift, visual, and on-site detection of TNP.

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PP-34

Sensitive and Selective Fluorescent Detection of Antibiotics and Picric Acid via a Polyimide-Based Covalent Organic Polymer

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Abstract: A simple and highly sensitive method for detecting picric acid and antibiotics is crucial for monitoring environmental and food safety, as well as clinical diagnostics. A synthesized covalent organic polymer (COP) with π-π conjugated frameworks shows strong fluorescence originating from the $n-\pi^*$ transition. The COP shows excellent sensing performance for picric acid and tetracycline hydrochloride in aqueous media. The polyimide-based COP is insoluble in all organic solvents and exhibits strong emission in acetonitrile (ACN) suspension. Among them, the detection limits of COP are determined to be 0.14 nm for tetracycline hydrochloride (TCH) and 0.062 nm for picric acid (PA). Most importantly, it demonstrated very good selectivity, with no response to other typical antibiotics and nitroaromatic compounds. Mechanistic investigations by combining fluorescence spectroscopy and density functional theory (DFT) calculations revealed that fluorescence quenching occurs through energy transfer (FRET) for tetracycline hydrochloride antibiotic and a combination of FRET and PET for picric acid detection. In brief, this work offers insights into the synthesis and application of fluorescent sensors based on COPs for the detection of multiple pollutants.

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PP-35

Optimization of the Synthesis of Ship-in-a-Bottle Zn(II)Salmphen Complex within Zeolite-Y via Photophysical Studies

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Abstract: A fluorescent Zn(II)Salmphen complex, encapsulated within zeolite-Y supercages, has been reported as a targeted antitumor drug and retains its fluorescence behaviour even after encapsulation[1]. The biocompatibility and tumour-targeting capabilities of host zeolite-Y make the encapsulated system beneficial for intracellular imaging[2]. To study the drug's mechanism of action and explore its intracellular imaging capabilities, the investigation of the photophysical properties of the zeolite-Y-encapsulated Zn(II)Salmphen complex appears to be indispensable. In this work, we describe the encapsulation of Salmphen ligand within Na-zeolite-Y, resulting in Na-Salmphen-Y, and within Zn-zeolite-Y, resulting in Zn(II)Salmphen-Y, using the flexible ligand method, and their photophysical properties, comprising absorption and emission measurements. Salmphen is a flexible Schiff base with ESIPT-coupled AIE properties; complexation with zinc metal results in chelation-enhanced fluorescence (CHEF). However, Salmphen confined within Na-zeolite-Y shows no significant emission, despite attaining rigidity within the zeolite nanopores. Encapsulation of the Salmphen ligand within the supercages of Zn-zeolite-Y results in considerable emission at 517 nm, red-shifted relative to that of the neat Zn(II)Salmphen complex appearing at 493 nm. The topology of the zeolite framework enforces the Zn(II)Salmphen complex to adopt nearly a planar structure, which otherwise would be a dimer with a tetrahedral arrangement around the zinc metal in its neat form. The emission intensity increases with increasing zinc content in the host Zn-zeolite-Y. However, increasing the amount of Salmphen ligand taken beyond a certain amount quenches the fluorescence. It is worth noting that the free Zn(II)Salmphen complex adsorbed on the surface of Na-Salmphen-Y exhibits photophysical behaviour quite similar to that of neat Zn(II)Salmphen. Thus, by optimizing the zinc metal content in host Zn-zeolite-Y or the amount of Salmphen ligand relative to host Zn-zeolite-Y, maximum encapsulation of the Zn(II)Salmphen complex can be achieved, as indicated by PXRD and electronic spectroscopic studies.

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PP-36

Electronic Substitution Effect on ESIPT-Driven pH and Amine Sensing: Exploring Mechanism

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Abstract: A more direct and easier method to evaluate food quality is essential to protect public health. The meat protein decomposes to ammonia and biogenic amines (BAs), so their overall quality and safety require sensitive detection. Here we have synthesized three luminophore probe molecules, derived from 2-(2-hydroxyphenyl) benzothiazole derivatives, it shows excited state-induced proton transfer (ESIPT) mechanism. As proton transfer rate can be controlled, it led towards pH and amine sensing, with limit of detection at 28.6 μM for ammonia and 61.34 nM for hydrazine, respectively. Also, both contact and contact modes were used for real life application for spoilage detection in chicken meat.

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PP-37

Solar-Light-Driven Photocatalytic Degradation of Crystal Violet Dye using S-C_3N_4/In_2O_3 Heterojunction

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Abstract: In this study, a high-efficiency S-C_3N_4/In_2O_3 heterojunction was engineered via a facile two-step hydrothermal strategy for the rapid remediation of organic dye pollutants. The structural, chemical, and morphological features of the as-prepared heterostructure were rigorously analyzed using PXRD, UV-Vis DRS, XPS, FE-SEM, and HR-TEM, which confirmed the successful anchoring of In_2O_3 nanoparticles onto the sulfur-doped carbon nitride nanosheets. The photocatalytic performance of the S-C_3N_4/In_2O_3 system was evaluated through the degradation of Crystal Violet (CV) dye under natural solar irradiation. The composite exhibited remarkable photocatalytic activity, achieving 99.18% degradation of the dye within a rapid 15-minute interval using a minimal catalyst loading of 20 mg. Optimization studies demonstrated that the degradation efficiency is highly pH-dependent, reaching a maximum in alkaline media (pH 9). This superior performance is attributed to the synergistic integration of the two components, which facilitates efficient charge-carrier separation at the heterojunction interface and effectively inhibits electron-hole recombination. Furthermore, the alkaline environment promotes strong electrostatic interactions between the deprotonated, negatively charged catalyst surface and the cationic CV molecules, significantly accelerating the adsorption-to-degradation kinetics. These findings underscore the potential of the S-C_3N_4/In_2O_3 heterojunction as a robust and sustainable photocatalyst for the solar-driven treatment of industrial textile effluents.

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PP-38

Zeolite Encapsulated Ni-Salmphen Complex: A Host-Guest Chemistry & Preliminary Study on Breast Cancer Cells

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Abstract: Cancer, being the second leading cause of death worldwide, is a major health challenge. Metal complexes are the dominant associates in the pool of chemotherapeutic agents and an appropriate drug delivery system can effectively enhance the efficacy of therapeutic agents. Zeolites are biocompatible drug delivery agents, and due to their porous framework, they have ability to 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-X and zeolite-Y, differentiated on the basis of their Si/Al ratio. Ni(II)-Salmphen-encapsulated zeolite material has been thoroughly characterized by FT-IR, UV-Vis, PXRD, and FESEM techniques. Both the encapsulated complexes exhibit the IC_{50} values within the range of 5-10 μg/mL against MCF-7 breast cancer cells. Moreover, they appear non-toxic towards non-cancer cells, showcasing high selectivity for 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 leaching of the encapsulated compounds has been analyzed using UV-Vis spectroscopy, HRMS, and nitrogen physisorption techniques. The pH studies and preliminary MTT assay results indicate promising stability & good cytotoxicity of Ni(II)-Salmphen entrapped in both the zeolites.

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PP-39

Quasi-Physical Growth and Characterization of Cobalt Oxide Nanowalls: Impact of Wet Oxidation and Thermal Treatment

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Abstract: Two-dimensional cobalt oxide (CoO_x) nanowalls were grown using a quasi-physical growth approach employing hot-water treatment (HWT) induced wet oxidation of vacuum-deposited cobalt thin films. The oxidation temperature and duration were systematically optimized to achieve uniformly distributed, vertically aligned nanowall architectures. Comprehensive structural, morphological, and compositional characterizations XRD, FESEM, XPS, Raman spectroscopy, and TEM confirm the formation of vertically oriented mixed-phase cobalt oxide nanowalls. FESEM analysis indicates that well-defined nanowall structures are optimally developed at an HWT temperature of 75°C. These as- grown nanowalls consist of mixed cobalt oxide and hydroxide phases along with a residual metallic cobalt layer. Subsequent thermal annealing promotes the conversion of Co and $Co(OH)_2$ into crystalline cobalt oxide, accompanied by partial degradation of vertical alignment. The proposed hot-water-based wet oxidation process offers a simple, low-temperature, cost-effective, and environmentally friendly route for directly growing well-adhered cobalt oxide nanowalls without the need for high-pressure systems or complex chemical precursors. Owing to their high surface area and porous morphology, these CoO_x nanowalls demonstrate strong potential for chemiresistive gas sensing applications and hold significant promise for advanced energy-related applications, including battery electrodes, electrocatalysis, and supercapacitors.

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PP-40

Intrinsic proton relay in poly-phosphamides to bolster proton exchange membrane fabrication and electrocatalytic proton reduction

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Abstract: Complex synthetic routes and over-swelling of the perfluoro/sulfonated Nafion-based proton-exchange membrane (PEM) materials at high temperatures and strong acidic pH lead to a continuous quest for stable non-fluoro organic polymers with high proton conductivity.[1] Herein, porous organic polymers containing tripodal polyamine (PPA-1a) and/or ethylenediamine (PPA-2) as the linker and possessing a phosphamide {P(O)-NH} moiety in the repeating unit, as confirmed by the ^{31}P and ^{13}C (CPMAS) NMR and other spectroscopic characterizations, are synthesized alongside a non-phosphamide polyamine (PPA-1b).[2] PPA-2 with SA_{BET} of ~11 $m^2\ g^{-1}$ leads to proton conductivity (σ) of 4.7×10^{-2} S cm^{-1} in aqueous pH 4.5 at 358 K, superior to some commercial Nafions. The low activation barrier (E_a) of 0.12 eV indicates facile proton-hopping within the PPA-2 frame following a Grotthuss pathway. The density functional theory (DFT) study predicts that protonation at both "-P=O" and "–NH" sites of the phosphamide is energetically favorable to facilitate the proton-relay within the polymeric frame of PPA-2. The fabrication of PEMs using only 1 wt% PPA-2 with the poly(methyl methacrylate) (PMMA) and poly(vinyl alcohol) (PVA), and the optically transparent membranes show structural stability after a successful proton-exchange study. The presence of redox-active P^V center in the $P^{V/IV}$ redox-couple indicates a proton-coupled-electron-transfer (PCET) process, and the proton adsorption on the {P(O)-NH} sites facilitates the Volmer step of the HER with a low overpotential of 311 mV at 10 mA cm^{-2}. In this study, phosphamide-based materials are exemplified as Nafion's alternative for PEM design and metal-free energy material for HER.[3]

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PP-41

Microenvironment-Regulated Ultraslow Microstructural Dynamics of Phenoxazine Dyes

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Abstract: Phenoxazine class of dyes, including nile red, cresyl violet, and nile blue, have been extensively used in chemical and biological studies, particularly for probing lipid membranes.[1–3] In this presentation, we will share our recent findings on a general phenomenon of hours-long spectral dynamics in the phenoxazine dyes, evidenced by systematic changes in their electronic spectra over an hour. Detailed mechanistic investigations reveal that such spectral dynamics of the dyes can be reduced by tuning microenvironments, where microsolvation (interactions of the dyes with their immediate solvent microenvironment) plays a key underlying role. These microsolvation-induced microstructural changes in a single dye species tend to follow zeroth-order kinetics. The half-life values of such processes systematically vary with solvent hydrogen bonding strength and ionic radius of the dyes' counter anions. Using lipid membrane model systems, this work showcases the importance of longer dye incubation time inside the bilayers for studying membrane properties. We believe that the observed phenomenon holds significance for the practical use of phenoxazine dyes in understanding chemical and biological systems. This work also advances the fundamental understanding of dye-solvent interactions and provides key guidelines for the optimized use of phenoxazine-based fluorescent probes in biophysical and analytical studies.[4]

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PP-42

Eco-Friendly Super-Hydrophobic ZnO Nanorod–Polymer Hybrid Thin Films for Sustainable Self-Cleaning Applications

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Abstract: Hydrophobic and superhydrophobic surfaces have attracted significant attention due to their potential for sustainable, low-maintenance technologies. In this work, asymmetric highly dense ZnO nanorods were fabricated on glass substrates using a simple, scalable two-step process: vacuum-evaporated Zn thin films followed by controlled thermal oxidation. The ZnO nanorods obtained at an oxidation temperature of 700 °C exhibited enhanced surface roughness, resulting in a water contact angle of 130°, indicating strong hydrophobic behaviour. To further reduce the surface free energy, a thin layer of 1 wt% polystyrene was deposited by spin coating, resulting in a transition toward Superhydrophobicity.

The resulting fluorine-free ZnO–polystyrene hybrid surface combines nanoscale surface texturing with eco-friendly surface modification, providing a practical approach for water-repellent, self-cleaning coatings. Such surfaces can significantly reduce water consumption, chemical usage, and maintenance requirements, making them attractive for sustainable applications. Potential applications include self-cleaning architectural surfaces, corrosion-resistant coatings, and biomedical interfaces. This study demonstrates a multidisciplinary approach integrating materials science, surface engineering, and sustainability-oriented design for future functional coatings.

PP-43

Isomeric Effects and Electronic Tunability in Conducting Polymers: A Computational Perspective

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Abstract: Conducting polymers are a unique class of organic materials that combine the electrical properties of metals or semiconductors with the mechanical flexibility and processability of polymers. Their conductivity arises from conjugated π-electron systems along the polymer backbone, which can be further enhanced through doping processes. *poly(benzimidazobenzophenanthroline)* (BBL) is one such n-type polymer, characterized by a planar structure and a naphthalene-based backbone. Although two isomeric forms of its monomer exist [1] , the highly symmetric backbone makes the identification and separation of *cis–trans* conformers nearly impossible. While this limitation may not significantly affect purely n-type organic transistors, it becomes critically important in ambipolar blends [2], where charge transport characteristics are highly sensitive to molecular structure. In this context, although experimental investigation of such systems is challenging, computational approaches offer a viable alternative by enabling precise control and localization of specific isomeric configurations. Density functional theory (DFT) has been employed to evaluate key electronic properties, including band gap, charge distribution, and absorption spectra. Additionally, morphological behavior can be studied using molecular dynamics (MD) simulations. A comprehensive computational analysis of isomeric effects can thus provide deeper insights into polymer blends and their bulk heterojunctions, as well as into chemical and electrochemical doping mechanisms, ultimately enabling the controlled fabrication of materials with tunable electronic properties.

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PP-44

VOC adsorption using NDI-based Covalent Organic Framework – A computational study

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Abstract: Covalent organic frameworks (COFs) have emerged as promising materials for adsorption studies due to its tunable porosity and chemical functionality. In this study, density functional theory (DFT) calculations were employed to evaluate the binding interactions between selected VOC (Volatile Organic compounds) molecules and the COF framework. Grand Canonical Monte Carlo (GCMC) simulations were further performed to investigate adsorption behavior, including gravimetric and volumetric uptake. Structural properties such as pore size distribution and density profiles were analyzed to understand adsorption mechanisms. Additionally, the isosteric heat of adsorption was evaluated to assess interaction strength and selectivity. The combined theoretical approach provides detailed insights into the adsorption performance of COFs, highlighting their potential for efficient VOC capture and sensing applications.

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PP-45

Accelerating Carbon Capture Materials Discovery: A Machine Learning Framework for Predicting CO_2 Adsorption and Structure-Property Relationships in MOFs

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Abstract: Metal-organic frameworks (MOFs) are promising candidates for carbon capture due to the ease with which the material properties can be tailored. MOFs can offer lower regeneration energy requirements and higher CO_2 capture selectivity compared to the other materials and techniques that are currently used for CO_2 capture. Rational design of effective materials for carbon capture applications demands a fundamental understanding of the CO_2 adsorption phenomenon occurring in the MOFs. Calculation of the CO_2 adsorption capacity of the MOFs by conventional trial-and-error experiments demands sophisticated experimental techniques and costly equipment. Additionally, calculating the CO_2 adsorption capacity of MOFs using molecular simulation techniques also incurs high computational costs. To overcome the above issues, a machine learning (ML) technique was applied to the prediction and understanding of the CO_2 adsorption phenomenon. A comprehensive dataset of the MOFs with diverse physical, structural, and chemical properties was used to train the ML model to effectively capture the CO_2 capture phenomenon. Benchmarking of the machine learning model's performance with respect to the CO_2 adsorption phenomenon was carried out by the application of effective statistical measures. These machine learning frameworks successfully reconstructed CO_2 adsorption isotherms across a diverse range of operating pressure regimes, with excellent agreement with simulated or experimental results. Apart from the prediction accuracy of the machine learning model with respect to the CO_2 capture phenomenon, another important aim of the research investigation was to obtain a deeper understanding of the physical chemistry phenomenon from the dataset. The SHAP (SHapley Additive exPlanations) analysis technique was applied to the dataset to effectively understand the driving forces behind the CO_2 adsorption phenomenon. This analysis showed the existence of a hierarchy of structural properties with respect to the CO_2 capture phenomenon. Additionally, the analysis revealed that, in addition to the thermodynamic operating pressure and the physical properties of the MOFs, the chemical properties also play a dominant role in the CO_2 capture phenomenon.

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PP-46

Structure-Activity Correlation in $NiCo_2X_4$ (X=S, Se, Te) Systems for Electrocatalytic Glycerol Oxidation

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Abstract: Electrocatalytic water splitting is one of the most promising ways for generating green hydrogen.[1] However, the overall efficiency of electrocatalytic water splitting is hampered by the sluggish kinetics of the oxygen evolution reaction (OER) at the anode.[2, 3] This issue can be resolved by replacing the OER with the more kinetically favorable glycerol oxidation reaction (GEOR).[4, 5] Herein, we have synthesized a series of nickel-cobalt-based spinels (AB_2X_4; X = S, Se, Te) as potent bifunctional electrocatalysts for HER and GEOR. The order of their activity towards GEOR is: $NiCo_2Se_4 > NiCo_2S_4 > NiCo_2Te_4$. The selectivity of products and glycerol conversion can be adjusted by varying the applied potential and temperature. Upon integrating $NiCo_2Se_4$ electrocatalyst as both cathode and anode, a two-electrode system (HER||GEOR) requires 1.497 V to achieve 10 mA cm^{-2} current density, which is 0.47 V lower than the conventional overall water splitting (HER||OER) to generate H_2. Theoretical results reveal the interaction/adsorption of glycerol molecules on different substrate surfaces, along with analyses of their electrostatic potentials and charge transfer.

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PP-47

pH controlled synthesis of end-to-end linked Au nanorod dimer in an aqueous solution for plasmon-enhanced spectroscopic applications

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Abstract: End-to-end linked nanorod dimer nanogap antennas exhibit superior plasmonic enhancement compared to monomers due to the coupling of localised surface plasmon resonances (LSPR) of individual nanorods. However, controlling the assembly to stop at the dimer stage is challenging. Here, we report a pH-controlled synthesis of Au nanorod dimer nanogap antennas in an aqueous solution using 1,4-dithiothreitol (DTT) as a linker. Neutral to acidic pH (4.0 to 7.0) favours dimer formation, while higher pH decreases dimer yield, stopping completely at pH 11.0. The reaction can also be halted in neutral and acidic solutions by abruptly increasing the pH to 11.0 or higher. At basic pH, both thiol groups of DTT deprotonate and acquire a negative charge, causing both thiolate ends to adsorb onto the positively charged cetyltrimethylammonium bromide (CTAB) micellar layer on the transverse surface of the Au nanorod, preventing dimer formation. TEM images confirm nanorod dimers, showing a good conversion yield (~80%) from monomers to dimers. Overall, out of all the DTT-induced NR assemblies, 70% are found to be dimers. The majority of these dimers (>90%) are end-to-end linked dimers, with a gap distance of ~1 nm, remaining intact for over two weeks. FDTD simulations demonstrate a significant enhancement of the light E field in the nanogap, ~80 times higher than in a homogeneous water environment and 11 times higher than in nanorod monomers. Simulations also show that E field enhancement varies with the angular separation of monomeric nanorods, being highest for end-to-end dimers (180°) and lower for side-to-side dimers (0°). Overall, we present an inexpensive method to design and control nanorod dimer nanogap antennas in aqueous solution, useful for plasmon-enhanced spectroscopic applications such as biosensing, chemical sensing, and biomedical devices.

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PP-48

Theoretical Investigation of CDFT based CDASE Scheme Derived Descriptors as Analogues of the Langmuir Constant

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Abstract: An alternative theoretical framework is proposed to explore qualitative trends of Langmuir constants (K_L) and adsorption rates for systems following pseudo-first- or pseudo-second-order kinetics forward and first-order backward direction.[1,2] Using Conceptual Density Functional Theory based descriptors (or Comprehensive Decomposition Analysis of Stabilization Energy based stabilization energy, to be more specific)[3] is used in place of the corresponding rate constants it is shown that when used in the form of rate of adsorption $r_{\text{ads}} \propto \Delta E_B(A)$ and desorption rates are expressed as $r_{\text{des}} \propto | \Delta E_{B(A)} + \Delta E_{SE(AB)} |$, and $K_L \propto \Delta E_{B(A)} / | \Delta E_{B(A)} + \Delta E_{SE(AB)} |$.[4] Computed trends of $\Delta E_{B(A)}$ for dyes malachite green (MG), methyl orange (MO), and BR46 on functionalized 3D adsorbents (NH2-SWCNTs, COOH-SWCNTs, SWCNTs)[5] and 2D materials (graphene, graphene oxide) largely correlate with K_L values. These trends of rate as well as K_L values are expected ones because surface functionalization of SWCNTs favours the kinetics and thermodynamics of adsorption than those on the pristine ones. The study demonstrates that CDFT-based analogues of rate and equilibrium constant can be used to study the trend of adsorption rates as well as Langmuir constants for both 2D and 3D adsorbents.

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PP-49

A Facile and Efficient Synthesis of BODIPY-Based Fluorescent Probes for Selective Detection of Hydrazine

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Abstract: A facile and ratiometric BODIPY-based fluorescent probe **4** was developed for the selective detection of hydrazine in solution phase. The BODIPY-based fluorophores **3** and **4** were easily prepared in high yields from the L-proline catalyzed reaction between *α*/*β*-formyl BODIPY **1a**/**1b** and 3-cyanoacetylindole **2**. Use of easily accessible substrates, benign solvent, catalytic amount of L-proline and high product yields are the advantageous features of the developed protocol. Prepared BODIPYs **3** (536 nm) and **4** (567 nm) showed bathochromic shifts (36-67 nm) in UV-Visible absorption maxima when compared to parent BODIPY (500 nm) in dichloromethane (DCM). The stable and economical BODIPY-based probe **4** exhibited rapid response and remarkable selectivity towards hydrazine when compared to other commonly occurring analytes. At low concentration, the BODIPY probe **4** (10 μM) is non-fluorescent, however, a significant enhancement in fluorescent (turn-on) was observed with the increasing concentration of hydrazine (0-100 μM). This change in fluorescent behaviour may be ascribed to intramolecular charge transfer (ICT) effect as supported by density functional theory (DFT) calculations. With a 4.3 μM detection limit, the BODIPY probe **4** was also found to be useful in detecting hydrazine in real environmental samples.

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PP-50

$MoSe_2$ - rGO based lateral memristive device for memory application

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Abstract: A memristive device can store information in its active layer as its resistance changes. These devices can exhibit two or more levels of resistance when subjected to an electric potential. This resistance can be maintained even after the applied voltage is removed. That makes them suitable for energy- and area-efficient memory and neuromorphic computing systems. A number of materials are used to fabricate these memristive devices, ranging from bulk transition-metal oxides to atomically thin 2D materials such as graphene, hBN, black phosphorus, and transition-metal dichalcogenides. Here, we proposed a lateral heterostructure of a few-layered 2D $MoSe_2$ with reduced graphene oxide (r-GO) to demonstrate its potential for resistive-switching devices. $MoSe_2$ is grown in the CVD system on a SiO_2/Si wafer and transferred onto 25 µm-spaced Ni electrodes patterned on the SiO_2/Si wafer using lithography. Characterizations such as Raman and FESEM are performed to confirm the successful transfer and growth of $MoSe_2$ using the polymer transfer technique. Later, a commercially purchased rGO solution is drop-cast onto the electrodes, onto which $MoSe_2$ is successfully transferred. Under repeated dual sweeps of Voltages applied over 50 cycles between two consecutive Ni electrodes. That produces the very large window hysteresis curves, which show bipolar, reliable switching. This hysteresis I-V curve is later plotted on a semi-log graph to calculate various parameters, such as on/off ratio (10^3), high-resistance state (10^7), low-resistance 10^4 ,states, Vset (7.5 V – 3 V) and Vreset voltages (2.3 V – 5.2 V), on power consumption, and off power consumption. Thus, the fabricated lateral device made of $MoSe_2$–rGO has potential for low-power-consuming memristive-based memory architectures.

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PP-51

Solvent Dependent Distinction of Vibronic Coherences and Enhancing Twisted Donor-Acceptor Systems' Absorption via Controlled Intensity Borrowings

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Abstract: Distinguishing vibrational and vibronic coherences in pump-probe spectroscopy remains a fundamental bottleneck without support from multidimensional spectroscopy, and has never been conclusively reported using pump-probe, as a robust strategy is lacking in the literature. Further, twisted intramolecular charge-transfer (TICT) states exhibit weak/dark absorption at orthogonal geometries, limiting their use in OLEDs/bioimaging. Moreover, thermally activated delayed fluorescence (TADF) triplet efficiency drops in polar media via larger ΔE_{ST} and non-radiative decay. We resolve these gaps in donor-acceptor (D-A) systems using 1,8-napthalimide derivatives (A1-A3, with anthracene, pyrene, and carbazole substituents, respectively, at various positions). We introduce a polarity-dependent strategy for sorting vibrational/vibronic coherences via a state-of-the-art 35-femtosecond pump-probe technique: LE-CT vibronic coherences emerge under resonance in n-hexane; DCM stabilizes CT, enlarges the electronic gap, and quenches vibronic signals, but vibrational coherences persist. Our unprecedented findings show how LE-CT mixing can boost TICT absorption: the effective transition dipole moment (TDM) scales with the angle θ between the TDMs of the coupled states. Aligned TDMs enhance absorption, while anti-aligned yield quasi-dark states. Finally, this is the first report showing a Dynamic TADF (non-polar)/TTA (polar) switching in a single deep blue emitter: A1 shows TADF in hexane (222% emission gain due to triplet contribution) and converts to TTA in DCM (179% gain), demonstrating the polarity robust superiority of TADF-TA switchable emitters over TADF-only. A2 yields pure blue TTA (CIE 0.15, 0.06; QY 0.44/0.69 degassed). We anticipate this study to enable versatile, high-efficiency D-A optical materials and help distinguish vibrational and vibronic coherences.

PP-52

One Pot Synthesized AIE Active Iridium(III) Photocatalyst for GSH Depletion and NADH oxidation Driven Redox Catalysis

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Abstract: Photodynamic therapy is a promising anticancer strategy but remains limited by oxygen dependence, aggregation-caused quenching, and the synthetic complexity of metal-based photosensitizers. Here, we report a first-of-its-kind one-pot-synthesized, aggregation-induced emission (AIE)-active monocyclometalated Ir(III) framework (AM, [2+1+1+1+1]) as a scalable, mechanistically advanced alternative to conventional multi-step [2+2+2] systems (AB). Compared to AB, AM exhibits superior excited-state behavior, including ~175-fold emission enhancement (vs ~46-fold) and prolonged triplet lifetime (17.8 μs), enabling efficient interaction with molecular oxygen and enhanced ROS generation. Importantly, AM integrates photoredox catalysis with NADH oxidation, sustaining redox cycling under both normoxic (O_2-mediated) and hypoxic (cytochrome c-mediated) conditions. AIE-driven aggregation further enhances catalytic efficiency, with higher NADH oxidation rates in physiological media (TOF $\approx 13\ h^{-1}$ for AM vs $6.8\ h^{-1}$ for AB). Nanoparticle formulation (~109 nm) amplifies these effects, enabling potent light-triggered cytotoxicity at nanomolar concentrations (~400 nM) with negligible dark toxicity. Mechanistically, AM induces multimodal cell death, combining apoptosis (~40%), mitochondrial dysfunction, and ferroptosis, supported by glutathione depletion (~36%), lipid peroxidation (~4.5-fold increase), and ferrostatin-1 rescue. Notably, these effects are retained in 3D tumor spheroids, resulting in a ~2-fold reduction in spheroid size. This work establishes a scalable AIE-enabled photoredox platform that overcomes key limitations of conventional PDT and advances the design of clinically relevant photosensitizers.

PP-53

Surface Chemistry Insights into Zn-Based Coordination Polymer Composites for Efficient CO_2 Conversion to Organic Carbonates

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Abstract: A composite of a one-dimensional Zn-based coordination polymer (ZnCP), synthesized from 1,2-bis(pyridin-3-ylmethylene)hydrazine (PHD) and $ZnBr_2$, was fabricated to explore polymer–framework interactions governing catalytic CO_2 conversion. Although ZnCP alone exhibits limited catalytic activity for the cycloaddition of cyclic epoxides with CO_2 due to restricted exposure of active Zn(II) sites, the matrix of the fabricated composite significantly enhanced its catalytic performance due to modified electronic charge redistribution and molecular reorganization.

The composite was characterized by IR, PXRD, and FESEM, which confirmed, while XPS revealed interfacial charge transfer and dipole-π interactions between polymer and ZnCP in the composite, suggesting exposure of catalytically active Zn(II) centers. These interactions modulate the electronic charge distribution of ZnCP, enhancing the accessibility of Lewis acid–base sites. NH_3- and CO_2-TPD analyses further indicated cooperative acid–base functionality within the composite, responsible for efficient, cocatalyst-free epoxide–CO_2 cycloaddition. Overall, the study highlights that the polymer not only stabilises the 1D ZnCP structure but also electronically activates it, demonstrating a promising strategy for designing functional polymer–framework hybrid membranes for effective CO_2 conversion and other catalytic applications. The heterogeneous nature of the catalyst is useful and easy to reuse. DFT studies were also performed to validate the experimental results and give insight into the composite interaction.

PP-54

Quinoline-Based Fluorescent Probes to Monitor Cancer Microenvironment

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Abstract: Cancer has emerged as a major global health challenge. One of the main reasons for the deadliness of this disease is its silent nature. Hence, timely detection is crucial for effective treatment and improved patient outcomes. In this context, disease linked overexpressed biomarkers such as proteins and enzymes serve as promising indicators for early-stage identification of the cancer microenvironment using optical probes. However, a significant limitation of many existing probes lies in their poor biocompatibility, often due to their large molecular size or the generation of undesirable by-products during their activity. In that regard, small molecular fluorescent probes are a good choice for the easy detection of the cancer microenvironment. Herein, we have synthesized quinoline derived small-molecular peptidyl optical probes to detect the overexpressed Cathepsin-B. Cathepsin-B (a cysteine protease) is mainly overexpressed in the lysosome in various types of cancer, including breast, colon and lung cancer. Initially, we have modified the quinoline-based fluoregenic system into a lysosome tracking analogue, to check the accountability of the fluorogenic core for entering into the lysosome. Then, for further advancement, we synthesized couple of Cathepsin-B responsive dark probe using the same quinoline core, which can detect the protease in a plate-based assay platform within 40 min.

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PP-55

Why Swelling of n-type Conducting Polymer, BBL, varies with the Molarity of Electrolytes?

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Abstract: Organic mixed ionic-electronic conductors (OMIECs) show great potential for advanced applications in biosensing[1], flexible and wearable energy storage[2], and neuromorphic computing[3], owing to their structural versatility and coupled ionic and electronic transport properties. To optimize the performance of OMIEC-based electrochemical devices, it is crucial to understand the complex relationships between chemical structure, charge transport, and morphological evolution during device operation[4,5]. In this study, we examine the swelling behavior of the n-type ladder polymer poly(benzimidazobenzophenanthroline) (BBL) during electrochemical switching in aqueous solutions with K^+ counterion concentrations ranging from 0.5 M to 4 M. We investigate this using molecular dynamics (MD) simulations as a computational microscopy technique, and validate our findings through experiments. When electrochemically reduced, the polymer backbone gains negative charges, which are balanced by the uptake of K^+ ions and water molecules. This process induces significant morphological changes and swelling within the polymer film. Our results indicate that polymer swelling depends strongly on the electrolyte molarity. At lower concentrations, the film exhibits considerably greater swelling and more extended polymer chain conformations compared to higher concentrations. This variation arises from differences in the hydration shell structures of the counterions at various molarities, which subsequently affect polymer morphology and ion uptake. Notably, the π-π stacked chains in the films remain intact in all cases; the morphological changes driven by water intake occur primarily in the lamellar regions between the polymer chains. These findings highlight the crucial role of electrolyte molarity in modulating the structural changes and electrochemical performance of BBL-based OMIECs. Ultimately, this work provides dynamic, molecular-level insights into the importance of selecting an appropriate electrolyte concentration to enhance the performance of electrochemical devices utilizing n-type conjugated polymers.

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PP-56

Synthesis of Pyropheophorbides as Red-Light Responsive Photosensitizers for Enhanced Photodynamic Therapy

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Abstract: The pharmacokinetic profile and anti-cancer activity of fluorinated and iodinated photosensitizers (PSs), the 3-(10 -(o-fluorobenzyloxy)ethyl pyropheophorbide and the corresponding meta-(m-) and para (p-) fluorinated analogs (methyl esters and carboxylic acids) were investigated.[1] Replacing iodine with fluorine in PSs did not make any significant difference in fluorescence and singlet oxygen (a key cytotoxic agent) production.[2] The nature of the delivery vehicle and tumor types showed a significant difference in uptake and long-term cure by photodynamic therapy (PDT),[3] especially in the iodinated PS. An unexpected difference in the pharmacokinetic profiles of fluorinated vs. iodinated PSs was observed. At the same imaging parameters, the fluorinated PSs showed maximal tumor uptake at 2 h post injection of the PS, whereas the iodinated PS gave the highest uptake at 24 h post injection. Among all isomers, the m-fluoro PS showed the best in vivo anti-cancer activity in mice bearing U87 (brain) or bladder (UMUC3) tumors. A direct correlation between the tumor uptake and PDT efficacy was observed.[4] The higher tumor uptake of m-fluoro PS at two hours post injection provides a solid rationale for developing the corresponding 18F-agent (half-life 110 min only) for positron imaging tomography (PET) of those cancers (e.g., bladder, prostate, kidney, pancreas, and brain) where 18F-FDG-PET shows limitations.

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PP-57

Green Synthesis of Ag, CuO, and Ag–CuO Nanoparticles Using Cymbopogon citratus: Structural Characterization and Enhanced Antibacterial and Antioxidant Performance

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Abstract: The production of environmentally benign nanomaterials with improved biological functionality is of great interest in nanomedicine. In this study, Ag, CuO, and Ag-CuO nanoparticles were synthesized in a green manner employing Cymbopogon citratus (lemongrass) extract as a natural reducing and stabilizing agent. The synthesized nanoparticles were characterized using XRD, SEM, TEM, and UV-Visible spectroscopy, which confirmed their crystalline structure, nanoscale shape, and altered optical characteristics. Band gap study indicates that Ag-CuO nanocomposites have better electronic interactions. Biological testing demonstrated that Ag-CuO nanoparticles have superior antibacterial activity against both Gram-positive and Gram-negative bacteria, as well as higher antioxidant capacity than their individual counterparts. Higher performance is ascribed to the synergistic actions of Ag and CuO, which cause greater reactive oxygen species production, membrane disruption, and interaction with intracellular biomolecules.

PP-58

Modeling of one-dimensional atomic-scale carbon strip decorated with transition metal adatoms for Magnonic applications

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Abstract: The present work reports a theoretical investigation of a one-dimensional atomic-scale carbon strip decorated with transition metal adatoms, focusing on its magnetic and magnonic properties. The electronic structure is studied using Density Functional Theory (DFT), elucidating the impact of transition metal adsorption on the host carbon system. By transforming plane-wave solutions into maximally localized Wannier orbitals and applying the magnetic force theorem, the exchange interactions are determined, enabling an accurate description of the underlying spin Hamiltonian [1]. Analysis of the magnetic configuration reveals the presence of both acoustic and optical magnonic modes in the terahertz frequency range [2], exhibiting well-defined dispersion that indicates coherent magnon propagation along the one-dimensional structure. To the best of our knowledge, this represents the first report of one-dimensional magnon propagation in such a transition metal-decorated carbon system, establishing a new platform for low-dimensional spin dynamics. The magnonic band structure is further shown to be tunable under external magnetic fields, allowing control over key properties such as bandgap and propagation characteristics. This tunability highlights the potential of the system for applications in magnonic and spintronic devices, including high-frequency signal processing, wave-based logic, and low-power information transmission [3].This work has also been reported in our recent publication in RSC Advances [4].

Figure: The magnon dispersion spectra for the carbon strip with Mn adatom along the path X'-Gamma-X.

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PP-59

Machine Learning-Assisted Hardness Prediction and Design of HEAs

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Abstract: High-entropy alloys (HEAs), particularly the Al-Co-Cr-Cu-Fe-Ni system, exhibit extremely high mechanical properties and are thus a potential candidate for high-technology structural applications. Nevertheless, it is time-consuming and resource-intensive to experimentally explore their compositional space as the possible combinations are very numerous. This paper presents a data-driven computational framework for predicting and optimizing the hardness of HEAs using machine learning (ML) methods. The study used a carefully chosen dataset of 337 alloys, all of which had been tested and shown to have hardness values between 110 and 905 HV. A physics-based feature engineering method was used, including thermodynamic and solid-solution-strengthening descriptors such as valence electron concentration (VEC), mixing enthalpy (ΔH_mix), and shear modulus-related factors. Two different modeling methods were adopted: (i) an interpretable ensemble learning framework based on gradient boosting, and (ii) a hybrid deep learning model that combined Transformer and multilayer perceptron architectures. The ensemble model had a coefficient of determination (R^2) of around 0.80, indicating better predictive performance. It also reduced the number of features by 84% without losing much accuracy. A binary classification model also successfully recognized high-hardness alloys (>600 HV) with an accuracy of about 82%. In contrast, the deep learning model's performance was only moderate. However, it enabled advanced interpretability via SHAP analysis and made inverse alloy design easier via metaheuristic optimization. This research finds that combining domain knowledge with machine learning effectively accelerates materials discovery. The proposed framework cannot only provide precise hardness predictions but also offer insights into composition-property relationships, thereby aiding the rational design of next-generation high-performance alloys.

PP-60

Comprehensive Computational Investigation of 6-(Benzyloxy) 1-Methyl-4-(Prop-2-en-1-yl)Naphthalene: DFT Analysis, Molecular Docking, and Dynamics Simulations

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Abstract: The naphthalene derivative 6-(benzyloxy)-1-methyl-4-(prop-2-en-1 yl)naphthalene (6BMPN) was investigated using density functional theory (DFT) at the B3LYP/6-311 ++ G(d,p) level. Geometrically optimised parameters were in strong agreement (R2 = 0.994 for bond lengths) with experimental data. No imaginary frequencies were observed in the frequency analysis, confirming that all 120 fundamental vibrational modes with their respective potential energy distribution (PED) assignments. Electron localisation function (ELF), molecular electrostatic potential (MEP), and Fukui functions identified atom C17 as the most reactive site (f^- = 0.0884, f^+ = 0.0642). Time-dependent DFT (TD-DFT) results demonstrated weak solvatochromism, with λmax shifting from 320 nm (gas phase) to 322–324 nm in polar solvents, and a band gap of 3.87 eV. Molecular docking simulations identified 4MYQ as the protein with the highest binding energy of -9.8 kcal/mol. 4MYQ-6BMPN complex was further validated employing 50 ns Molecular dynamics simulations over yielding a RMSD of 0.5 nm and a radius of gyration (2.0 nm). In silico drug likeness predicted elevated gastrointestinal absorption and moderate bioavailability (0.55). These integrated computational results demonstrate that 6BMPN exhibits promising structural, electronic, and biological features, suggesting its potential as a PDE4B inhibitor and nonlinear optical (NLO) material.

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PP-61

Green Synthesis and Photocatalytic Degradation of Methylene Blue, Rhodamine B, and Crystal Violet Using Green-Synthesized ZnO Nanoparticles Under Sunlight

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Abstract: In this study, ZnO, nanoparticles doped with various concentrations of transition metals, i.e., 2%, 4%, 6%, 8%, and 10% were synthesized and characterized using a green sol-gel method with saffron flower anther **extract** as a biogenic reducing and stabilizing substance. The obtained materials are systematically analysed for their structural, optical, and magnetic properties by techniques such as X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, high- resolution transmission electron microscopy (HRTEM), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS). The green-synthesized transition metal doped ZnO was investigated for its photocatalytic activity under direct sunlight using methylene blue (MB), rhodamine B (RhB, and crystal violet (CV) as prototype aromatic dyes. UV–Vis spectra of pure and doped ZnO nanoparticles revealed an important shift in the optical band gap with increasing concentration of dopant, implying dopant-induced strong modification of the electronic structure. A degradation efficiency of up to 96% was achieved for all three dyes after 140 minutes, while the intermediate degradation efficiency was 96% (MB), 88% (RhB), and 94% (CV) within 60 minutes. These findings imply the photocatalytic prospect of bio-derived ZnO nanoparticles for environmental remediation applications. Green synthesis of nanoparticles not only reduces environmental impact in the production process but also delivers efficient photocatalysts with specific features for the degradation of dyes.

PP-62

Experimental Exploration of Compression Moulded FRP and FML Composite Plates under High-Velocity Impact

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Abstract: Now a days every structural member design requirement is to provide a structure which offers durability, design flexibility, life and strength to weight ratio. FRP and FML composites poses most of the properties. Whereas the dynamic behaviour of composites under impact load is unpredictable. The primary objective of this study is to explore and compare their ability to withstand impact forces experimentally. Impact testing of the structures operating in the services like automotive, aerospace, robotic, military and defence industries plays vital role. This study explores the impact response of two types of most important composite materials they are fibre-reinforced polymer (FRP) laminates and fibre-metal laminate (FML) in the plates form exposed to high-velocity impacts. Kevlar Epoxy and Aluminium-Kevlar structures were manufactured by using compression moulded fabrication technique followed by hand layup method. In compression moulding technique the composite is compressed up to four hours at a pressure of 20 bar and temperature of 80^0c. A gas-gun experimental setup was used to launch projectiles on the plates at high velocity. Several key impact parameters like energy absorption, residual velocity, and ballistic limit were observed and measured. The findings of this study provide valuable insights for designing of composite structures for high-performance. The improved impact resistance of FMLs makes them a strong candidate to be used in applications endure extreme impact response. The outcome of the work can contribute to the development of safer and more efficient composite materials for future engineering solutions.

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PP-63

STRUCTURAL AND DIELECTRIC PROPERTIES OF X $MgFe_2O_4$- (1-X) $BaTiO_3$ BY CHEMICAL CO-PRECIPITATION METHOD

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Abstract: $MgFe_2O_4$-$BaTiO_3$ based composites with weight fractions x = 0.2, 0.4 and 0.6 were synthesized using solid-state route method. Structural, morphological and dielectric properties of $MgFe_2O_4$-$BaTiO_3$ nanoparticles were investigated. Structural characterization was studied by X-ray diffraction (XRD) where cubic phase formation of magnesium ferrite nanoparticles was confirmed. The size of nanoparticles was calculated by Scherrer formula using X-ray diffraction (XRD) peaks and surface morphology was studied by using scanning electron microscopy (SEM) image. The average size of nanoparticles was found to be 24.89 nm. The dielectric permittivity and loss tangent of the samples were determined in the frequency range from 100Hz to 120MHz. Magnesium ferrite has a cubic structure of normal spinel-type which is a soft magnetic n-type semi-conducting material and Barium Titanate has a perovskite structure, having a number of applications in sensors operating in hazardous environment, etc.

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