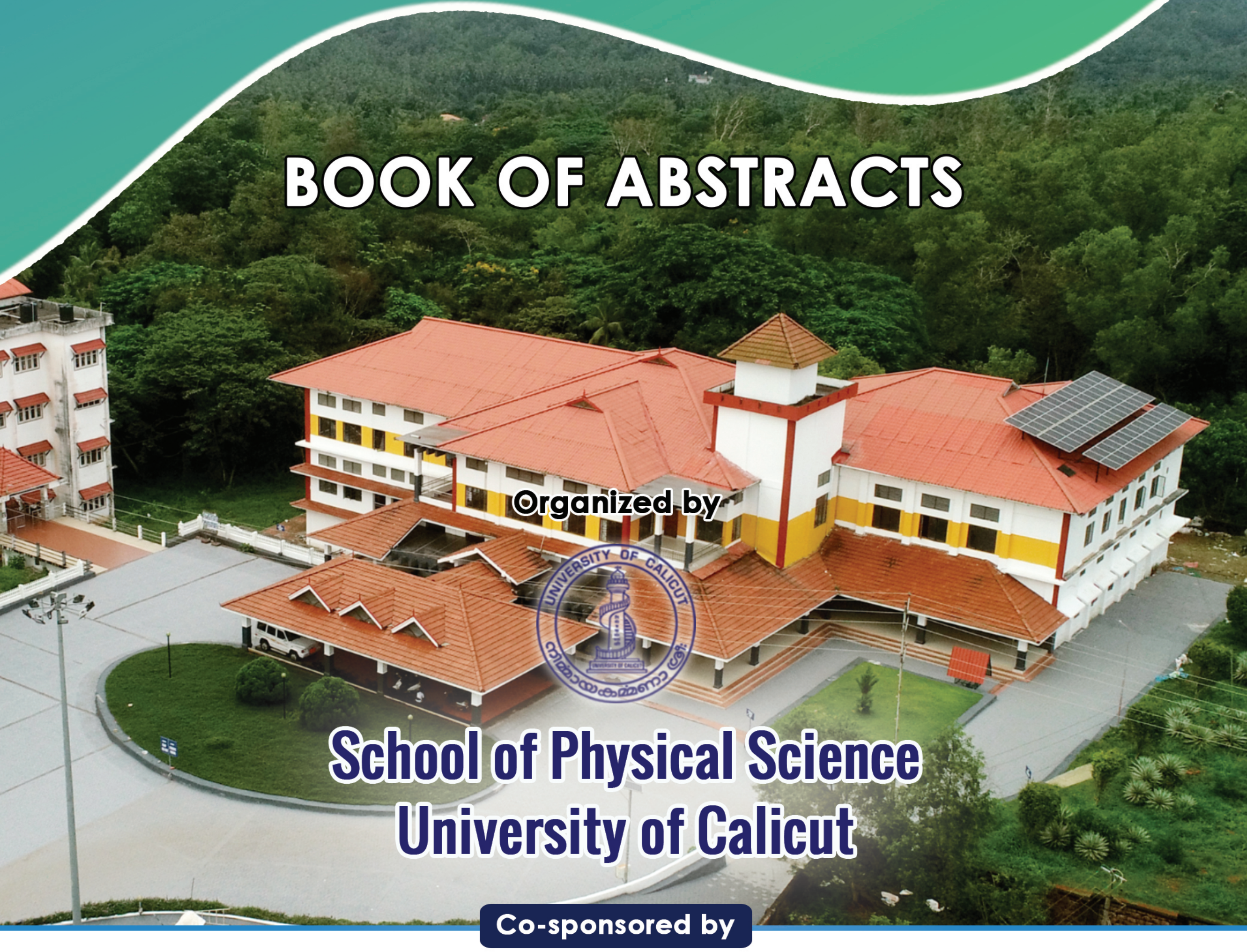
INTERNATIONAL CONFERENCE ON ADVANCED MATERIALS FOR SUSTAINABILITY

ICAMS 2023

21-23, December 2023



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ICAMS 2023

International Conference on Advanced Materials for Sustainability

21st – 23rd, December 2023

Book of Abstracts

Organized by

School of Physical Sciences
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Prof. (Dr.) M.K. JAYARAJ
Vice-Chancellor

UNIVERSITY OF CALICUT
*(Re-accredited by NAAC with **A⁺** Grade)*

Message

Dear Colleagues,

It is a matter of great happiness that the School of Physical Sciences is organizing the International Conference on Advanced Materials for Sustainability (ICAMS 2023) from December 21 to 23, 2023. As the Vice-Chancellor of the University of Calicut, I am honoured to welcome scholars, researchers, experts and industry partners from diverse fields who have converged here to share their insights and contribute to the advancement of knowledge in science, technology and innovation.

The ICAMS 2023 will provide a platform for the exchange of ideas, the dissemination of cutting-edge research, and the fostering of collaborative efforts among academics and professionals. Over the three days, we will have the opportunity to listen and learn from illustrious researchers, teachers, and academicians from across the country and beyond. I believe that the University of Calicut is extremely fortunate to receive and host dozens of eminent delegates and hundreds of keen participants who will all contribute to the event in their own ways.

I encourage each participant to actively engage in discussions, network with fellow researchers, and seize the opportunity to form collaborations that have the potential to redefine the landscape of their respective fields. Such cooperative efforts would be the most fitting outcome of this conference which itself is a joint venture of the Departments of Nanoscience and Technology, Chemistry and Physics.

I thank everyone who has been instrumental in organizing this Conference including Co-patrons, Advisors, and the Local Organizing Committee, for their tireless efforts, vision and collective outlook. I eagerly look forward to listening to the experts and participating in the discussions that would cover various aspects of state-of-the-art Materials Science.

I wish the ICAMS 2023 a grand success.

Prof. M. K. Jayaraj

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Dr. M. Nasser
Pro-Vice Chancellor

UNIVERSITY OF CALICUT

Dated: 18.12.2023.

MESSAGE

It is heartening to note that the School of Physical Science is organizing an International Conference on **Advanced Materials for Sustainability (ICAMS 2023)** from 21 to 23 December 2023. The importance of advanced materials for sustainability is crucial to catalyze collaborative efforts and knowledge exchange. The conference will certainly provide a platform for experts, researchers, and industry leaders to share advances and foster interdisciplinary dialogue. I am confident that the conference will spark partnerships and inspire new research directions. The event will highlight the critical role of advanced materials in addressing global challenges, emphasizing their significance in building a sustainable and resilient future for our planet.

I wish the organizing committee all the success in this endeavour.

Dr. M. Nasser,
Pro Vice Chancellor.

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Foreword

The discipline commonly known as *Materials Science* thrives on extensive cooperation between researchers from various branches of science. Almost all the major advancements in this truly interdisciplinary field have originated from collaborations across conventional boundaries of research areas. Therefore, it is entirely apposite that three Departments of the University of Calicut jointly organise the **International Conference on Advanced Materials for Sustainability (ICAMS) 2023.** The Departments of Nanoscience & Technology, Chemistry and Physics, under the School of Physical Sciences, have joined hands to assemble renowned scientists, industry partners and young researchers at the University of Calicut. ICAMS 2023 will set the stage for hundreds of participants to interact, exchange ideas, inspire each other and initiate cooperative efforts for moving towards the goal of *Sustainability*. Delegates ranging from renowned experts from all over the globe to the young and curious researchers of the locality will enrich the conference. We are honoured and thrilled to welcome all the participants to the picturesque campus of the University of Calicut. We, along with all other participants, look forward to taking part in informative and productive sessions on the latest developments in advance materials. Let us hope that the conference will enlighten and inspire the participants, enrich the field and sow the seeds for longstanding and fruitful collaborations. We thank the organising team of ICAMS 2023 for arranging an event of this scale with careful planning, persistent hard work, and seamless cooperation.

Welcome you all to ICAMS 2023.

Chairperson

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Vice-Chairperson

PREFACE

There is no aspect of human life that is untouched by Materials. The science of the latter is therefore, a large canvas whose boundaries overlap with many other branches of knowledge. For the practitioners of the art, it becomes essential to regularly meet, interact, gauge where the area is headed, appreciate how it is influencing other sciences and estimate how much it is getting influenced by them. The opportunity to do exactly these will be provided for all the participants of the ‘International Conference of Advanced Materials for Sustainability (ICAMS) 2023’ organised by the School of Physical Sciences, University of Calicut. True to the interdisciplinary nature of Materials Science, ICAMS also is being realised by the cooperation of three Departments, namely Nanoscience & Technology, Chemistry and Physics, of the University of Calicut. ICAMS is expected to be a stage where ideas and developments are shared, new alliances are forged, and long-lasting memories are formed.

This book of abstracts, compiled by the Editorial team, consists of the snippets of the scientific discourse that forms the heart of ICAMS. The abstracts of 14 Plenary lectures, 12 invited lectures, 31 oral presentations, and 71 posters will undoubtedly reflect the diversity, breadth and far-reaching influence of the subject theme of the conference. The reader will find topics ranging from established sectors of Material Sciences to the most recent developments in emerging areas of it.

The editorial team wishes to thank the advisory committee, organising committee, faculty members, research scholars and staff of the participating Departments for the valuable advice, assistance, cooperation and support. We also thank all the sponsors who generously supported the event.

Happy Reading

Editorial Team, ICAMS 2023
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Plenary Lectures

Invited Lectures

Oral Presentations

Poster Presentations

PL 01

2D Materials-based Smart Membranes and their Applications

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Permeation through nanometre-pore materials has been attracting unwavering interest due to fundamental differences in governing mechanisms at macroscopic and molecular scales, the importance of water permeation in living systems, and relevance for filtration and separation techniques. The latest advances in the fabrication of artificial channels and membranes using two-dimensional (2D) materials have enabled the prospect of understanding the nanoscale and sub-nm scale permeation behaviour of water and ions extensively. In particular, several laminate membranes made up of 2D materials show unique permeation properties, such as ultrafast permeation of water and molecular sieving. In my talk, I will discuss our recent results on controlling molecular transport through various 2D materials-based membranes by an external parameter and will discuss the prospect of developing next-generation intelligent membranes based on 2D materials. Specifically, I will discuss two themes: pH-dependent water permeability switching and its memory in MoS_2 membranes and the controlled release of ions from graphene oxide membranes for healthcare applications.

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PL 02

(Car)borane Cluster Molecules in Self-Assembly on Flat and Colloidal Metal Surfaces

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Carborane clusters have become an important class of molecules for self-assemblies. Their rigid molecular structures and rich isomeric forms enable to investigate particular physical properties of their 2-D assemblies while keeping the surface pattern either identical or close to identical. The respective self-organized monolayers exhibit fewer types and lower total number of surface defects, partly as a consequence of their low conformational freedom. In our laboratories we have been using these molecules as basic constituents for better understanding of some of the most fundamental self-assembly principles and intermolecular interactions that lead to a certain supramolecular structure and function. We shed more light on several key aspects such as the interaction of these molecules with flat gold and silver surfaces, we analyzed and showed the effect of their dipole moment orientation and magnitude on the surface properties changes and, not the least, we opened these monolayers to further chemistries by introducing additional functional groups that are in their SAMs exposed from the surface. This interdisciplinary contribution summarizes several of the above-mentioned aspects but also shows how these species can be advantageously used to generate new types of stable interfaces for further research and applications in bio-medicinal sciences.

PL 03

Excitons and Free Carriers in Semiconductor Quantum Dot System

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The size- and composition-tunable bandgap and emission color of metal chalcogenide and halide perovskite quantum dots are two fascinating inventions in nanoscience and nanotechnology.[1-3] These unique properties accompany these tiny crystals to various basic research disciplines and promise the development of brilliantly luminescent displays, tunable lasers, and high-efficiency photovoltaics. However, exciton deactivation by defects and charges[4-6] prevents applying these materials to on-demand light sources or quantum computing. Such defects and residual charges are correlated with the energy/intensity of the excitation light and the nature and density of defects. Additionally, the development of incessantly luminescent quantum dot devices is challenging due to exciton splitting, delocalization, and nongeminate nonradiative recombination in higher-order structures. This presentation highlights the excitonic and charge carrier properties of individual and self-assembled quantum dots of metal chalcogenides and lead halide perovskites,[4-12] including photoluminescence and electroluminescence blinking of a few quantum dots. The characteristics of luminescence blinking are discussed by correlating charging and blinking with the intensity of excitation light, the density of intrinsic defects, and the presence of electron donor/acceptor molecules.

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PL 04

Metavalent Bonding

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A distinct type of *metavalent* (intermediate to *met*allic and co*valent*) bonding (MVB) was recently proposed to explain an unusual combination of anomalous functional properties of group IV chalcogenide crystals, whose electronic mechanisms and origins remain mysterious. Through theoretical analysis of evolution of bonding along continuous paths in structural and chemical composition space, we demonstrate emergence of MVB in rocksalt chalcogenides as a consequence of *weakly* broken symmetry of parent metallic simple-cubic crystals of Group V metalloids. Stronger symmetry breaking structural and chemical fields, however, transform them *discontinuously* to covalent and ionic semiconducting states respectively. MVB involves an electron engaged in bonding and antibonding pairwise interactions alternating along linear chains of atoms, which facilitate electronic delocalization and long-range electron transfer in response to polar fields and cause unusual properties. Understanding of MVB is central to design of quantum materials exhibiting thermoelectric, ferroelectric and nontrivial electronic topological properties.

* Work done in collaboration with Raagya Arora and C. N. R. Rao

PL 05

Affordable Clean Water Using Advanced Materials

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Sustainable nanotechnology has made substantial contributions in providing contaminant-free water to humanity. In this talk, I will present the compelling need for providing access to clean water through nanotechnology-enabled solutions and the large disparities in ensuring their implementation. I will discuss the current nanotechnology frontiers in diverse areas of the clean water space with an emphasis on applications in the field and provide suggestions for future research. Extending the vision of sustainable and affordable clean water to environment in general, I note that cities can live and breathe well by adopting such technologies. By understanding the global environmental challenges and exploring remedies from emerging nanotechnologies, sustainability in clean water can be realized. I will suggest specific pointers and quantify the impact of such technologies, particularly in the context of India.

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PL 06

Secondary Nucleation Triggered Supramolecular Materials

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Supramolecular polymers formed by the noncovalent association of monomers have evolved over the last two decades as the most promising candidates for the design of dynamic, adaptive, and recyclable materials. Study of dynamic and adaptive supramolecular polymers has now entered an era that demands assemblies with more structural and dynamic control. The synergy between structural and temporal control is important for the advent of supramolecular polymers to be employed as functional adaptive materials. Thus, taking cue from the biological self-assembly process, kinetically controlled seeded growth has been recently shown to provide length, dispersity, and sequence control on the primary structure of dynamic supramolecular polymers.[1,2] However, command over the molecular organization at all hierarchical levels for the modulation of higher order structures of supramolecular polymers remains a formidable task. In this context, a surface-catalyzed secondary nucleation process, which plays an important role in the autocatalytic generation of amyloid fibrils and during the chiral crystallization of small monomers, offers exciting possibilities for topology control in synthetic macromolecular systems by introducing secondary growth pathways compared to the usual primary nucleation–elongation process. However, mechanistic insights into the molecular determinants and driving forces for the secondary nucleation event in synthetic systems are not yet realized. Recently, we have filled this dearth by showing an unprecedented molecular chirality control on the primary and secondary nucleation events in seed-induced supramolecular polymerization.[3] I will be discussing our recent attempts to use surface catalyzed secondary nucleation process, to modulate the topology of supramolecular polymers and to modulate the functional outcomes of supramolecular materials.[4,5]

Figure 1: *Schematic representation of primary and secondary nucleation events in synthetic supramolecular polymerization process.*

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PL 07

Van der Waals Gap Engineering of Two Dimensional (2D) Materials

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Most of the Two Dimensional materials have a finite van der Waals gap (v-gap) in between the layers which provides a clear separation between the in-plane and through plane electronic interactions. Although the carrier transport and associated unique features are studied in accurately prepared and precisely characterized monolayers, many technological applications such as nanoelectronics, electrocatalysis, biosensing, solar energy conversion, and energy storage use multilayers which are conveniently prepared using inexpensive and scalable chemical methods. For example, among various two-dimensional (2D) materials, graphene possesses similar interlayer spacing of multiwalled carbon nanotubes (0.32−0.35 nm) which could be modulated by several strategies such as the intercalation of cations and anions, the nature of the solvent, and surface functionalization. The resultant graphene nanoribbons (∼40 nm diameter) formed by the ionic liquid-assisted transformation of multiwalled carbon nanotubes of an average diameter (∼21 nm) along with graphene quantum dots having an emission wavelength of 445 nm are more useful for some of the specific applications. This electrochemical approach not only reveals the introduction of multiple heteroatoms at room temperature but also modulates the van der Waals gap between the layers of multiwalled carbon nanotubes, which could have significant implications for the mechanical and electrical properties. The tunability of this spacing depends on the nature of the ionic liquid, the size of the incoming ions, the applied potential, and the time. In this lecture several examples of v-gap engineering will be demonstrated for specific application like Na/Li ion batteries and fuel cells.

PL 08

Inorganic and Organic Materials for Electrocatalysis, Sensors, and Energy Storage

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Studies on electrochemical phenomena have seen an emergence in the last few decades, particularly in the context of energy conversion and storage. Fundamental as well as applied research involving electrochemical interfaces have gained considerable momentum, due to the enormous interest in materials chemistry. Various families of materials based on layered chalcogenides, nitrides, carbides and organic-based ones have significantly contributed to this development. Our group has been involved in understanding interfaces of various kinds that include both organic and inorganic materials. The present lecture will describe some of our efforts on electrocatalysis, energy storage, sensors and solid-state devices. Using the fundamental knowledge on interfacial science, it is possible to further delve into applications based on energy storage, such as batteries, capacitors and fuel cells. The present lecture will discuss results from our group in the above mentioned areas.

PL 09

Design Strategies for Solid Electrolytes and Interfaces for All-solid-state Li/Na Batteries

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In the current scenario, Li-ion batteries are the unparalleled choice to power electric vehicles owing to their appreciable energy and power density. Replacing liquid electrolytes with solid counterparts offer improved safety and also help overcome the energy-density limitations of current Li–ion batteries, so as to make them suitable candidates for the growing electric vehicle sector. However, several issues such as poor solid-solid interface and lithium dendrite formation at higher current densities remain to be addressed, in-order to realize commercial implementation of the technology.[1] Several studies have been focused on the interface engineering to improve the electrochemical compatibility, ion transport and mechanical stability. Here, some of our recent efforts on the design and development of solid electrolyte materials and the anode-solid electrolyte interfaces toward fabricating efficient all-solid-state Li/Na batteries will be discussed.[2,3]

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PL 10

Role of materials in Biosensors and bioimaging: Pre-clinical experiences

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Bionanosensors represent a cutting-edge intersection of nanotechnology and biosensing, offering unprecedented capabilities in detecting biological entities at the nanoscale. These sensors leverage the unique properties of nanomaterials to interface with biological systems, enabling highly sensitive and selective detection of various biomolecules. The integration of nanomaterials with biological recognition elements, such as enzymes, antibodies, or nucleic acids, allows for the specific identification and quantification of target analytes, ranging from proteins to DNA.

The development of bionanosensors holds immense promise across diverse fields, including medical diagnostics, environmental monitoring, and food safety. Their miniature size and enhanced sensitivity make them ideal for point-of-care applications, facilitating rapid and on-site detection of diseases. Moreover, bionanosensors exhibit potential in real-time monitoring of biological processes, providing valuable insights into cellular functions and dynamics.

Moreover, nanomaterial-based contrast agents have also emerged as essential components in medical imaging. Nanoparticles, quantum dots, and other engineered nanomaterials exhibit unique optical, magnetic, or acoustic properties that enhance contrast in imaging modalities such as magnetic resonance imaging (MRI), computed tomography (CT), and ultrasound. These contrast agents improve sensitivity and specificity, enabling the visualization of anatomical structures and pathological changes with greater precision.

Key challenges in these fields include optimizing the stability and reproducibility of nanomaterial-based sensor and imaging platforms, ensuring biocompatibility, and addressing issues related to signal-to-noise ratios. As research progresses, bionanosensors and nano contrast agents are poised to revolutionize the landscape of diagnostics and monitoring, offering innovative solutions with implications for personalized medicine, early disease detection, and advancements in our understanding of biological systems at the nanoscale.

We have been working in the field of development of nanobiosensors and materials for imaging applications for last few years. I will be discussing some of them including gold-graphene hybrid based nanotags for developing the filter system for circulating tumor cells, bipyridine based molecule for the imaging of zinc translocation during epilepsy, dopamine sensor during neuronal cell differentiation, design of multianalyte sensor using quantum dots etc., and iron oxide materials for MRI and materials with optical property for fluorescence imaging.

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PL 11

Photophysical Properties of Donor-Acceptor Systems Involving Quantum Dots, Nanocrystals and Organic Molecules

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In the recent past, there has been a growing interest in understanding the excited state dynamics of quantum dots (QDs) due to their potential role in energy harvesting and biomedical applications. The present talk reveals the recent results obtained from our laboratory regarding the excited state dynamics and emission properties of CdSe QDs, Graphene QDs, lead halide nanocrystals, and novel 2D materials based QDs.[1] The excited state dynamics of quantum dots (CdSe QDs) and nanocrystals were monitored using femto second laser flash photolysis system, in the presence and absence of other quantum dots (GQDs) as well as organic donor-acceptor systems. The results from the study indicate the evidence of electron transfer along with the hole-trapping process by surface defects in the QDs. More importantly, the consequences of improved charge transfer have been established through the measurements of enhanced photoconductivity, indicating that suitable organic molecular interface can potentially enable high charge carrier dynamics in QD/perovskite nanocrystal-based donor-acceptor systems. Details of the work will be presented.

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PL 12

Active colloids in liquid crystals

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Colloidal particles dispersed in liquid crystals create elastic distortion and act as an elastic multipolar source that results in topological defects. Invariably such defects have been considered an undesirable feature in liquid crystal display devices. The defect-decorated particles interact via novel anisotropic elastic forces which are tunable and the particles can be guided to create 2D and 3D colloidal crystals. Another interesting manifestation is the ability of the particles to propel due to the breaking of symmetry in electrohydrodynamic flow. Studies on motility and collective dynamics of such particles as active colloids are natural experimental and theoretical challenges. In this talk, I will present a summary of our recent works on liquid crystal colloids, a fast-growing area of soft matter research for directed assembly and controlled transport.

PL 13

Advancing Electrochemical Energy Devices: Tailoring Mixed Transition Metal Oxides for Enhanced Oxygen Reduction Reaction

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The oxygen reduction reaction (ORR) is a pivotal electrode process in electrochemical energy devices, particularly in direct methanol fuel cells (DMFCs). However, the sluggish kinetics of ORR at the cathode has been a persistent challenge, impeding the overall performance of DMFCs. State-of-the-art Pt/C catalysts, while effective, are marred by issues such as methanol oxidation activity, nondurability, and high costs. Addressing these concerns, there is a need for an alternative, that includes characteristics such as efficiency, methanol tolerance, durability, and cost-effectiveness. At this juncture, mixed transition metal oxides (MTMO) have emerged as promising candidates, with a particular focus on Ag-based compositions. Tuning the d-band center of these materials has been identified as a critical aspect of augmenting their performance in the ORR. We explored the structure-dependent ORR activity of $AgVO_3$, shedding light on its potential as a catalyst. Additionally, the synergistic contribution of AgCl to ORR activity, achieved by strategically shifting the d-band center, and the incorporation of SnO_2 are investigated. These methods not only enhance ORR activity but also improve durability, presenting a multifaceted approach to catalyst development. This research contributes to the ongoing efforts to develop highly durable and high-performance ORR catalysts that address the limitations associated with conventional Pt/C catalysts.

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PL 14

Toward the Creation of High-Performance Energy and Environmental Catalysts: Controlling the Aggregation of Metal Atoms with Atomic Precision

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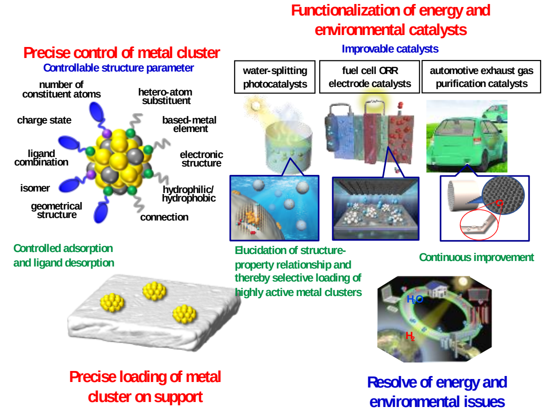

Figure 2: *Graphical summary of the presentation.*

In order to build a sustainable society, it is indispensable to create new innovative materials that can solve the problems of the current society. Strict control of the structure of materials at the nanoscale is expected to lead to the creation of such materials. Ultrafine metal clusters, in which several to several dozen metal atoms are aggregated, have novel electronic/geometric structures and physicochemical properties/functions that are different from those of bulk metals composed of the same elements. In addition, doping (alloying) of different elements to these metal clusters results in a variety of structures, properties, and functions. Thus, metal clusters have high potential as constituent units for innovative materials. However, in order to understand the functions of metal clusters and to apply them as materials, it is essential to establish techniques to strictly control the chemical composition and geometric structure of metal clusters. We have established several techniques to strictly control the chemical composition and geometric structure of metal clusters. We also succeeded in establishing a method to control the supported metal clusters to enhance the functionality of advanced water splitting photocatalysts, fuel cell electrocatalysts, and automotive exhaust gas purifying catalysts. Accordingly, we have achieved the highest water-splitting activity for UV-responsive $BaLa_4Ti_4O_{15}$ water-splitting photocatalysts, created platinum electrocatalysts with higher catalytic activity for oxygen reduction than those currently used in fuel cells, and succeeded in developing highly functional catalysts for automotive exhaust gas purification. These our research is unique in that it consistently achieves the atomic-level control of the metal clusters throughout the entire research, from synthesis to control on the support. This presentation summarizes our recent works concerning these topics.

IL 01

Smart Materials and Devices for Multifunctional Fenestration in Energy-Efficient Sustainable Buildings

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An efficient solution for the vicious problem of global warming demands for more adept energy utilization. Therefore, new molecular and supramolecular systems with designed functions are being actively explored for driving next-generation clean and efficient energy technologies. In this context, smart materials and devices with low energy footprint capable of modulating their optical properties under electrically and thermally stimulated conditions have led to a watershed moment in the area of energy management. Multifunctional smart fenestration systems that regulate heat and light transmission leading to efficient indoor energy management, has added several new dimensions to the classical concept of energy-saving smart glass technologies. We have successfully demonstrated high-performance nanoscale thermo- and electro-responsive materials and devices that exhibit a practical combination of low energy operation and efficient color/transparency switching along with good redox, photochemical and cycling stabilities, write-erase efficiency, and easy processability.[1,2] These materials were further integrated into devices and large-area smart window prototypes that exhibited up to 7 ^{o}C reduction in indoor temperature. Our results also corroborate that the energy storage aspects of such smart materials can be effectively directed towards combining energy saving and energy storage using a single system.[3,4] Significantly, the multi-state optical switching of these supramolecular assemblies can also be translated into logic operations and volatile memory.[5] Such multifunctional fenestration systems, that integrate smart functions with energy storage and memory operations, are critical towards achieving universal energy access, energy sustainability, and ensuring reliable power supply.

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IL 02

Analysing the Role of Counterions and Additives in Catalysis: A DFT Approach

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The computation of transition state models using Density Functional Theory (DFT) is an established method of choice for the mechanistic elucidation of a wide array of regio- and stereoselective reactions.[1] This is further employed to analyse the role of solvent, additives, counterions etc in the rate and selectivity determining steps of a reaction. With this, making improvements in the future reaction scheme design, which represents a major synthetic challenge, became easier.[2] To this end, I will discuss the strategies we have applied for the study of C−N coupling and α-alkylation reactions.[3] The detailed chemical insights in the presentation will unravel the mechanism of the reaction, importance of additives and solvents, and factors controlling the origin of selectivity by employing DFT methods. Furthermore, how these obtained insights and methods can be proposed to apply in future for refining the transition state models for the catalyst design will be discussed. The key focus of the presentation is the efficient use of the synergy between the theory and experiment to overcome the current inherent challenges for novel catalyst design.

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IL 03

Advanced Carbon-based Electrocatalyst Support Materials for Durable Proton Exchange Membrane Fuel Cells

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Global energy demands are projected to grow 36% over the current level by the year 2030. Polymer electrolyte membrane fuel cells (PEMFCs) are promising candidates for the reliable and efficient conversion of hydrogen, produced from fossil or renewable sources, into electric power in automotive, distributed power generation, and portable electronic applications on a large scale. However, the large-scale implementation of fuel cell technology for use in commercial residential or transportation applications is hindered largely by the high cost and durability issues of the materials associated with PEMFCs. The thriving development of nanomaterials and nanotechnologies brings opportunities for high-activity Pt catalysts and support materials. Nonetheless, the limited activity and poor durability of Pt itself put pressure on the cost and performance of fuel cells. PEMFCs still suffer from the insufficient durability of their constitutive materials: the Pt or Pt-alloys or non-precious metal catalysts used as electrocatalysts, catalyst support materials, the proton exchange membrane (PEM), the ionomer, and the gas-diffusion layers.

Carbon-based support materials, such as nanotubes, Vulcan carbons, graphene, aerogels, carbon nanofibers, boron-doped diamond, nanocoils, carbon nanohorns and hollow graphitic spheres, have been proposed as catalyst supports for PEMFCs in order to maximize the utilization of nanocatalyst. Among these materials, carbon nanofibers and graphene have been identified as a suitable candidate due to their high surface area, high electrical conductivity and thermal stability. However, the sluggish ORR causes a large over potential during the start-up/shut-down operation which leads to electrochemical oxidation of the carbon support. This electrochemical oxidation (corrosion) leads to the separation of Pt electrocatalyst particles which then become electronically isolated, leading to poor utilization of Pt and degrades their performance. On the other hand, few efforts have been made by employing inorganic based support materials to overcome the stability issues. Even though these materials possess high stability towards electrochemical corrosion, they suffer from inadequate porosity, solubility in aqueous environment, poor electronic conductivity, low surface area to incorporate catalyst, low thermal stability. Focusing on the structure–activity relationship, the fundamental problems raised from active components and robust supports, this talk will emphasis on novel material design strategies for durable PEM fuel cells.

IL 04

Design and Synthesis of Novel Macromolecules with Tuneable Properties for Environmental Remediation and Biological Applications

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Structural diversity and tuneable properties achieved in synthetic macromolecules uniquely qualify them for a wide array of applications in material and biomedical sciences. However, having an efficient and simple modular synthetic platform to make those macromolecules is challenging. This motivated us to develop a novel synthetic platform which focuses on the production of new properties along with producing new material. In this seminar, I will talk about two new classes of macromolecules: (i) non-conventional synthetic polymer, named as Sequence-Defined Polymer (SDP) and (ii) functionally tuneable Organic Polymer (OP) and their applications for environmental remediation and biological sciences. One unique functional group namely, dithiocarbamate (DTC) has been strategically incorporated in both the cases, as DTC is known to be a potential functional group for material as well as biomedical applications. DTC-based SDP (DTC-SDP) showed excellent performance in detection of environmental pollutants at very low level (up to picomolar) in contaminated water as well as living cells. On the other hand, DTC-based OP (DTC-OP) was found to be highly efficient in removing several types of toxic environmental pollutants including heavy metals, dyes, pharmaceuticals, volatile organic compounds, oxo-anions, radioactive contaminants in a matter of few seconds. On a separate note, DTC-SDP was found to be a potential platform for developing antibacterial drugs. DTC-SDP was also employed to develop highly sensitive serum proteins-selective staining agent. In addition to DTC, we have also developed other classes of materials with key functional groups e.g. triazole and amine and explored them for various applications including selective detection of biologically important compounds like cholesterol, cancer biomarker, drugs etc. Taken together, we will discuss the low-cost multipurpose macromolecules developed in our lab for environmental remediation and biological applications.

IL 05

Nanoparticle Protein Framework Hybrid Materials

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The existing porous synthetic materials encompasses zeolites, mesoporous structures, covalent organic frameworks, and metal-organic frameworks. In this presentation, I introduce a novel "hybrid porous material" that is constructed through the hierarchical self-assembly of supramolecular protein polymers and gold nanoparticle cross-linkers. The protein employed in this approach is the chaperonin GroEL, a biomolecular machine known for capturing denatured proteins within its cavities, facilitating their refolding, and releasing them through the action of adenosine-5′-triphosphate.[1] Previously, Aida and colleagues had developed GroEL protein supramolecular polymers through DNA hybridization of GroEL containing complementary DNA sequences on their apical domains (^{DNA}GroEL).[2] To create a nanoparticle protein framework (NPF), DNA-appended gold nanoparticles (^{DNA}AuNP) were hybridized with ^{DNA}GroEL using either a one-pot or stepwise approach (see Figure 1).[3] In the one-pot method, an equimolar mixture of monomers resulted in the formation of NPF clusters, albeit with smaller pore sizes compared to those formed using the stepwise approach. With the stepwise method, an intermediate comonomer composed of multiple GroELs on AuNP was isolated. The pore size of the resulting NPF (30 to 70 nanometers) could be adjusted based on the linker supramolecular polymer and the core size of the AuNP (5 to 30 nm). Furthermore, NPF could encapsulate relatively large guests, with sizes up to approximately 40 nanometers.

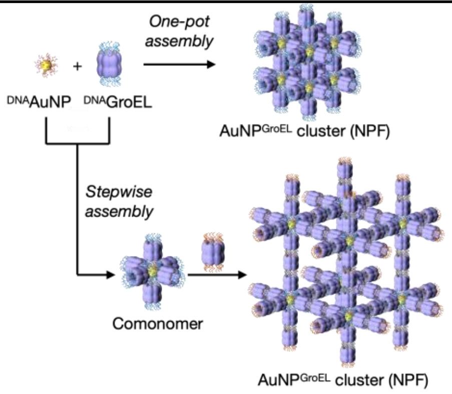

Figure 1: *Scheme showing the methods for NPF construction using ^{DNA}GroEL* and ^{DNA}AuNP.

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IL 06

Seeing Nanoscale Assemblies in 3D

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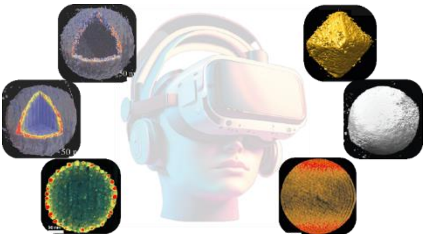
Figure 3: *An overview TEM tomography assisted 3D reconstructed colloidal superstructures.*

Transmission electron microscopy (TEM) imaging has revolutionized modern materials science, nanotechnology, and structural biology. Its ability to provide information about materials' structure, composition, and properties at atomic-level resolution has enabled groundbreaking discoveries and the development of innovative materials with precision and accuracy. Electron tomography, single particle reconstruction, and microcrystal electron diffraction techniques have paved the way for the three-dimensional (3D) reconstruction of biological samples, synthetic materials, and hybrid nanostructures at near atomic-level resolution.[1,2] TEM tomography using a series of two-dimensional (2D) projections has been used extensively in biological science. In recent years, it has become an important method in synthetic nanomaterials and soft matter research. I will discuss how TEM tomography offers unprecedented morphological details of 3D objects, internal structures, packing patterns, growth mechanisms, and self-assembly pathways of self-assembled colloidal systems.[3-8] I will also present how it provides valuable data for computational simulations for predictive design and reverse engineering of nanomaterials with desired structures and properties.

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IL 07

Molecular Basis for Probabilistic Origin of Alzheimer's Disease: Emergence of a Real-time Nanoscale Structural Risk Factor

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Figure 1: *A schematic illustration nanoscale enzymatic processing subunits of APP at excitatory synapse.*

Decades of extensive research have firmly established that alterations in the proteolytic processing of Amyloid Precursor Protein (APP) are pivotal in the development of Alzheimer's disease (AD). However, the exact role of synaptic APP, finely regulated within axo-dendritic and synaptic compartments, remains poorly understood. This knowledge gap exists due to limited insights into the molecular mechanisms governing the localization and mobility of the amyloidogenic machinery at individual synapses. Within synapses, the composition of the postsynaptic membrane is intricately orchestrated, encompassing both passive molecule diffusion and active processes like endo- and exocytosis. Our laboratory is dedicated to unravelling the stochastic molecular changes that influence amyloidogenesis at individual synapses. We have unveiled distinct functional domains within synapses where APP, β-secretases, and γ-secretases exhibit diverse distributions and participate in lateral diffusion. Alterations in APP characteristics directly affect APP processing and the accumulation of amyloids at synapses. These findings underscore the critical roles of nanoscale aggregation and the regulation of lateral diffusion in shaping the onset and progression of AD. Furthermore, it appears that molecular determinants affecting APP lateral diffusion and reversible trapping contribute to APP proteolysis and AD-related changes. Over the past decade efforts from our lab compared across different AD models, support the existence of a "**structural risk factor**" that can be dynamically and precisely regulated at the nanoscale, opening new avenues in the fight against AD.

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IL 08

Hierarchical Organization of Bio-Mimetic Supramolecular Polymers

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Morphological evolution during the hierarchical assembly process of chiral supramolecular polymers has always been a fascinating subject among supramolecular self-assembled structures.[1,2] A wide variety of chiral building blocks, like peptide amphiphiles, amphiphilic lipids, and proteins, are known to form self-twisting architecture. However, understanding the connection between molecular chemistry and morphological selection remains a challenge and, thus, an exciting topic of research. In the present talk, we are trying to find a correlation between molecular geometry and its supramolecular outcome, resulting in distinctive properties. We found that depending on the conformational flexibility of the polycyclic aromatic hydrocarbon functionalized-dipeptide conjugate leads to the hierarchical organization of flat nanoribbons into microcrystals via a non-classical crystallization mechanism.[3] However, a similar system with geometrical constraints forms nanotubes from the metastable helical nanoribbons through a series of intermediates. The details of these interesting hieratically organized bio-mimetic supramolecular polymer systems will be presented.

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IL 09

Ultralow Pt Catalyst for Efficient Oxygen Reduction Reaction

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Pt-based electrocatalysts are considered the best option for both the oxygen reduction reaction (ORR) and the hydrogen oxidation reaction (HOR) in polymer electrolyte membrane fuel cells (PEMFCs), despite the ORR having lower reaction kinetics and the high amount of Pt required for efficient ORR at operating temperatures below 200 °C. The overall performance of a fuel cell depends largely on the ORR, making it necessary to use a significant amount of Pt, which significantly contributes to the total cost of the device. Alternative electrocatalysts, such as heteroatom-doped carbon, metal oxides, Fe-Nx doped carbon (FeNC), and Fe-Sx-doped carbon, exhibit ORR activity with excellent fuel tolerance and stability compared to Pt/C under alkaline conditions (pH>7). However, their stability and ORR activity are poor compared those with of Pt at low pH values. Fe/C/Ni-NC exhibited ORR activity under acidic conditions, but with an overpotential of 100 mV, which was higher than that of Pt/C. Modifying the chemical and surface properties of Fe/C/Ni-NC had little impact on the ORR activity. Nevertheless, the ORR activity still experiences an overpotential. Therefore, a new strategy is required to develop an electrocatalyst that can achieve activity comparable to that of Pt/C at low pH without significantly contributing to the overall catalyst cost. The use of a single precious metal atom (in this case, Pt) on a carbon alloy plays a crucial role in reducing the gap between the Pt and non-Pt catalysts. However, methods such as atom layer deposition or related synthesis protocols are not suitable for bulk-scale catalyst preparation. Recently, we found that heating a blend of FeCN-based non-PGMs and Pt salt (equivalent to 2 wt. %) to undergo a simple heat treatment, a Fe3PtN type alloy is formed on a non-PGM surface. The Fe3PtN nanoparticles were evenly distributed on the surface. This Fe3PtN-supported FeCN catalyst displayed an ORR performance comparable to that of a 46 wt.% Pt/C catalyst at low pH levels, with high mass activity and electrochemical stability. This presentation will recount the journey of developing electrocatalysts from non-Pt to ultra-low Pt catalysts for the ORR.

IL 10

Mechanical Conformity in π-Conjugated Molecular Crystals

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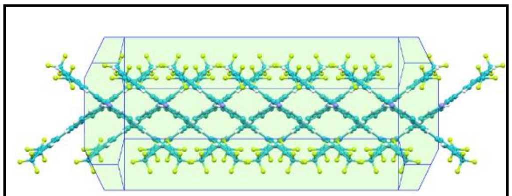

Figure 1: *Representative crystal packing that can sustain mechanical stress.*

Flexible optoelectronics emerged as the need of the hour due to increasing demand for wearable and conformable devices. The key requirement of these devices is to withstand mechanical deformations without compromise in device performance. Crystalline organic π-conjugated molecules as active materials can offer an enhanced performance due to their superior charge and exciton transport properties over the semi-crystalline/amorphous counterparts. Organic molecular crystals are generally brittle and shattered into pieces on subject to subtle mechanical perturbation, which limit its application. A greater part of the fragile nature arises from the anisotropic packing of molecules in the crystal lattice, where the applied force dissipated in an asymmetric manner along the molecular planes resulted in the rapture of the three-dimensional network. Seminal research work commenced by different groups brought about the consensus that the isotropic dissipation of applied stress is the key towards the mechanical compliance of the crystals. In a large variety of systems, the bending ability is due to a) interactions topology acting in the orthogonal directions b) corrugated structures and buffering weak and dispersive interactions and c) structural isotropy. However, most of the observations on mechanically compliant crystalline materials are serendipitous in nature. A more intense research is required to derive a rule of thumb design concepts to develop crystalline materials with mechanical compliances. Diverse structural motifs and synergetic interactions reported in the available literature that governs the mechanical compliances to applied stress in single crystals, untangling and differentiating the precise aspects responsible for mechanical conformity remains a major challenge. In my talk, I will be discussing our efforts in these directions on a few optoelectronically relevant molecular structures and our strategies to fine tune the molecular packing for mechanical conformity.

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IL 11

Thermally activated delayed fluorescence emitter for OLEDs

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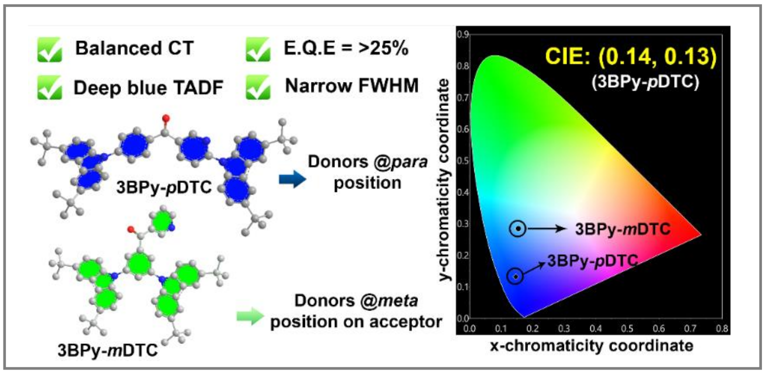

Metal-free organic emitters with thermally activated delayed fluorescence (TADF) characteristics are emerging due to the potential applications in optoelectronic devices, time-resolved luminescence imaging, and solid-phase sensing.[1-3] An efficient blue organic light-emitting diode (OLED) device with high color purity is challenging issue with technological relevance. Herein, we will demonstrate the role of donor substitution position in a thermally activated delayed fluorescence (TADF) emitter to achieve deep blue emission with improved color purity without reducing the device performance. The 3BPy-pDTC emitter exhibits narrow emission spectra with the FWHM of 58 nm. The OLED device using 3BPy-pDTC dopant provided a high EQE of 25% with deep blue emission maximum at 458 nm. 3BPy-pDTC shows color purity in deep blue emission as compared to its meta substituted counterpart 3BPy-mDTC.

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IL 12

Insights into the Role of Structure and Composition of Ion-Solvent Complexes in the Reductive Decomposition of Li-Ion and Post-Li Ion Battery Electrolytes

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Despite their high theoretical capacity, the practical application of metal anode-based batteries is severely impeded by the inherent instability of the organic electrolytes used in these batteries. The high reactivity of organic electrolytes toward metal anodes leads to electrolyte decomposition, anode corrosion, release of flammable gasses, and safety issues due to dendrite formation. [1] In this regard, a stable electrode-electrolyte interface (EEI) is crucial and interface engineering was found to be an excellent approach to improve the electrochemical performance of batteries. Thus, identifying the critical reactivity descriptors that can provide insights into the kinetics of the EEI formation by the decomposition of electrolytes on the electrode surface is of large importance. Herein, we employed quantum chemical computations and ab initio molecular dynamics simulations in conjunction with enhanced sampling techniques to scrutinize the role of the structure and composition of ion-solvent complexes in the reductive decomposition of some of the commonly used electrolytes on the alkali and alkaline earth metal anode surfaces used in Li-ion and post-Li ion batteries. The computations also provide insights into critical chemical reactivity descriptors for predicting the kinetics of these reactions.[2]

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OP 01

Crafting Highly-Porous Hexagonal 3D Carbon Structures for Energy Storage Application

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Keywords: Porous carbon, Hexagonal hierarchical nanostructure, Supercapacitor

Three-dimensional hierarchical hexagonal porous carbon was synthesized from *Ailanthus Triphysa* sawdust for the first time. A two-step carbonization process results in etching of the carbon structure caused by $ZnCl_2$ activation and tailoring pores over the carbon structure caused by gasification. The $ZnCl_2$ acts as an activating agent, a template and a facilitator of the activation process, and its concentration regulates the porosity as well as specific surface area of the carbon nanostructures. There are two distinct types of pores in the prepared carbon i.e.mesopores and micropores. The highest specific surface area of 1757.80 m^2/g was obtained when the ratio of $ZnCl_2$ is four times higher than that of the sample. The highly porous activated carbon exhibits excellent electrochemical storage properties in an aqueous neutral electrolyte of 0.1 M Na_2SO_4. A redox-enhanced electrolyte like 0.1 M Na_2SO_4 with 0.03 M KI combination improvise the specific capacitance and cyclic stability. The specific capacitance of the redox-enhanced electrolyte combination increases to 104 F/g (30.11 mAh/g)at 5 mV/s and cyclic stability of 50000 with a retention of 95% during continuous charge-discharge cycles.

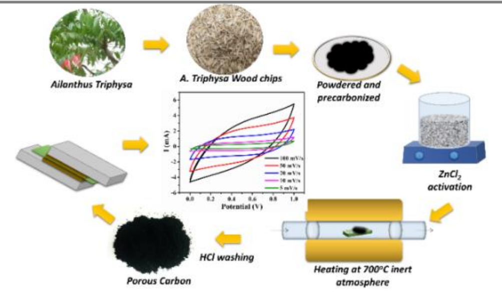

Figure 1: *A schematic representation of highly porous activated carbon from Ailanthus Triphysa.*

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OP 02

Polyaniline-based Biomimetic Self-sensing Supercapacitor

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Keywords: Polyaniline, reactive current sensors, supercapacitor, solid-state device

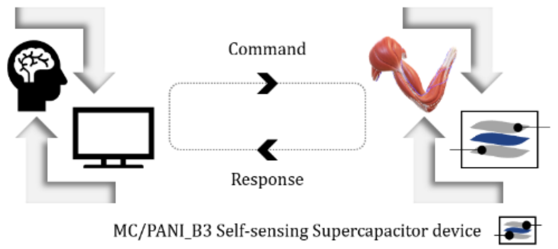

Figure 1: *Illustration of brain/muscles feedback loop juxtaposed with the processing unit and MC/PANI_B3 self-sensing supercapacitor device.*

Conducting polymers, mimicking the electrochemical reactions of biological muscles within their reactive dense gel-like structure, offer a biomimetic platform with self-sensing characteristics in addition to their energy storage capabilities.[1] Harnessing the electrochemistry of methylcellulose-polyaniline (MC/PANI) composites, this research delves into their potential applications as reactive current sensing supercapacitors, with electrical energy as sensing parameter, to fabricate multifunctional devices with single connectivity.[2] The MC/PANI_B3 composite-based symmetric solid-state device was fabricated andrecords cathodic and anodic current sensitivity of 8.77 mJmA^{-1} and -8.86 mJmA^{-1}, respectively. Besides it possesses a specific capacitance of 300 Fg^{-1} with a current density of 0.5Ag^{-1} with cyclic retention of 87.01% over 2000 cycles. With the simultaneous transmission of input and output signals through the same connecting wires, akin to biological muscles, the device juxtaposes the perpetual feedback loop between the brain and biological muscles (Figure 1).

At its core, MC/PANI emulating biological processes offers a transformative blueprint for multifunctional devices. Their inherent reactive properties and unique electrochemical reactions position them as frontrunners in biomimicry, offering a pathway to develop next-generation technologies capable of dynamic sensing and advanced functionalities. Thence, integrating biological inspiration into material science paves a pivotal step toward highly responsive and efficient devices, spanning energy storage to sensor technologies.

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OP 03

Supercapacitive Performance Analysis of Nickel Disulfide Electrode in Li_2SO_4 Electrolyte

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Keywords: Supercapacitor, Nickel Disulfide, Microwave-hydrothermal

The current energy crisis necessitates high-performance electrochemical energy storage devices like supercapacitor to store energy.[1] The specific capacitance of a supercapacitor is mainly coupled with its electrode characteristics hence selection of proper active material to prepare the supercapacitor electrode is mandatory. Among the various available choices such as carbon materials, electronically conducting polymers, transition metal oxides, transition metal dichalcogenides (TMDs), etc., TMDs have received great attention in the recent past. In the family of TMDs, transition metal sulfides are attracted the scientific community due their excellent charge storage characteristics.[2] Herein, we report the facile synthesis of novel hierarchical nickel disulfide (NiS_2) nanosheets via. microwave-assisted hydrothermal approach using nickel chloride and thiourea as precursors. The microwave-assisted hydrothermal approach avoids the demerits underlying with the conventional hydrothermal approach such as long reaction time, non-uniformity, reduced yield, lower crystallinity, etc. The microstructure and surface morphology of NiS_2 nanosheets are examined using scanning electron microscopy and energy dispersive X-ray spectroscopy. The electrochemical performances of the NiS_2 electrode are examined by electrochemical impedance spectroscopy, cyclic voltammetry, and galvanostatic charge-discharge measurement. The electrochemical performances of the electrode were tested in a three-electrode cell configuration using NiS_2/nickel, platinum wire and Ag/AgCl electrode as working, counter, and reference electrodes, respectively, in Li_2SO_4 aqueous electrolyte. The NiS_2 electrode delivered a gravimetric capacitance of 66.11 F/g with a corresponding area specific capacitance of 0.79F/cm^2 at a scan rate of 3mV/s. The present study proclaims the development of novel electrode comprising of layered NiS_2 nanosheets for supercapacitor application.

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OP 04

Investigation on Structural, Morphological, and Electrochemical Performance of La_2FeMnO_6 Double Perovskites

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Keywords: La_2FeMnO_6, Sol-gel method, Electrochemical Performance

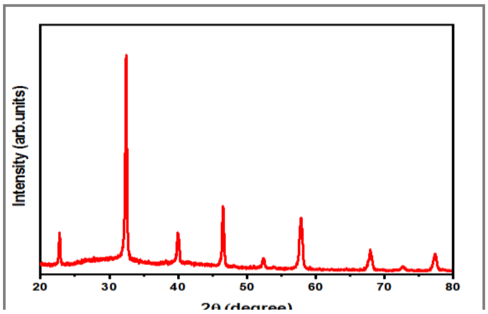

Figure 1: *XRD pattern of La_2FeMnO_6*

The incipiency of urbanization and industrialization has brought several environmental deteriorations like global warming, energy crisis, pollution, etc. This leads to the search for reliable and renewable energy sources that can meet the rise in global energy demand to a great extent.[1] The fabrication of energy storage devices such as supercapacitors, solar cells, rechargeable batteries, fuel cells, etc. can overcome the shortage of natural energy sources and the depletion of fossil fuels. Supercapacitors possess high power densities, fast charge–discharge properties, and long lifetimes and are widely used in electric vehicles, smart grids, portable devices, etc.[2] La_2FeMnO_6 double perovskite was prepared via the sol-gel method. The XRD pattern revealed the cubic structure with a pm-3m space group. The SEM image confirms the formation of randomly distributed quasi-spherical morphology of the perovskite. The electrochemical performance was analyzed using a three-electrode system. The CV curves are highly symmetrical even at higher scan rates with a quasi-rectangular shape. The specific capacitance of La_2FeMnO_6 double perovskite was calculated to be $10.4mFg^{-1}$ at a scan rate of 5mV/s. The GCD profiles were symmetric with approximately isosceles triangular shape which further confirms the EDLC behavior of La_2FeMnO_6 electrode material. The cyclic stability test confirms that 96% of initial specific capacitance was retained even after 5000 cycles which implies that long – term stability and practical use of the prepared sample.

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OP 05

Enhancing Interplanar Spacing in V_2O_3/V_3O_7 Heterostructures to Optimize Cathode Efficiency for Zn-Ion Batteries

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Keywords: Zinc Ion Batteries, Aqueous, Cathode, heterostructures, Vanadium oxide

The development of advanced cathode materials is crucial for enhancing the performance of Zn-ion batteries, which have gained significant attention due to their high energy density and potential for cost-effective energy storage solutions. In this study, we present a novel approach to improve the electrochemical performance of Zn-ion batteries by expanding the interplanar distance of V_2O_3/V_3O_7 heterostructures. V_2O_3/V_3O_7heterostructures were synthesized through a facile hydrothermal method, and their crystal structures were systematically characterized using various analytical techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The XRD analysis revealed the successful formation of V_2O_3/V_3O_7 heterostructures with an expanded interplanar distance attributed to the intercalation of water molecules between the layers. Electrochemical studies were conducted to evaluate the performance of the V_2O_3/V_3O_7 heterostructures as cathode materials for Zn-ion batteries. The expanded interplanar distance facilitates the insertion/extraction of Zn ions, leading to significantly improved electrochemical properties. Specifically, the V_2O_3/V_3O_7 heterostructures exhibited a high specific capacity of 330.9 mAhg^{-1}@ 0.1 A g^{-1}. It also showcased excellent rate capability and coulombic efficiency of 98.6 % and 99.4 % respectively even after 200 cycles.

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OP 06

Unveiling the Potential: Black Zinc Oxide as a Pioneering Material for Supercapacitor Innovation and Electrochemical Investigations

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Keywords: Black zinc oxide, Supercapacitor, electrode, Electrochemical technique

The creation of a cost-effective, high-performance supercapacitor is crucial in light of the current energy crisis. Nanotechnology has become increasingly influential across various fields due to its diverse applications. Among the myriad types of nanoparticles, metal oxide nanoparticles stand out, with ZnO nanoparticles being particularly well-explored. This study concentrates on the hydrothermal synthesis of black zinc oxide (BZO) nanoparticles. The distinctive structural features of BZO, including a high surface area and excellent electrical conductivity, facilitate swift ion diffusion and charge transfer, ultimately boosting the specific capacitance and energy density of supercapacitors. This research lays the groundwork for advanced supercapacitors with improved electrochemical performance, contributing to ongoing initiatives aimed at addressing energy storage challenges in diverse applications.

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OP 07

Unlocking Specific Capacitance of Morphology Controlled MnO_2 and its Functioning in High Energy Asymmetric Supercapacitor

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Keywords: MnO_2, Supercapacitor, High Specific Capacitance, KOH Electrolyte.

Achieving high capacitance is a major step to obtain high energy density for the supercapacitors. In this work, morphology-controlled MnO_2 is synthesized using a simple co-precipitation process and their charge storage characteristics are analyzed in different electrolyte conditions. MnO_2 spheres showed high specific capacitance in alkaline electrolyte which is nearly two-fold higher than the neutral electrolytes. Moreover, the rate capability of the MnO_2 spheres in KOH is highly enhanced when compared with the other tested electrolytes. Further, lab scale MnO_2 || AC asymmetric prototype was fabricated and their electrochemical performances were analyzed. The asymmetric configuration showed excellent cycle life with capacitance retention and round trip efficiency of 70 % and 99% respectively up to 95k cycles which indicates the good practical viability of the tested system in an alkaline electrolyte. Therefore, using an alkaline electrolyte with the pseudo-capacitive MnO_2 electrode will be an effective way to unlock its specific capacitance.

OP 08

Fabrication and Characterization of Lead-Free, Air Stable Cs_2SnI_6 Thin Films

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Keywords: Perovskite, Thermal evaporation, Photovoltaics, Lifetime

The field of perovskite photovoltaics glimpsed a commendable hike in power conversion efficiency from 3.5% to 25.5% in the last decade. Nevertheless, its toxicity and instability put a stop to the commercialization of the perovskite solar cell. This scenario demands the development of air stable, cost-effective and non-toxic perovskites with high power conversion efficiency.[1,2.]

In the present work, Cs_2SnI_6, thin film, a vacancy ordered air stable double perovskite is grown by thermal evaporation method. Both co-evaporation and sequential evaporation of CsI and SnI_2 are attempted to fabricate Cs_2SnI_6 thin film along with additional Sn. The as-deposited film is identified as Black phase γ- $CsSnI_3$, exhibits a phase change and then later changes to Cs_2SnI_6. Also, the as-deposited film is annealed in iodine vapour at 200^0 C for 30 minutes to obtain Cs_2SnI_6. An impurity phase (CsI) is observed in both phase changed and annealed films but the presence of CsI is comparatively lower in annealed film and it shows enhanced stability and better morphology. For attaining the phase pure film, the CsI/SnI_2 compositional ratio of annealed film is varied, and we obtained phase pure film for $CsI/SnI_2 =1$. The phase pure film shows an optimal band gap of 1.5 eV and its morphology and composition were studied using scanning electron microscopy with energy dispersive X-ray analysis. X-ray photoelectron spectroscopy validates the presence of elements and their oxidation states. Depth-wise elemental analysis using XPS confirmed the uniform distribution of both elements and phase in the material. The work function and valence band maximum were determined by the Ultraviolet photoelectron spectroscopy. The time-resolved Photoluminescence measurement revealed the superior lifetime of 9.59 μs for the polycrystalline Cs_2SnI_6 thin films. The phase purity, optimal bandgap, compositional uniformity and exceptional lifetime of the fabricated Cs_2SnI_6 thin film make it an ideal candidate for photovoltaic applications.

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OP 09

Spontaneous Curvature Induction in an Artificial Bilayer Membrane

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Keywords: Self-assembly , Asymmetric membrane , Vesicles , Structural Dynamics

Maintaining lipid asymmetry across membrane leaflets is critical for functions like vesicular traffic and organelle homeostasis.[1,2] However, a lack of molecular-level understanding of the mechanisms underlying membrane fission and fusion processes in synthetic systems precludes their development as artificial analogs. Here, we report asymmetry induction of a bilayer membrane formed by an extended π-conjugated molecule with oxyalkylene side chains bearing terminal tertiary amine moieties (**BA1**) in water. Autogenous protonation of the tertiary amines in the periphery of the bilayer by water induces anisotropic curvature, resulting in membrane fission to form vesicles and can be monitored using time-dependent spectroscopy and microscopy. Interestingly, upon loss of the induced asymmetry by extensive protonation using an organic acid restored bilayer membrane. Our study unveils mechanistic insight into the dynamic transformation of bilayer membranes into vesicles.

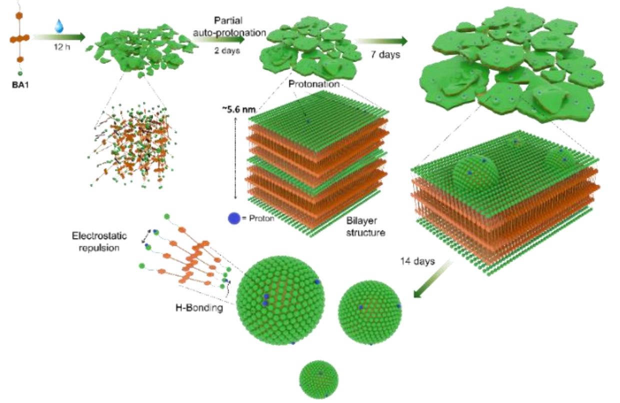

***Figure 1:** The schematic illustration of the spontaneous curvature induction in a self-assembled bilayer membrane.*

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OP 10

The Effect of 3d Atoms in 2D Single Molecule Magnets

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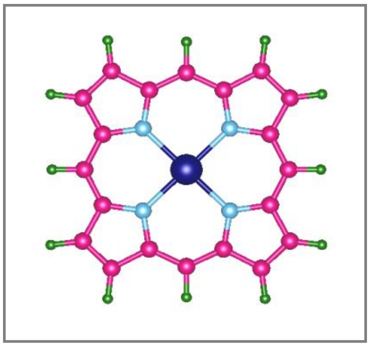
Keywords: Single Molecular Magnets, 3d metalloporphyrin



Two-dimensional organometallic material has picked up steam due to its diverse applications. Metalloporphyrins and their derivatives manifest as promising candidates as Single Molecular Magnets (SMM). The smooth structures and quantum phenomena are fascinating as the aforementioned properties can be enhanced by doping. The SMMs have gained crescent interest for their use in data storage, magnetic switches, spin filters, spintronic devices, and magnetic refrigeration.

The current study involves the tuning of electronic, magnetic[1] and optical properties of 3d Metalloporhyrin. It is possible to tune the properties above by the addition of an electronegative adsorbent to pristine metalloporphyrin. The figure provided includes the D4h metalloporphyrin structure

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OP 11

Self-assembly of some Amphiphilic Azo-Cardanol Compounds: Gelation and Liquid Crystalline Properties

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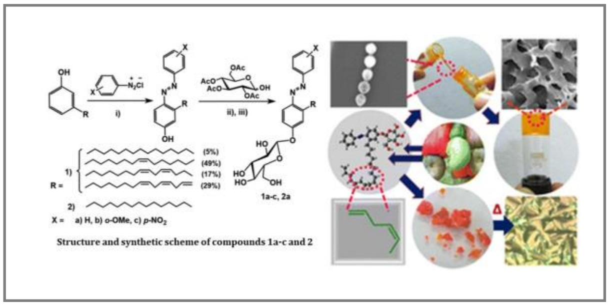
Keywords: Cardanol-azo dyes, Self-assembly, Gels, Liquid Crystals.

We present here the utility and scope of cardanol, a plant-based phenol for the design of functional soft materials with improved properties. The target amphiphilic azo-cardanol compounds (**1a-c** and **2**a) were synthesized and characterized by various spectroscopic methods. The analysis of their self-assembly was fascinating.[1,2] These compounds were found to form various nanostructures in solution, gel, and liquid crystalline phases. Their self-assembly into bicelles and microgel-like structures, as well as thermotropic smectic type liquid crystalline phases, will be discussed based on dynamic light scattering (DLS), scanning electron microscope (SEM), transmission electron microscope (TEM), polarizing optical microscope (POM) and X-ray diffraction studies



Structure and synthetic scheme of compounds 1a-c and 2

A subtle change in the structure of compounds such as substitution on the aromatic ring, and the saturated/unsaturated nature of the alkyl chains were found to have a profound effect on the self-assembly of these cardanol derivatives. The compound **1a** was found to form a viscous and gel phase in solvents under suitable conditions. On the other hand, **2a** with a saturated alkyl chain formed only gels and notably, it did not form a viscous phase in the solvents considered. Based on combined textural, DSC, and XRD analysis, we confirmed the only mesophase seen in **1a, 1b** and **2a** as smectic A phase. The observation that the unsaturated alkyl chain in cardanol induces the formation of micelles and bicelles in solution, gives insights for the development of new cardanol-based functional materials.

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OP12

Electronic Structure and Electric Field Response in Twisted Double Trilayer Graphene: Theory and Experiment

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Keywords: Graphene, band structure, tight-binding model

Twisted Graphene based systems with superlattice electronic bands have recently emerged as a platform for realizing correlated and topological states with a high degree of control and tunability. Extensive studies have been carried out on monolayer graphene and Bernal-stacked bilayer graphene via transport experiments and theoretical calculations. Moire systems with trilayer graphene remain largely elusive. This work reports the discovery and characterization of electronic properties of twisted double ABC-stacked trilayer graphene (TDTG) by transport measurements. We also report theoretical calculations that describe the band structure of TDTG as a function of twist angles and displacement fields using tight binding Hamiltonians. This work demonstrates the existence of an intrinsic bandgap at the charge neutral point in small-angle TDTG. Both experiments and theoretical calculations reveal the tunability of the bandgap by tuning displacement fields and twist angles.

OP 13

Origin of Low Lattice Thermal Conductivity through Micro-Structural Defects in Ni Substituted Bi_2S_3 for Enhanced Thermoelectric Performance.

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Keywords: Dislocations, carrier mobility, phonons scattering and electrical conductivity

Bismuth sulphide (Bi_2S_3) is a V-VI group semiconductor which are a prominent material in mid-temperature (303 K to 623 K) thermoelectric applications. In this work, $Bi_{2-x}Ni_xS_3$ (x = 0, 0.025, 0.05 and 0.075) were prepared by hydrothermal method along with the hot-press technique. Increasing Ni concentration on Bi_2S_3 leads to a high power factor due to the significant enhancement in electrical conductivity. In particular, the x= 0.075 sample reached the maximum electrical conductivity of 9835.98 Sm^{-1} at 623 K, owing to the presence of Ni at the interstitial sites of the Bi_2S_3 lattice, which gives an extra electron, which significantly enhanced the power factor of 170.82 $\mu Wm^{-1}K^{-2}$. Furthermore, the phonon thermal conductivity of the samples decreases with temperature. The x = 0.025 sample exhibited a remarkably low lattice thermal conductivity value of 0.432 $Wm^{-1}K^{-1}$ at 623 K, which primarily due to the enhanced multiple phonon scattering by the presence of various defects. Consequently, the x = 0.025 sample attained a enhanced thermoelectric (zT)value of 0.17 at 623 K *via* the combination of high power factor and low- phonon thermal conductivity.

Reference

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OP 14

Nonlinear Optics in Metal-organic Complex through Hyperpolarizability and Sum Over States Analysis

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Keywords: DFT, HRS, NLO, Hyperpolarizability, SOS

Density functional theory (DFT) simulation was used to conduct quantum mechanical studies on the electronic structure and hyperpolarizabilities of copper-based metal-organic complex. To attain high precision, hybrid functionals were used, such as cam-B3LYP/def-PVTZ/LANL2DZ level of theory. TD-DFT calculations show that the compound exhibits good electronic excitations up to 30 levels, and accounting for high oscillator strength values results in a band gap diagram. Nonlinear optics (NLO) is a discipline that studies nonlinear phenomena under the effect of strong coherent light incident on the nonlinear medium. Polarizabilities are among NLO's key constituents.[1] Both static and dynamic types of Polarizability (α), first hyperpolarizability (β), and second hyperpolarizability (γ) and their vibrational dependent parts were also calculated.[2] Additionally, quantify the Hyper-Rayleigh scattering (HRS) connection; this method measures the molecules' hyperpolarizability. The (hyper)polarizability vs. number of states graph, which looks at the sum over states (SOS) of all excited states (hyper)polarizabilities, shows how consistent the predicted value is. Perform two- and three-level models of (hyper)polarizability using SOS techniques.[3] Additionally, look at the (hyper)polarizability density to ascertain each atom's contribution. Using Multiwfn, plotting the hyperpolarizability density as an isosurface and plane map is comparatively easy. This quantity is very useful when analyzing the nature of the (hyper)polarizability of a particular molecule.

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OP 15

Magnetoresistance and Enhanced Thermoelectric Performances in Ni-Mg Dual Cation Doped $CuCrO_2$ Crystallites

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Keywords: Thermoelectric properties, Magnetoelectric coupling, Magnetoresistance, VSM, Xray diffraction.

Mitigating the decline in performances of thermoelectric materials within the intrinsic excitation region remains a significant hurdle.[1] The magnetic transition from ferromagnetism to paramagnetism offers a viable avenue for addressing this challenge effectively.[2] Here, we synthesized crystallites of Ni-Mg dual-doped $CuCrO_2$ to investigate magnetic phase transitions with the aim of exploring their potential for thermoelectric applications. The introduction of Ni^{2+} resulted in the induction of a ferromagnetic phase, confirmed by VSM investigations, and the non-magnetic Mg^{2+} induced modifications to this ferromagnetic phase by introducing magnetic frustrations. The magnetic transport characteristics were explored through anisotropic magnetoresistance studies unveiling the captivating interaction between the non-magnetic Mg^{2+} insertion and the magnetic phenomena. The analysis of magnetoresistance (MR) studies clarify the notable changes in carrier concentration and mobility as the temperature fluctuates. The magnetic phase transitions were visualized by monitoring the behavior of the Seebeck coefficient with changing temperatures and provided insights into the creation of carrier reservoirs within the ferromagnetic phase and the sudden release of carriers during the paramagnetic phase. The scattering and subsequent effects through magnetic phase transition modulate the thermoelectric (TE) performances. The highest conductivity of 6779 S/m and Seebeck coefficient of 348 μV /K at 700 ∘ C leading to an outstanding power factor of 0.722 mW/mK2. Achieving a remarkable feat, the Ni-Mg dual cation doped CuCrO2 demonstrated an exceptional performance with a thermal conductivity of 2.84 W/mK and the highest ZT value of 0.25 at 700 ∘ C solidifying its uniqueness among Cu-based delafossites.

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OP 16

Thermal Response of Double-Peak Nematicons in a Periodic Potential

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Keywords: Nematic liquid crystals, nematicons, double-peak nematicons, thermal response coefficients, periodic potential

The spatial optical solitary waves in nematic liquid crystals (NLCs) are referred to as nematicons. The nematicons are widely used in all-optical interconnects, readdressable configurations, all-optical steering, and routing devices.[1] The thermal response of nematicons in a periodic potential has been studied numerically by employing the finite difference method. The model equations of the system are given by,

$$2i\frac{\partial X}{\partial z}+\frac{\partial^2 X}{\partial x^2}+\frac{\partial^2 X}{\partial y^2}+Xsin^2\xi+\frac{1}{2}Ye^{\frac{iz}{1+\gamma(\tau)}}sin2\xi+V(x,y)X=-2\mu X,$$

$$2i\gamma(\tau)\frac{\partial Y}{\partial z}+\frac{\partial^2 Y}{\partial x^2}+\gamma(\tau)^2\frac{\partial^2 Y}{\partial y^2}-Ysin^2\xi+\frac{1}{2}Xe^{\frac{-iz}{1+\gamma(\tau)}}sin2\xi-V(x,y)Y=-2\mu\gamma(\tau)Y,$$

$$\nu(\tau)\nabla^2\xi+(|X|^2-|Y|^2)sin2\xi+2Re\left(X\,Y^*e^{\frac{-iz}{1+\gamma(\tau)}}\right)cos2\xi=0,$$

where, $V(x,y)=V_0(cos^2x+cos^2y)$. Since the potential is periodic, the system supports Bloch waves. The thermal response coefficient (τ) is the solution of the heat equation, $\mu_T\nabla^2\tau=-|X|^2-|Y|^2$.

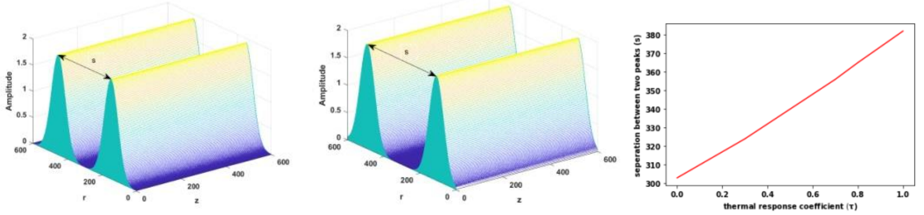

***Figure 1**: Evolution of amplitude for (a) τ=0, (b) τ=1.0. And (c) thermal response coefficient versus seperation between two peaks*

For a certain potential strength of V_0=1.7 and propagation constant of μ=1.9, double-peak nematicons are obtained. The separation between two peaks changes considerably in the presence of thermal response as shown in Fig. 1(a) and 1(b). As the thermal response coefficient increases, the separation between peaks increases linearly as depicted in Fig. 1(c).

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OP 17

Facile Metal Catalyzed Low-Temperature Synthesis of Magnetic N-Doped Carbon Nanotubes (N-CNT)

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Keywords: magnetic N-CNT, CVD, low-temperature route, antibiotic removal

High tensile strength, π-conjugated graphitic structure, high surface area, exceptional chemical and thermal stability, etc. make carbon nanotubes (CNT) ideal for a range of applications, including biomedical fields, environmental remediation, energy storage, hydrogen storage,biosensors, etc.[1,2] Typically, arc discharge, laser ablation, and chemical vapour deposition (CVD) methods are used to prepare CNT. CVD produces CNT with a higher yield and purity and uses transition metals catalyzed pyrolysis of hydrocarbons in the presence of an inert atmosphere at high temperatures (650–1000°C). Here we present a facile comparatively low-temperature route for the preparation of magnetic nitrogen-doped carbon nanotube (N-CNT) catalyzed by a transition metal without the use of inert gases. A thorough analysis was conducted on the morphology, structure, and properties of magnetic N-CNT, and its use in antibiotic removal has been investigated. The impact of various reaction parameters, kinetics, adsorption isotherms, and recyclability were carefully investigated. The magnetic N-CNT exhibited increased activity in antibiotic adsorption when compared to the bare materials prepared, primarily as a result of the π-π interaction with the N-CNT's graphitic planes. At room temperature, the magnetic N-CNT demonstrated 86% antibiotic removal in a short duration. Adsorption experiments followed pseudo-second-order kinetics and the Freundlich isotherm. The separation of magnetic N-CNT after antibiotic adsorption is represented in Figure 1.

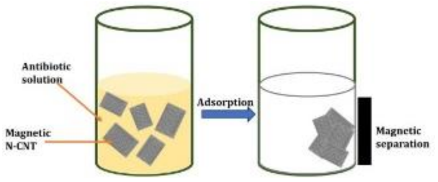

Figure 1: *Pictorial representation of the separation of magnetic N-CNT after antibiotic adsorption.*

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OP 18

Enhanced Antibacterial Activity of Gd Doped ZnO Nanoparticles Synthesised by Coprecipitation Method

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Keywords: Rare earth elements, Coprecipitation, ZnO, Antibacterial activity

Rare earth doped metal oxide nanoparticles have recently gained much attention in biomedicine for noninvasive biological applications due to their unique optical properties. In the present study antibacterial activity of pure ZnO and Gd doped ZnO nanoparticles was comapred. Pure ZnO and Gd doped ZnO were synthesized by coprecipitation method using zinc nitrate hexahydrate and gadolinium nitrate hexahydrate as precursor materials.[1] The structural, compositional and morphological characterization was done by XRD, Raman spectroscopy, EDAX and SEM. XRD analysis revealed the hexagonal wurtzite structure of the nanoparticles. The XRD peaks were shifted with Gd doping.[2] EDAX analysis confirmed the presence of Gd^{3+} in the ZnO lattice.[2] Antibacterial activity of pure ZnO and Gd doped ZnO nanoparticles was evaluated against Gram positive and Gram negative bacterial pathogens, *Staphylococcus aureus, Escherichia coli, Klebsiella sp, and Pseudomonas sp* according to guideline set by Clinical Laboratory Standards Institute using disc diffusion method.[3] The present study showed that Gd doped ZnO nanoparticles has efficient antimicrobial potential than pure ZnO nanoparticles against both Gram postive and Gram negative pathogens. So rare earth doped metal oxide naoparticles could be more efficient in antibiotic treatment.

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OP 19

Synthesis and Characterization of Pure ZnO Nanoparticles and 2D: ZnO Nanocomposites & Comparative Analysis of their Properties

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Keywords: Graphite, $Ti_3C_2T_x$ MXene, Zinc oxide, Morphology, Gas Sensing

This work is focused on the synthesis of ZnO nanoparticles and 2D: ZnO nanocomposites followed by the characterization of the samples for their comparative analysis. Graphite and multi-layered $Ti_3C_2T_x$ MXene are the two 2D materials considered in this work. The primary aim of the work is to identify the effect of morphology on gas sensing properties of the samples. The second aspect of the work focuses on identifying the best composition of 2D materials to be integrated with ZnO nanoparticles to obtain the best results. This element of the work has been proceeded by comparing two different compositions, specifically, 5% and 10% of 2D materials. The structural, functional, optical, morphological, and elemental properties of the samples have been studied. ZnO is synthesized using the chemical coprecipitation technique and the solvothermal method is followed for the preparation of 2D: ZnO nanocomposite. Among its numerous applications zinc oxide is noted for its gas-sensing properties because of its highly crystalline framework and large surface area. However, the requirement for high operating temperatures and easy agglomeration are two of its major drawbacks.[1] 2D-based nanocomposites have the potential for diverse applications due to their large surface area and tunable properties. 2D materials called MXenes ($Ti_3C_2T_x$) have recently gained significant attention as gas sensors because of their metallic conductivity and outstanding stability.[2] Thus, integrating the unique advantages of 2D materials and ZnO provides a nanocomposite with synergistic effects having enhanced gas-sensing properties. After CNTs (Carbon Nanotubes), Graphene and its derivatives have been studied recently for improving the gas sensing application.[3,4] Still, no studies on MXene-zinc oxide nanocomposites and their compositional variation have been done so far, regardless of their exceptional properties. The prepared multi-layered $Ti_3C_2T_x$ MXene-ZnO nanocomposite shows many improved characteristics. Moreover, in the current scenario, studying gas sensing properties is crucial for detecting and controlling the rising levels of toxic gases in the atmosphere, food, and water.

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OP 20

Luminescent Metal Organic Framework Based Sensor for Selected Pharmaceutically Active Compounds

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Keywords: Metal-organic supramolecular framework, Luminescent sensor, Antibiotic detection, Quenching, Tetracycline

Pharmaceutically active compounds, unlike other emerging contaminants, persist in their bioactive form, raising greater concerns. Hence, detecting trace levels of these contaminants in the environment has become a growing concern. Various pharmaceutical agents, such as antibiotics, analgesics, beta-blockers, antidepressants, non-steroidal anti-inflammatory drugs (NSAIDs), analgesics, and estrogens, have been detected in water samples within a range of ng/L to μg/L. While chromatographic techniques are crucial for identifying and quantifying these contaminants, practical applications demand less complexity. There is a growing need for sensing techniques with high sensitivity and selectivity. The development of Metal–Organic Frameworks (MOFs) as a sensing platform appears promising for studying environmental contaminants.[1] Their properties include high surface area, tunable pore size, a high density of active sites, and significant catalytic activity. Here, Copper (I) Iodide and mercaptobenzothiazone (MBT) based MOF, termed CuI-MOF in solution state is proposed as a selective sensor platform for specific antibiotics.[2] It was synthesized using a modified solvothermal method. The structure of CuI-MOF was determined via powder X-ray diffraction and solid-state NMR, revealing a distinct chair-like configuration. Theoretical calculations suggested that the fluorescent emission of CuI-MOF originates from the charge transition between the [Cu_4I_4] core and the MBT ligand. CuI-MOF demonstrated remarkable sensitivity as a luminescent sensor for detecting tetracycline hydrochloride (TCH) in aqueous solutions as well on immobilized CuI-MOF on solid support using polyion mediated LBL technique. Impressively, it exhibited a higher efficiency in quenching TCH compared to other antibiotics, while retaining its sensing capabilities. This investigation underscores the importance of molecular copper(I) iodine materials in the surveillance of water quality, marking a significant advancement in the identification and analysis of environmental contaminants.

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OP 21

Rapid and Sensitive Surface Enhanced Raman Spectroscopy Detection of Melamine using Silver Nanoparticles Anchored Hexagonal-Boron Nitride Nanofibers

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Keywords: Melamine, SERS, Hexagonal Boron Nitride, Label-free detection

Melamine is a nitrogen-rich chemical compound that is sometimes illegally added to food products, including milk, to increase the apparent protein content. While melamine itself is not inherently harmful, its presence in food, especially in high levels (above 2.5 ppm (19.8 μM) for non-infant products and 1 ppm (7.9 μM) for infant) milk products, can lead to serious health issues including kidney disease and even to death in babies.[1] Currently, various methods have been developed to detect adulterant melamine in assorted food samples, but all these require hectic sample preparation, extensive solvent consumption, complicated operation procedure and long analysis time. Therefore, it is of particular importance to develop simple, rapid, cost-effective, and sensitive methods for detection of melamine in food.[2] Surface-Enhanced Raman scattering (SERS) is a powerful technique for rapid, accurate, non-destructive, and label-free detection which offers notable advantages in trace and ultra-trace detection.[3] Herein, silver nanoparticles anchored electrospun hexagonal boron nitride were developed as substrate to construct a novel SERS sensor for the sensitive detection of melamine in food samples. The electron h-BN fibres with a high surface area to volume ratio facilitates the deposition of Ag nanoparticles providing the abundant hot spots for the electromagnetic enhancement and the suitable charge transfer path to induce the chemical enhancement[4].The sensing material was characterized structurally and morphologically using XRD, SEM and TEM analysis. Finally, the developed sensing material was used to detect melamine at various concentrations within the permitted range from 5 uM to 250 uM, demonstrating the possibility of the developed substrate to detect melamine at trace-level concentrations down to 5 uM. Hence, this study offers a new approach for the rapid and sensitive detection of adulterant melamine in milk samples.

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OP 22

Silver Supported Multi-walled Carbon Nanotubes based SERS Substrates for the Detection of Sulfate Ions in Water Residues

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Keywords: Sulfate Ion, SERS substrate, Muli-walled Carbon nanotube

Sulfates are (SO_4^{2-}) a family of chemicals that contain the fully oxidized ionic form of sulfur, in combination with metal and/or hydrogen ions. The increasing concentration of sulfate will cause several diseases, e.g., Diarrhea, Dehydration, and gastrointestinal disorders, etc..[1] Analytical methodologies for SO_4^{2-} detection have been developed for many years. Spectrophotometric, and potentiometric readouts stand out for the specific application of water analysis among the available techniques. Previous detection methods are time consuming and cost effective.[2] Therefore, the development of accurate analytical methods for identifying and detecting contaminants in water analysis is greatly demanded. In this scenario, Surface Enhanced Raman Spectroscopy (SERS) offers fast, sensitive, and high-throughput analysis of water contaminants.[3] A rapid, label-free, accurate sensor that is suitable for the assessment of water quality is greatly demanded. Herein, we report the synthesis, characterization and evaluation of the SERS sensor properties of Ag supported multi-walled carbon nanotubes (MWCNT)-based SERS substrates for the detection of sulfate ions in water residues. Structural and morphological analysis have been carried out using X-ray diffraction (XRD), Raman spectroscopy and Scanning Electron Microscope (SEM) etc. This investigation can pave the way to novel strategies for designing and fabricating low-cost, high-performance SERS substrates for real time applications.

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OP 23

Synthesis, Characterization, and Metal Ion Recognition Properties of A Triazole Linked Schiff Base Derivative of Pillar[5]Arene

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Keyword: Pillar[n]arenes, host-guest chemistry, supramolecules, triazole, metal ions, halogens

Metal ions play vital roles in various biological and physiological processes, hence they are closely related to our day-to-day life. Its deficiency and overload are detrimental to human life. Therefore, it is essential to develop appropriate techniques for the detection of metal ions with the highest selectivity and lowest detection limit. Though there are several synthetic receptors known in the literature for the selective detection of ions and molecules, the receptors based on supramolecular systems have several advantages due to their unique characteristics. Among various supramolecular systems, pillar[n]arenes have shown excellent binding affinity towards various guest molecules.
A Schiff base containing naphthylimine connected to the pillar[5]arene platform through a triazole liner, (1) has been synthesized and characterized by spectroscopic methods such as ^{1}H and ^{13}C NMR and ESI MS. It has been found that pillar[5]arene derivative, 1 is selective towards Fe^{3+} among thirteen metal ions studied by visual color changes while it is selective towards Cu^{2+} and Fe^{3+} by UV-Visible spectroscopy. Further, the sensor molecule 1 is found to be selective for Al^{3+} by fluorescence *turn-on* mechanism while the Al^{3+} complex of 1 exhibits selectivity towards F^- among halogens.

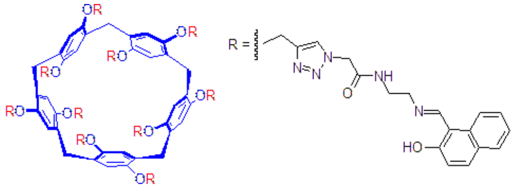

***Figure 1**: Structure of pillar[5]arene based Schiff Base* [1]

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OP 24

Luminescence Enhancement and Stark Splitting Studies on Li Co Doped $Gd_2O_3:Eu^{3+}$ Micro Phosphors

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Keywords: Phosphorescence, Rare earth Oxides, XPS,XRD, Photoluminescence

Various concentrations of Lithium-Europium doped Gadolinium Oxide powders are synthesized by a high-temperature solid-state solutions method. X-ray diffraction pattern of the compounds revealed single-phase crystal formation, matching with the predominant monoclinic phase of Gd_2O_3. The core level electron emission spectra revealed the formation of highly valence-stable compound systems with shell structures corresponding to Li^+, Eu^{3+} and Gd^{3+} electronic states. In-depth analysis of photoluminescence spectra with multiple emissions in the yellow–red region corresponding to transitions of $^5D_0$ – $^7F_2$, $^5D_0$ – $^7F_1$, and $^5D_0$ – $^7F_0$ which arise due to europium and Lithium brought out respective components corresponding to polarisation anisotropy.

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OP 25

Arsenic Detection Unveiling the Potential of Potentiometric Sensors

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Keywords: Sodiumarsenite, Potentiometric sensor, Ion imprinted polymer, Precipitation polymerisation.

Long-term exposure to low levels of arsenic in drinking water causes human health problems, including cancer, heart disease, and nerve effects. Arsenic poisoning in ground water happens by means of human activities such as mining, burning of fossil fuels, industrial waste disposal, and agricultural practices using arsenic-containing fungicides, insecticides, and herbicides. Different analytical methods, such as inductively coupled plasma[1], atomic absorption spectroscopy[2], stripping voltammetry[3], neutron activation analysis[4], and polarographic techniques[5], have been used for arsenic determination in different samples. But the above methods are inconvenient for routine analysis. Potentiometric sensors have attracted great interest because they are simple and economically viable when compared to other electrochemical sensors. Here, a novel potentiometric sensor for the trace level detection of arsenic (III) in ground water using an ion-imprinted polymer (IIP) was developed. The developed sensor exhibits a Nernstian response in a concentration range of 1×10^{-9} M to 1×10^{-2} M with a slope of -17.7 mV and a limit of detection of 1×10^{-10}M. The characterization of the IIP was done using FESEM and EDX. The developed sensor is highly sensitive and selective for the As(III) ion.

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OP 26

Controlled Synthesis and Engineering of One-dimensional Titanium Dioxide Nanofiber for Water Purification

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Keywords: Electrospinning, TiO_2 nanofibers, Phase transition, Defect states, Water treatment.

Over few decades, the environmental degradation specifically, air and water pollution have emerged as the primary worry impacting human society evolution. To overcome this, various semiconductor nanomaterial with different morphology has been reported focusing to develop a cleaner environment. In this context, the generation of one-dimensional (1D) nanofibers with interconnecting network of semiconductor and polymer has been developed and got attention with intense area of research. For this, electrospinning technique being an all-round and feasible for the fabrication of self-standing 1D nanofibers with mass production. It involves an electrohydrodynamic process, where the charged polymer melt elongates and ejects out to form thin long fibers when an electric field is applied along with the control of other electrospinning, solution and ambient parameters. A well optimized nanofibers attains extraordinary properties such as high aspect-ratio, low density, high pore volume and more importantly shorten the charge transport resistance and allow electrons to travel longitudinally through the 1D path.[1] This makes highly attractive to explore titanium dioxide (TiO_2) nanofibers towards water treatment. Based on these properties we have investigated the influence of the crystal structure and band position engineering of mixed-phase TiO_2 nanofibers and defects induced due to the surface electric dipole layer plays a vital role towards the increment activity of dye degradation.[2] We have studied in detail the effect of ratio of sacrificial polymer PVP with titanium precursor on annealing. It clearly demonstrates how the titania phase transformation from anatase to rutile can be adjusted, not only by varying the temperature but also by changing the ratio between titanium salt and sacrificial PVP during electrospun synthesis which enhance the charge carrier dynamics and increase the performance of the catalyst.[3]

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OP 27

Harmonizing Adsorption, Kinetics, and Ultrasound-aided Sonocatalysis for the Removal of Congo Red from Aqueous Solution Using CuS Nanoflakes

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Keywords: Adsorption, ultrasound, sonocatalysis and congored

This study investigates removing and degrading Congo Red (CR) dye from water using CuS as an adsorbent and catalyst. In contrast to adsorption, where dyes are trapped on the surface of adsorbent materials, sonocatalysis for dye degradation utilizes ultrasound and the adsorbent(catalyst) to break down dye molecules into less harmful substances like CO_2 and H_2O. CuS exhibits these dual capabilities as an effective adsorbent and a catalyst, making it well-suited for adsorbing and degrading Congo Red in waste water under ultrasonic radiation. In this study, high-purity CuS nanoflakes have been successfully synthesized at room temperature via a quick, simple, and efficient grinding approach. The X-ray diffraction (XRD) patterns and Raman spectra indicated that the as-prepared CuS was of high purity, and scanning electron microscope (SEM) images showed the flakes-like nanostructure. A batch adsorption experiment was performed to investigate the effects of dye concentration, quantity of adsorbent, reaction duration, temperature, and ion strength on Congo Red (CR) dye removal performance. The results of modelling studies proved that Langmuir isotherms and pseudo-second-order kinetics best represented the isotherm data and adsorption kinetics. The maximum adsorption capacity was identified as 248 mg/g. Adsorption studies yielded valuable data to optimize the adsorption process and guide the design of water treatment systems aimed at removing dye pollutants from wastewater. Efficient degradation of adsorbed dye molecules occurs through the irradiation of ultrasonic sound in the aqueous solution. The hydroxyl radicals and superoxide radicals generated sonochemically play a crucial role in decomposing dye molecules into CO_2, H_2O, and other minerals. A significant reduction (~99%) in the concentration of CR dye was achieved after extended irradiation (~90 minutes at 20 kHz) of ultrasound.The mechanisms leading to the degradation of CR under sonocatalytic irradiation conditions and the effect of various factors, such as the ultrasound frequency and reaction pH, have been explained in detail. The valuable mechanistic aspects obtained from studies are essential for adequately implementing sonochemical techniques into actual water purification processes and, thus, receive extreme environmental relevance.

OP 28

Effect on the Orientation Angle of TiO_2 with Tin Porphyrins Containing One and Many Anchoring Groups in MCSS for Water Splitting

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Keywords: Artificial Photosynthesis, Surface Interface Spectroscopy, Water Splitting, MCSS

Molecular Catalyst Senzitised systems (MCSS) are one of the interesting candidates to use as photocatalysts for the overall water splitting using the visible region of solar radiation. The physical and chemical properties at the interface microenvironment influence the electron transfer and water activation process in MCSS.[1] To explore the effect on orientation angle by the number of anchoring groups on the tin porphyrins (Sn-Por), we have synthesized and studied two tin porphyrins: one with four carboxylic anchoring groups and the second one with one carboxylic anchoring group. The axial ligand microenvironment of the two molecules was studied by spectrophotometric titration, and the pKa values show that the active form of the catalyst exists under neutral and mildly acidic conditions.[2] The orientation angle of the Sn-Por was studied by surface interface spectroscopy (SIS) using a very fine layer (less than 10 layers) of TiO_2 over a waveguide glass. The absorbance ratio for the P-polarised light to S-polarised light was higher for the adsorption through one anchoring group compared with four anchoring groups, indicating a higher orientation angle for the former(Figure 1).

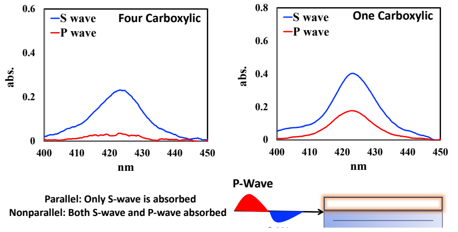

Figure 1: *SIS of MCSS Flims Exposed to MeCN/*H_2O*(8/2, v/v)*

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OP 29

Platinum-Grafted Twenty-Five Atom Gold Nanoclusters for Robust Hydrogen Evolution

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Keywords: Precision nanoclusters, hydrogen evolution reaction, catalysis, electrochemical activation, supramolecular assembly

Atomically precise noble metal nanoclusters (NCs) enhance electrocatalytic activity, crucial for surface-sensitive reactions.[1] Gold NCs despite poor electrocatalytic performance for HER, show improved reactivity with hetero-atom doping.[2,3] Advances in electrocatalytic water-splitting applications are promising, but thiolate ligands' strong adsorption can impede active sites, requiring careful adjustment for optimal performance without aggregation and coalescence. Electrochemical activation of $Au_{25}(PET)_{18}]^-$ NCs, involving partial removal of thiols without affecting the metallic core, exposes Au-sites adsorbed with hydrogen, facilitating electroless grafting of platinum (Fig. 1a). The exposed Au-sites feature the (111)-facet of the fcc-Au_{25} NCs as assessed by Pb-UPD (Fig. 1b). The platinum-grafted NCs outperformed with a lower overpotential of 0.117 V_{RHE} compared to electrochemically activated NC (0.353 V_{RHE}) at 10 mA cm^{-2} and is comparable with commercial Pt/C (Fig. 1c). Due to the possible metallophilic interactions, the modified NCs show unique supramolecular self-assembly characteristics as observed in electron microscopy and tomography. [1].

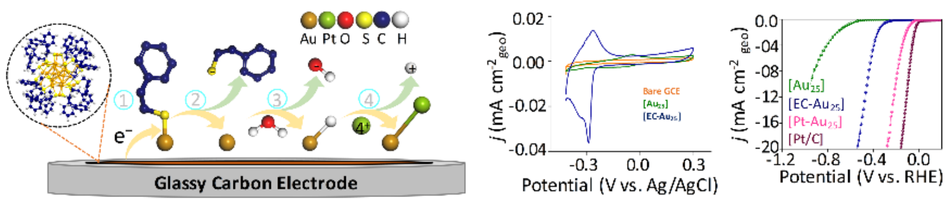

Figure 1: *(a) Scheme of electrochemical activation and subsequent Pt-grafting. (b) CV of Pb-UPD at 20 mV s−1. (c) HER polarization curves in 0.1 M H2SO4 at 5 mV s⁻*

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OP 30

A Novel TPA-Based Dendritic Organic D–Π–A Dye for High Performing Indoor Photovoltaic DSSC.

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Keywords: Dye sensitized solar cells,Indoor light,triphenylamine dyes

The development of metal-free organic dyes for DSSC applications led to the emergence of a new class of dyes. Most organic dyes are based on the structural framework of donor–π–acceptor (D–π–A) design. Due to its push-pull structure, charge transfer occurs within the molecule when dye absorbs light. The transmission of charges is crucial for light harvesting. Among the metal-free organic dyes, the triphenylamine dyes, holding the record for validated efficiency of over 15.2%, are excellent candidates for highly efficient DSCs . Triphenylamine is an excellent donor moiety used in DSCs. The triphenylamine unit was originally utilized as an electron donor in organic dyes by Yanagida and coworkers.[1]Numerous dendritic TPA derivatives with various π-bridges, including vinyl, ethynyl, aryl, and heteroaryl, have been created and investigated as DSSC dyes.[2] In 2016, Vinayak *et al* reported three novel D-π-A type dyes TPAA1, TPAA2, and TPAA3. Here in we report a novel dendritic triphenylamine dye RJ-C6 which act as an excellent co-sensitizer and gave best indoor efficiency when compared with the established dye XY1b.

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OP 31

Synthesis of Efficient Bi-anchoring Phenothiazine Derivatives for Dye-Sensitized Solar Cells

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Keywords: Phenothiazine, Photosensitizer, Light harvesting properties

It is an enormous challenge for scientists to discover new energy sources to meet the expanding demands of human society. Scientists are striving to create new renewable energy sources as the world's conventional energy sources become more scarce due to the growing energy needs of the world's population. Solar cells and other photovoltaic devices are the result of research in this field. On Earth, solar energy is a copious and easily accessible energy source. Without affecting the environment, photovoltaic devices directly convert solar radiation into electricity. Despite their great efficiency, inorganic solar cells are difficult to produce due to high manufacturing costs. Lately, there has been an increase in the importance of researching new effective sensitizers, particularly cheap pure organic dyes that are free of metals. Due to its affordability and transparency, dye-sensitized solar cells (DSSCs) are an alternative to traditional silicon-based solar cells.[1] The most important factors for DSSC commercialization are enhanced photovoltaic performance, long-term stability, and affordable, ecologically friendly materials. The donor-π-acceptor configuration is the most commonly recognized structure for photosensitizers. Numerous dyes with multiple anchoring moieties have been reported in recent scientific literature. Organic sensitizers that double anchor have a number of advantages over those with a single anchor, such as (i) a bathochromic shift in the absorption spectra; (ii) strong binding to the semiconductor; (iii) maximum stability; and (iv) an increased number of injected protons.[2] Double anchoring compounds are needed to refine the architecture and create more potent DSSCs. These compounds show increased light-harvesting properties and are more stable compared to their single counterparts.[3] In this work, we focused on the synthesis of phenothiazine-basedbi-anchoring organic dyes with π-spacer and acceptorfor efficient DSSC application.

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OP 32

Thermoresponsive Metal-Organic Hybrid for Multistate Logic Gate and Smart Window Applications

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Keywords: Metal-Organic hybrids, logic gates, Smart windows

The metal complexes that perform memory operations and molecular logic-enabled systems responding to temperature constitute a fascinating research topic as temperature is not a precision stimulus.[1] There are thermochromic systems that perform bistable or non-volatile memory operations which require reversibility in thermochromic behaviour and the readout to remain constant upon application of constant temperature.[2] In this work, we have used simple metal bipyridine complexes that are thermochromic in nature to demonstrate multi-state volatile memory and arithmetic operations. With the aid of temperature-dependent optical spectroscopy, we demonstrated the reversible thermochromic effects to result in cross-coupled NOR gate-based logic gates, counters and colour/opacity variable dynamic window prototypes. Interestingly, this simple metal bipyridine combination and Cetyl trimethyl ammonium bromide (CTAB) allow us to fabricate smart window prototypes that show color-to-color and color-to-colorless transitions.[3]

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PP01

Scalable Preparation of High-Quality Graphene for Binder-Free Flexible Supercapacitors

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Keywords: Less-defective graphene, green method, large-scale production, flexible supercapacitor

Scalable and ecologically friendly methods for graphene production are becoming a major requisite in this modern scarcity to explore the practical applicability of graphene-based materials[1,2]. We present a green approach for the large-scale production of less-defective graphenewhere graphite exfoliation is attained via polymer-assisted mechanochemical treatment. The well-exfoliated graphene sheets and their less-defective nature along with the functionalization at the edges are demonstrated from various characterization techniques such as HRTEM analysis, Raman spectroscopy, FTIR spectroscopy, XRD, and XPS analyses[3,4]. The high specific capacitance and improved cycle life in a three-electrode configuration indicate the superiority of graphene as a supercapacitor electrode material. The electrodes show remarkable energy storage capabilities derived from the EDLC contribution of graphene as well as the pseudocapacitance resulting from the oxygen functionalities at the edges. A flexible symmetric supercapacitor is constructed out of the less-defective graphene using a gel electrolyte that ensures quick ion transport to the electrodes. The flexible device showed excellent supercapacitor performance and maintained the electrochemical properties at different bending states. The real-time analysis of the supercapacitor device is, assessed by connecting five devices in series to light an LED, which further suggests the potential of the prepared less-defective graphene in future flexible electronics.

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PP 02

Metal Hydroxide Based High-Energy Aqueous Supercapacitor

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Keywords: β-$Ni(OH)_2$, Tungsten Carbide, Composite Electrode, Hybrid Capacitor, High Energy Density

In the present work, Ni $(OH)_2$ and metal carbide composites are prepared and used as positive electrodes in aqueous supercapacitor applications. The materials' phase structure and elemental composition have been analyzed using XR and EDS. The electrochemical characterizations such as CV, GCD, and EIS of the samples have been recorded in a KOH electrolyte medium. The prepared compositeas a positive electrode in a capacitor delivered much-improved cell performance than the bare metal hydroxide, where activated carbon is used as the negative electrode. The capacitor device delivered a maximum specific energy of ~Wh kg^{-1} at ~0.3 Ag^{-1} in a KOH electrolyte. Further, the practical feasibility of the as-prepared composite materials was explicated by fabricating a flexible pouch-type supercapacitor using PVA-KOH hydrogel, and their characteristic performance was analyzed. Thus, the present metal hydroxide and metal carbide composite highly improved the cell performance. Hence, the proposed composite is believed to be a potential candidate for high-energy supercapacitor application as the positive electrode.

PP 03

Less-Defective Graphene as Electrode Material for Flexible All-Solid-State Supercapacitors

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Keywords: Electrode, Graphene, Supercapacitor

Graphene has emerged as a widely utilized electrode material for supercapacitors, owing to its remarkable properties such as high electrical conductivity and large surface area.[1, 2] In this study, an innovative mechanochemical, low-cost exfoliation method is employed to synthesize less-defective graphene in large-scale. This novel approach ensures that the graphene network maintains high conductivity without introducing undesirable functionalities or defects. The structural and morphological characteristics of the graphene sheets are investigated using various characterization techniques, including X-ray diffraction, Raman spectroscopy, scanning electron microscopy, and high resolution transmission electron microscopy, revealing the successful formation of less-defective graphene. Then, these graphene sheets are employed as electrode material in supercapacitor. A flexible all-solid-state supercapacitor suitable for wearable applications is fabricated, and its performance is assessed using various electrochemical techniques such as cyclic voltammetry and galvanostatic charge-discharge measurements. The stability of the device is also scrutinized by conducting cyclic voltammetry for 1200 cycles. The device retained 97% of its initial capacitance after 1200 cycles. The results demonstrate the suitability of this graphene material for high-performance energy storage devices, emphasizing its potential for advanced applications in the field.

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PP 04

Electrochemical Investigations on Ionic Liquid for Energy Storage Applications

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Keywords: EDLC, supercapacitor, ionic liquid

Electrical double layer supercapacitors (EDLC) have been pioneered as energy storage devices in the renewable energy market owing to their superior power density, cycle durability, and shelf life.[1,2] Supercapacitor with aqueous electrolytes exhibits superior power density at lower energy density, whereas supercapacitor with nonaqueous electrolytes exhibits superior energy density due to the large voltage window of nonaqueous electrolytes. Thus, the choice of a nonaqueous electrolyte solution is of technical importance in the development of high- performance supercapacitor. In this work the electrode electrolyte interaction with both conventional and ionic liquid were studied by cyclic voltammetry (CV). Here the combination of conventional and selected ionic liquid electrolyte exhibit high electrochemical voltage window which can be effectively implemented for supercapacitor application. A maximum specific capacitance of 31.1 F/g is attained for KOH + IL electrolyte with voltage window of 2V.

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PP 05

Cobalt Doped Tin Oxide Nanoparticles an Effective Catalystfor H_2 Evolution Reaction

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Keywords: Doping,Electrochemistry, Water splitting, H_2 production

Electrolytic water splitting, an attractive strategy to achieve clean and sustainable H2 fuel, has received increasing worldwide concern with the ongoing energy crisis and climate change.[1] In recent years, clean hydrogen production as a promising new energy has attracted the large amount of research. Water splitting can convert and store electrical energy into chemical energy such as H_2 and O_2 through the two key electrochemical processes: the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) taking place in the cathode and anode, respectively.[2] In this work, we report a co-precipitation method to synthesize Co doped SnO_2 nanoparticlesas electrode materials with excellent the electrocatalytic properties for water splitting are discussed in detail. This work is relevant since the real synergistic effect in these hetero-structured catalysts is not yet fully understood and should be explored.Co-precipitation derived cobait doped SnO_2 electrocatalyst has persuaded unparalleled synergistic effect in the field of bi-functional electrocatalyst due to its multiple active sites assisting OER and HER. The slope was determined to be 142 mV.dec^{-1}, 169 mV.dec^{-1}, 113 mV.dec^{-1}, and 132 mV.dec^{-1} for $Sn_{(1-x)}Co_xO(x = 0, 0.03, 0.05, 0.07)$ electrocatalysts, respectively. The more favourable reaction kinetics for HER are indicated by the lower Tafel slope. It can be seen that the HER on the 5% Co-doped SnO_2 catalyst followed the Volmer-Heyrovsky pathway[3] because the electrocatalyst's Tafel slope (113 mV.dec^{-1}) is almost 120 mV.dec^{-1}. Therefore, metal doping into transition metal-based phosphides may be a promising strategy for the remarkable bifunctional electrocatalyst for water splitting.

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PP 06

Visible light driven Water Activation Sensitized by Vanadium based Molecular Photoanodes

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Keywords: Artificial photosynthesis, molecular catalyst, porphyrin

The environmental impact and climate change implications associated with fossil fuels highlight the necessity of shifting towards sustainable alternatives. One of the most promising areas of research in sustainable energy is photoelectrochemical water splitting, wherein solar energy is converted to storable chemical fuels. Bio-inspired molecular catalysts for visible light driven water activation serves a central role in the field of artificial photosynthesis. Herein, we have synthesized and characterized vanadium (IV)-incorporated porphyrin molecules having neutral, cationic and anionic ligands (VTPyP, VTMPyP, and VTCPP). Electrochemical benchmarking of the synthesized V(IV) porphyrins exhibited catalytic current in the presence of water. In the absence of water, V(IV)TMPyP in acetonitrile showed one-electron redox wave due to porphyrin ring ($E_{1/2}$ = 1.7 V vs. SHE). However, V(IV)TMPyP exhibited a large irreversible catalytic cyclic voltammogram in aqueous conditions (1.3 mA.cm^{-2} at 1.4 V vs. SHE at pH = 12.4) which indicates water molecules surely activated on the oxidized V(IV) porphyrin species. Subsequently, sensitization of SnO_2 or TiO_2 nanoparticle decorated FTO electrodes were performed using neutral V(IV)TPyP through axial ligand and anionic V(IV)TCPP using the carboxylate side chain. The photoelectrodes were characterized using spectrophotometric and fluorescence analysis. The photoelectrochemical response of V(IV)Porphyrin/Semiconductor photoanodes were tested under different conditions. The effect of visible light on *I-V* plot of V(IV)Porphyrin/SnO_2 in the presence of iodide ion as the sacrificial electron donor exhibited a photocurrent of 1.4 mA.cm^{-2} and utilization of water as the electron donor in the neutral condition exhibited a photocurrent of 0.16 mA.cm^{-2} at 0.0 V vs. Ag/AgCl. The efficient photo-electrochemical responses of V(IV)TPyP/SnO_2 photoanodes will be highly beneficial for the construction of molecular artificial Z-Scheme systems for artificial photosynthesis.

PP 07

$ReSe_2$ Based Electrocatalyst for Hydrogen Evolution Reaction

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Keywords: Transition metal dichalcogenides, Rhenium diselenide, Hydrogen Evolution Reaction, Electrocatalyst.

Renewable energy sources are attracting significant interest due to increased energy demand. Hydrogen, being environmentally clean and safe, can be considered the future clean fuel. Hydrogen evolution reaction (HER) is the half-cell reaction of the water splitting reaction leading to the formation of hydrogen gas. Till date, the state-of-the-art catalyst known for HER is platinum. Transition metal dichalcogenide (TMD)-based catalysts such as MoS_2, WS_2, $MoSe_2$, etc., are considered as an alternative for platinum and finding great interest in HER due to their high electrochemical performance. Recently, $ReSe_2$, one among the TMDs with an indirect band gap, has attained great research interest due to its impressive electrocatalytic performance towards HER.[1],[2] An efficient HER electroctalyst was developed using $ReSe_2$ by hydrothermal approach. The effect of reducing agents in the synthesis were also studied. The $ReSe_2$ samples synthesized using different reducing agents exhibited an overpotential of 182 mV and 209 mV at 10 mA/cm^{-2} current density. The electrochemical analysis revealed that the synthesised catalysts exhibited comparable onset potential with that of Pt/C.

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PP 08

Turbostratically Aligned Graphene Sheets via an Environmentally Benign Ball Mill Method for Supercapacitor Applications

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Keywords: Turbostratic graphene, supercapacitor, ball-milling

Renewable energy sources are apt to address the energy needs in a rapidly growing technologically advanced society. Owing to the instability concerns, these energy sources are not very dependable for continuous usage. The development of energy storage technologies like supercapacitors is required to provide the energy needed in this competition. Supercapacitors are smaller devices with lower maintenance costs than batteries, as well as possess high power density, and cycle life. Here, graphene is synthesized via mechanochemical exfoliation with the assistance of a carbohydrate-derived milling agent, followed by calcination.[1] The CH-π and OH-π interaction of milling agent to the graphitic layers is shown in Figure 1. Using the characterization methods such as XRD, FTIR spectroscopy, Raman spectroscopy, FESEM, TEM, BET, TG and XPS, the turbostratic alignment of edge functionalized less-defective few-layer graphene is evidently revealed.[2] The electrochemical properties were thoroughly investigated using cyclic voltammetry, galvanostatic charge discharge, and electrochemical impedance spectroscopy. The prepared graphene possessed a specific capacitance comparable with the theoretical capacitance of graphene. The developed system has excellent cyclic stability of 100% capacitance retention in 10000 repeated runs.

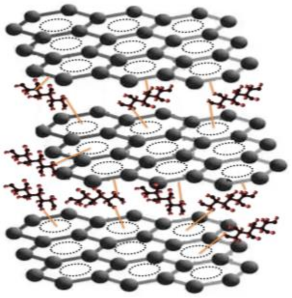

Figure 1: *Representation of CH-π and OH-π interaction of the milling agent with the graphitic layers*

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PP 09

Low-Temperature Solvothermal Growth of Co_xS_y Nanospheres on Conducting Substrates as Efficient Electrodes for Hydrogen Evolution Reaction

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Keywords: Electrocatalysis, Hydrogen evolution reaction, Solvothermal reaction, Co_9S_8, Co_3S_4

Electrochemical water splitting is widely regarded as a sustainable method for green hydrogen production. Cost-effective hydrogen production through hydrogen evolution reaction (HER) requires highly active and low-cost alternatives to traditional noble metal-based catalysts such as platinum.[1] Despite the progress in the development of efficient and non-noble metal-based electrocatalysts, their performance still falls behind platinum in terms of HER activity and stability. Furthermore, many existing synthesis methods are suitable for laboratory conditions, require expensive synthesis facilities, and are difficult to scale up to the industrial level due to the complexity of the methods involved.[2] In this work, we discuss a feasible, one-step solvothermal synthesis method to grow different sizes of cobalt sulfide (Co_xS_y) nanospheres made up of Co_3S_4 and Co_9S_8 on carbon cloth (CC), which can be directly employed as a self-standing working electrode for catalyzing HER, without any use of polymer binders. The current synthesis method is facile and economical, requires less time, and can be processed at a very low temperature (80 °C), compared to many other previous reports on solvothermal methods.[1,2] In addition, we studied the influence of utilizing various cobalt precursors during the solvothermal synthesis process and their effects on the morphological and electrocatalytic performance of the resulting Co_xS_y nanospheres. The synthesized samples were analyzed using field emission scanning electron microscopy, transmission electron microscopy, Raman spectroscopy, X-ray diffraction, energy dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy techniques. Electrocatalytic measurements revealed that incorporating multiple cobalt precursors during the synthesis is shown to have a positive influence on their HER electrocatalytic performance due to the changes in the particle size distribution and the number density on CC. The as-synthesized electrocatalyst materials (Co_xS_y/CC) showed good catalytic performance with reliable stability for HER in both acidic (0.5 M H_2SO_4) and alkaline media (1 M KOH).

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PP 10

Fluorine-Free Synthesized Tantalum Carbide (Ta_2C MXene) as an Efficient Electrocatalyst for Water Reduction and Nitro Compound Reduction

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Keywords: Ta_2C Mxene, Nitroreduction, Hydrogen Evolution Reaction

One of the eco-sustainable ways to generate hydrogen, which is considered a clean energy source, involves the electrochemical process. On the other hand, identifying the most effective heterogeneous catalyst is crucial for amine synthesis from nitro compounds in order to determine the optimum catalytic activity, stability, and reusability. Herein, we report the preparation of a 2D tantalum carbide MXene via the fluorine-free etching method and its application in catalysis (nitro reduction) and electrocatalysis (HER and nitro reduction). It is well-known that due to their layered structure, Mxenes show better catalytic activities, and hence they find applications in catalysis. Ta_2AlC (MAX phase) and Ta_2C (MXene) were evaluated for their electrocatalytic activity in the hydrogen evolution reaction. The electrocatalyst Ta_2C MXene exhibited overpotentials of 223 mV to reach 10 mA / cm^2 current density when tested under standard HER conditions (0.5 M H_2SO_4), and furthermore, the electrocatalytic reduction behavior of Ta_2C MXene towards the electrochemical reduction of 4-NP was tested in 1 M KOH. Galvanostatic electrolysis was performed in a divided cell using Ta_2C modified carbon cloth as the cathode, and Pt as the anode separated by a Nafion membrane, and it showed 72% product conversion and 96% faradaic efficiency. The progress of the galvanostatic electrolysis was monitored using ex situ Raman and UV-Vis spectroscopy. Similarly, the reducing behavior of Ta_2C towards the reduction of 4-nitrophenol to 4-aminophenol in the presence of $NaBH_4$ was tested. The Ta_2C MXene displayed improved catalytic activity with pseudo-first-order kinetics. Ta_2C nanoparticles completely reduced all three nitro compounds (10 mL each), 4-NP (216 mM–17 min), 2,4-dinitrophenol DNP (163 mM–25 min) and 2,4,6-trinitrophenol TNP (131 mM–36 min). Furthermore, in all these studies, the Ta_2C MXene exhibited improved catalytic performance and stability.

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PP 11

Tuning of Metal Grafted $BiVO_4$ Photoelectrodes for Solar Fuel Production

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Keywords: Green hydrogen production, electrocatalysis, sustainable chemistry

The energy resources around the globe needs a drastic transition with time since sustainability is being seriously threatened by CO_2 emissions from fossil fuels as a result of rapid economic development. To address the conflict between increasing energy demand and serious environmental concerns of earth derived fossil fuels, it is essential to consider alternative renewable energy sources. Among various green energy carriers, hydrogen (H_2) is considered as a potential candidate for the future due to its greenness and high energy density. The photo-electrocatalytic (PEC) assemblies for utilizing water as the non-sacrificial reductant considered as the key-step for green hydrogen production. However, photon flux density problem under normal solar irradiance for achieving four-electron oxidation of water through multi-photon excitation of the photo-responsive materials limits the scalability of solar fuel devices. Identification of alternative reductants to bypass the photon-flux density bottlenecks of visible light driven oxygen evolution reactions (OER) with thermodynamically more favourable and kinetically faster oxidation reactions would be beneficial for future energy devices through synchronized energy production and environmental remediation. Herein, we synthesized and characterized Bismuth vanadate ($BiVO_4$) semiconductor nano-particles with band gap of 2.4 eV in pure monoclinic form.[1] Metal grafting method has been adopted to overcome the low interfacial charge transfer rate and high recombination of photoinduced electron-hole pairs which limits the applications of bare $BiVO_4$ nano-particles. Various metal grafted $BiVO_4$ nano-particles decorated FTO electrodes were prepared. The photoelectrochemical testing of the photoanodes by using Pt as the counter electrode were performed. The photo-response of the Rh^{3+} grafted $BiVO_4$ photoanodes were significantly improved (0.4 $mA.cm^{-2}$) upon visible light irradiation in comparison with bare $BiVO_4$ film (0.007 $mA.cm^{-2}$). The role of various metal ions on the $BiVO_4$ lattice will be discussed for the visible light induced water activation. Furthermore, applications of the metal grafted $BiVO_4$ photoanodes for the key reactions to bypass photon-flux density bottleneck of OER and to achieve value-added products instead of oxygen at photoanode coupled with green hydrogen production will be discussed.

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PP 12

Three-Dimensional Porous Graphene Network as Anode Material for Asymmetric Supercapacitor

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Keywords: Holey graphene; mechanical exfoliation; 3D porous graphene; asymmetric supercapacitor

Three-dimensional graphene nanostructures are excellent platforms for high-performance supercapacitors owing to their high conductivity, large surface area, more active sites, and exceptionally high diffusion rate of electrolytes.[1,2] Here, holey graphene is prepared via mechanical exfoliation of graphite with a sugarcane-derived sweetening agent followed by hydrothermal reaction and further controlled heat treatment, where the method is devoid of the use of any additional precursors to induce in-plane holes in the graphene sheets. A novel method for the introduction of three-dimensional array of porous graphene is also introduced here that resulted in excellent supercapacitor electrode material due to the superior conductivity and diffusion pathways along with the pseudocapacitance offered by the functionalities on graphene. The potential of the 3D porous graphene as an anode material is utilized for the fabrication of an asymmetric supercapacitor which offers a wide potential window. The practical applicability of the asymmetric supercapacitor was also investigated here which is represented in Figure 1 and the results further confirms the superiority of the present three-dimensional porous graphene as an anode material in future energy storage devices.

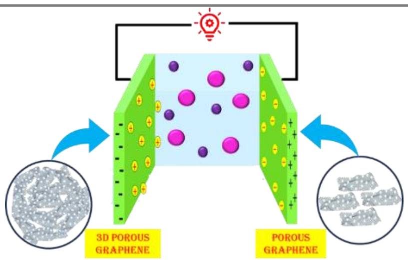

Figure 1: *Schematic representation of the investigation of the practical applicability of the 3D porous graphene as anode material.*

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PP 13

Eggshell Powder- PVA Composite Based Triboelectric Nanogenerator; An Energy Harvest from Residual Waste

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Keywords: Triboelectric nanogenerator, Triboelectrification, Polyvinyl alcohol

The thirst for energy demand drives a man to discover more eco-friendly, inexpensive, renewable, and sustainable energy sources. We are living in a highly technological world where using many small electronic gadgets makes life easier. The use of chemical batteries in such devices is not only unecological but also uneconomical. Thus, as a solution, Zhong Lin Wang and his coworkers invented Triboelectric nanogenerators (TENGs) in 2012 to convert any low-frequency mechanical energy like human motion, vibration wind energy, etc to useful electrical energy.[1,2] Triboelectrification and electrostatic induction are the principles underlined behind the TENG operation. The easiness of fabrication, cost-effectiveness, and diverse choice of material selection boost the practicality of TENG in a wide variety of application fields. In this research work, we report a novel, simple, and low-cost Polymer-based TENG with eggshell powder as filler (ESP-TENG). The Polyvinyl alcohol (PVA) films with different filler concentrations and polypropylene sheet act as tribomaterials. The output peak-to-peak voltage of the contact-separation mode of TENG by manual tapping was investigated and the load performances of TENG were studied by driving the commercial LEDs. The PVA-eggshell powder composite films were characterized by XRD and FTIR-ATR. Thus, the work outlines the simply fabricable ESP-TENG, that can be used for the clean and green mechanical energy harvesting technology.

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PP 14

Cobalt Hydroxide Based High-Energy Aqueous Supercapacitor

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Keywords: β-$Co(OH)_2$, Tungsten Carbide, Composite Electrode, Hybrid Capacitor

Two important characteristics of electrochemical capacitors—good rate capability and extended cyclic performance—are strongly influenced by the electrochemical stability, composition, charge-storing method, etc., of the electrodes[1]. $Co(OH)_2$-based composite is prepared and used as positive electrodes for aqueous supercapacitor application in the present work. Electrochemical characterization techniques such as CV, GCD, and EIS have been used to quantify the electrochemical behavior of the samples in a KOH electrolyte medium. The prepared composite as a positive electrode in a capacitor delivered superior cell performance than the bare metal hydroxide when activated carbon was used as the negative electrode. Further, the practical feasibility of the as-prepared composite materials was illuminated by fabricating a flexible pouch-type supercapacitor using PVA-KOH hydrogel, and their characteristic performance was analyzed. Cobalt hydroxide and metal carbide composite highly enhanced cell cyclic stability, with over 65 percent capacitance retention even after 15000 cycles.

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PP 15

Role of NiO Nanostructures in the Enhanced Hydrogen Storage Properties of Oxidized Lithium Borohydride

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Keywords: Hydrogen storage; $LiBH_4$; NiO; activation energy; binding energy

Storing of hydrogen in solid-state materials has become a promising technology for mitigate the energy crisis. Under this scenario, $LiBH_4$ has been received great attention among the other physisorbent and chemisorbent materials, due to its hydrogen storage capacities. However, several key issues are associated with $LiBH_4$ during practical applications. In order to counter these issues, oxidized $LiBH_4$ was seperately blended by NiO nanorods (NiONR), nanoplates (NiONP) and nanoflowers (NiONF) using the ultrasonic-assisted wet-impregnation method. Then, the physico-chemical properties were investigated systematically for the oxidized $LiBH_4$, $LiBH_4$/NiONR, $LiBH_4$/NiONP and $LiBH_4$/NiONF systems. Later, hydrogen charging experiments were conducted at three different temperatures (RT, 100 and 150°C) under 10 bar H_2 pressure for 30 mintues. Hydrogen charged samples were dehydrogenated using TGA technique under Ar medium from RT to 275°C. We found that the oxidized $LiBH_4$, $LiBH_4$/NiONR, $LiBH_4$/NiONP and $LiBH_4$/NiONF systems are released 0.87 wt.%, 1.27 wt.%, 1.66 wt.% and 1.76 wt.% of H_2 between RT-275°C. From these results, $LiBH_4$/NiONF has better hydrogen uptake/release kinetics than other systems due to its advantages of physico-chemical properties [1,2].

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PP 16

Studies on Structural, Morphological, and Electrochemical Properties of Pristine and Co Doped Cr_2O_3

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Keywords: Cr_2O_3 nanoparticles, Pseudocapacitance Capacitive, Cyclic voltammetry (CV), Galvanostatic charging/discharging (GCD)

Supercapacitors are receiving considerable attention due to the increasing demand for electric energy storage.[1] Pseudocapacitors show higher energy densities than EDLCs.[2] Metal oxides possess multiple oxidation states, leading to multiple redox reactions that can be used in pseudocapacitors.[3] Pseudocapacitance followed by higher specific energy density is exhibited by a few transition metal oxides (TMOs) along with their excellent cyclic life. While, some other TMOs have at least shown the signatures to be the pseudocapacitive candidates.Cr_2O_3 and 1 % Co doped nanostructures have been successfully synthesized by modified auto combustion method. Structural and morphological aspects, vibrational spectra and optical properties are evaluated. X-ray diffraction profiles revealed that both Cr_2O_3 and Co doped Cr_2O_3 are indexed in the rhombohedral structure with an R-3c space group, as 072-3533 JCPDS card number. Energy band gap gives 2.96 eV and 2.75 eV for pristine and Co doped samples. Surface morphology was identified from the Scanning Electron Microscopy (SEM) and the particles are appeared to spherical shape morphology. Electrochemical performances were evaluated through cyclic voltammetry, galvanoscopic charge discharge and electrostatic impedance spectroscopy. The remarkable electrochemical performances of Cr_2O_3 show it can be used for energy storage applications.

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PP 17

Innovative Bottom-Up Synthesis of Iron Oxide-Carbon Hybrid Materials for Enhanced Electrochemical Performance

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Keywords: Iron oxide-Carbon hybrid system, Electrode material, Supercapacitor

Metal oxide-carbon composites are widely studied as electrodes for lithium-ion batteries and electrochemical capacitors.1-3 The common preparation method for such composites consists of mixing some type carbon material with a metal oxide, where both the components are synthesized separately. In the present study, iron oxide-carbon hybrid material is synthesized by a novel bottom-up approach, starting with a phenolas carbon precursor and iron nitrate as the precursor for metal oxide. Initially, the phenol is treated with formaldehyde to obtaina resin, which enables an efficient conversion of phenol into graphitic carbon by later processing. This resin is then allowed to complex with ferricions and dried to a highly homogeneous precursor for the hybrid material. The dried solid precursor is heat-treated further under different conditions to obtain iron oxide-carbon hybrid system. Apart from additives, several parameters associated with the synthesis and heat-treatment is optimized to obtain a nano-structured electrode material. The materials are characterized using powder x-ray diffraction, Scanning electron microscopy, BET surface area analysis and FTIR spectroscopy. Electrochemical performance of the materials is measured using Cyclic Voltammetry.

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PP 18

Fabrication of Scalable Pigmented Superhydrophobic Coatings for Self-Cleaning Applications

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Keywords: Superhydrophobic Coatings, Self-Cleaning, Pigmented Paints

Superhydrophobic coatings with self-cleaning capability is recently grabbing attention of researchers for its innovative applications. Polyurethane based polymers are promising ingredient for superhydrophobic nanoformulation due to its mechanical durability, scalability and efficient optical transparency[1]. Herein, we have developed a polyurethane based colored superhydrophobic nanoformulation. The superhydrophobic property was achieved by creating optimum surface roughness and modifying surface with low surface energy material. Moreover, various metallic pigments were used for imparting colours to the superhydrophobic coatings on various substrates adapting simple spray coating method[2]. The water contact angle of the coating was found to be greater than 150° and roll-off angle was less than 5°, implying that the surface is superhydrophobic. Such pigmented superhydrophobic coatings can find potential applications in paints and can be also used for many outdoor applications[3].

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PP 19

Polyaniline/Graphene Nanocomposites Preparation via a Green Strategy and Application as Supercapacitor Electrode Materials

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Keywords: Graphene, liquid phase exfoliation, PANI/G, in-situ polymerisation, supercapacitor

Environmental contamination and resource depletion necessitate alternative energy sources and storage methods, and supercapacitors are promising candidates for energy storage due to their high power density, long cycle life, and fast charge-discharge rates.[1] Here we present a combination of polyaniline (PANI) with graphene for energy storage applications. A novel method is introduced for graphene production using green solvents since the commonly used solvents in the synthesis of graphene are toxic in nature. Polyaniline/graphene (PANI/G) nanocomposites with different aniline concentrations are prepared via in-situ polymerization in graphene dispersion. The schematic representation of PANI/G formation is shown in Figure 1. Different characterization techniques are used to investigate structure and morphology. Well coverage of graphene layers with PANI is revealed by morphological investigations via SEM and TEM. The increased capacitance of PANI/G nanocomposites in comparison with bare PANI and graphene is due to the synergistic effect of the combination.[2] In addition, PANI prevented the layer restacking observed in bare graphene whereas graphene diminished the volume shrinkage of PANI in charge-discharge cycles.

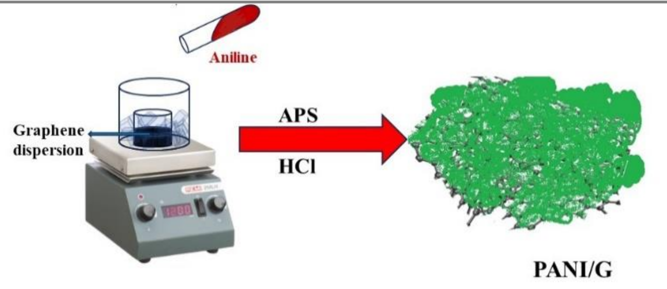

Figure 1: *Schematic representation of PANI/G preparation*

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PP 20

Preparation of Diverse Stable MOFs and their Electro Catalytic Capabilities towards Desulfurization, Water Splitting and various Nitrophenol Reduction

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Keywords: Desulfurization, Carbonization of MOFs, Nitrophenol reduction

Metal-organic frameworks (MOFs) are gaining popularity as electrocatalysts in a variety of energy resources [1,2] and sensor applications due to their large specific surface area, high porosity, variable pore size and organized pore organization. Herein, we report synthesis of carbonized monometallic MOFs involving Co, Al and Ni as metal nodes, benzene tricarboxylic acid and 4,4 bipyridine as linkers, their characterization using various surface analytical techniques and their employment as modal catalysts for water splitting, electrooxidation of thiophene, benzothiophene and dibenzothiophene and reduction of 4-nitrophenol. Electrochemical studies using linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS) revealed that Co-C MOF has the lowest onset potential with a lower Tafel slope and charge transfer resistance value (R_{ct}) for the electrooxidation of thiophene (Fig. 1), benzothiophene and dibenzothiophene respectively. The high catalytic activity of Co-C MOF may be due to its higher surface area and larger pore volume than that of Al- C MOF and Ni-C MOF, as a result of vast number of redox-active sites for electrochemical processes, as revealed by BET analysis. In addition, the catalytic activity was evaluated for the conversion of various nitrophenols to aminophenols, where Co-C MOF showed outstanding activity with minimal reduction time and high-rate constant value.

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PP 21

Discovering the Interaction Profile of Camptothecin Functionalised Silver Nanoparticles with ctDNA: Multi- Spectroscopic and Calorimetric Approach

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Keywords: Silver, ctDNA, Interaction, Cytotoxicity, A549 cells.

Natural drug functionalised silver nanoparticles have gained significant interest in pharmacology related applications due to their therapeutic efficiency.[1] This work aims to discuss the relevance of the camptothecin functionalised silver nanoparticles (CMT-AgNPs) in the field of nano-medicine. The influence of nanoparticles inside the human body and their interactions with biological macromolecules need to be studied prior to specific applications.[2] We have primarily analysed the anticancer activity and cytotoxicity of CMT-AgNPs and then investigated the binding strategy of CMT-AgNPs with calf thymus DNA (ctDNA) through a series of spectroscopic and calorimetric methods. The synthesised CMT-AgNPs were characterized using UV-Visible, fourier transform infrared (FTIR) spectroscopy, XRD and high-resolution transmission electron microscopy (HRTEM). Also, an exhaustive in vitro MTT assay was conducted by CMT-AgNPs against human lung cancer cell lines and L929 cell lines. The green synthesised CMT-AgNPs arestable, spherical in shape, size of 10±2 nm average diameter and shows good anticancer activity. A group of experimental techniques such as UV–Visible spectrophotometry, fluorescence dye displacement assay, circular dichroism (CD) and viscosity analysis unraveled the typical groove binding mode of CMT-AgNPs with ctDNA. The CD measurement evidenced the minor conformational alterations of double helical structure of ctDNA in the presence of CMT-AgNPs. The information deduced from the isothermal titration calorimetry (ITC) experiment is that the binding was exothermic and spontaneous in nature. Overall, we believe that camptothecin functionalised silver nanoparticles is a potential prospect for pharmaceutical applications.

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PP 22

From Nanoscale Precision to Macroscopic Impact: Self-Assembled Nanoclusters and Luminescence-Driven Device Fabrication

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Keywords: Metal nanoclusters, Self-assembly, Luminescence, Light-emitting diodes, Anticounterfeiting

Atomically precise monolayer thiol-protected noble metal nanoclusters (NCs) emerged as a fascinating area of nanoscience research in the past two decades.[1] NCs are distinct pieces of matter, that possess ultra-small metal cores (< 2 nm), composed of a few to hundreds of atoms protected with a definite number of ligand shells. In the recent past, new and improved protocols were developed to fabricate monodisperse NCs. The molecular composition of monodisperse NCs has been solved by using mass-spectrometry and single-crystal diffraction studies. NCs show size-dependent electronic, optical absorption, photoluminescence, and magnetic properties. NCs have been used as attractive nanoscale building blocks for the fabrication of three-dimensional superstructures via a colloidal self-assembly process. Such self-assembled architectures play an important role in harvesting the enhanced and collective optical properties from the neighbouring NCs. Driving forces such as hydrogen bonding, electrostatic interactions, van der Waals interactions, dipolar interactions, C-H⋯π/π⋯π interactions, metal chelation, metal-metal interactions, amphiphilicity, light-triggered dipole-induced interactions, and external templates have been implemented to achieve such assemblies.[2] The organic synthetic toolbox has allowed the rational design of a variety of NCs with specific functional moieties on their surfaces. Particularly, anchoring photoresponsive ligands on the surface of NCs can be utilized as nanoscale building blocks for photoresponsive NC assembly.[3,4] One could foresee that such smart self-assembled superstructures with enhanced photophysical properties are needed to develop future precision devices. The luminescence property of NCs can be efficiently used to probe toxic metal ions/molecules, monitor biological events, production of anticounterfeiting ink,[4] and light-emitting device fabrication.

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PP 23

Enhancing the Stability and Reusability of Ag_3PO_4 Nanoparticles by Introducing a Thin Silica Shell

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Keywords: Ag_3PO_4, Photocatalytic dye degradation, Cyclic Voltammetry

A semiconductor photocatalyst, known for its potential and cost-effectiveness, holds promise in the degradation of harmful organic contaminants in water. Ag_3PO_4 has proven to be a highly efficient visible-light photocatalyst, facilitating the oxidation of water and the degradation of dyes. In this research, the limitations inherent in Ag_3PO_4 were successfully addressed by applying a thin silica shell coating. The silica-coated Ag_3PO_4 exhibited sustained photocatalytic activity even after undergoing five cycles of photodegradation, whereas the bare Ag_3PO_4 experienced a 50% decline in photocatalytic activity. The study highlights the ability of the thin silica shell to enhance photostability, preserving photocatalytic efficacy through multiple cycles of dye photodegradation. XPS analysis revealed a greater formation of Ag0 on the surface of bare Ag_3PO_4 compared to silica-coated Ag_3PO_4, contributing to the decline in photocatalytic activity after five cycles of photodegradation. Electrochemical studies identified key intermediates such as $OH^{\cdot}$, O_2^{-}, etc., formed during water oxidation, playing a crucial role in the photodegradation of dyes. This investigation offers valuable insights for the design of core-shell semiconductor nanostructures tailored for reusable photocatalytic applications.

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PP 24

Structural, Morphological, and Antioxidant Studies of Green Synthesized Gold Nanoparticles Using *Trichopus Zeylanicus* Leaf Extract

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Keywords: Green synthesis, Trychopus Zeylanicus, Gold nanoparticles, Antioxidant Property

Biosynthesized nanoparticles are gaining attention because of biologically active plant secondary metabolites that help in green synthesis and also due to their unique biological applications. This study reports a facile, eco-friendly, reliable, and cost-effective synthesis of gold nanoparticles (Au NPs) using the aqueous leaf extract of *Trichopus Zeylanicus* and their antioxidant activity[1]. The plant *Trychopus Zeylanicus* is a rare medicinal plant found in the Agastyar hills of Kerala. The local 'kani' tribe uses it as a healthy food for getting instant stamina, ever-green health, and vitality[2]. The prepared Au NPs were crystalline and stable with a mixed morphology. The formation of Au NPs was confirmed by using UV-visible absorption spectroscopy. FTIR analysis was performed to find the roles of the micro and macromolecules present in the leaf extract in the synthesis and the stabilization of the AuNPs. The crystalline nature of Au NPs was confirmed with the help of XRD analysis. TEM and SEM were used to determine the morphology of Au NPs. The evaluation of antioxidant activity of Au NPs shows that they possess a good potency in a dose-dependent pattern to trap DPPH free radicals.

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PP 25

Precision Nanocluster-Based Toroidal and Supertoroidal Frameworks Using Photocycloaddition-Assisted Dynamic Covalent Chemistry

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Keywords: Precision nanoclusters, coumarin, [2+2] photocycloaddition, toroidal superstructures, drug delivery

Ligand-protected atomically precise nanoclusters (NCs) derived from coinage metals are ideal building blocks to construct self-assembled superstructures.[1] Though photon-assisted supramolecular reversible self-assembly in precision NCs has been reported, long-range self-assembly based on photochemical reactions on the NC surface has yet to be investigated.[2,3] Herein, we present the synthesis and light-induced reversible self-assembly of coumarin tethered Au_{25} NCs via [2+2] photocycloaddition reaction. Photoactivation of functionalized NCs dispersed in tetrahydrofuran results in the formation of uniform toroidal superstructures (Scheme 1). Further, prolonged illumination of NCs under 365 nm results in the formation of honeycomb frameworks due to the inter-toroidal coupling. The electron microscopic and tomographic results suggests that the initially formed spherical superstructures are fusing to form the toroids. As a proof-of-concept, a cross-photocycloaddition reaction between coumarin-tethered NCs and 5-fluorouracil is demonstrated as a model photo-controlled drug release system, allowing systematic loading and unloading of the drug during the assembly and disassembly. Such systems with appropriate modifications will be an ideal probe for addressing noninvasive drug delivery and theranostics in the future.

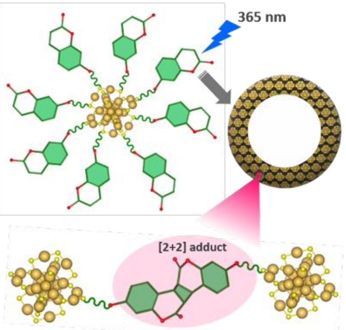

***Figure 1**: Illustrative showing the photo-dimerization and self-assembly of coumarin-tethered NCs.*

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PP 26

Study of the Effect of Silver Nanoparticles in Methylene Blue Sensitized Poly Vinyl Alcohol-Acrylamide Photopolymer for Holographic Applications

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Keywords: Holography, holographic recording medium, silver nanoparticle incorporated recording medium

Photopolymers are preferred in various holographic applications because of being self-developing along with high resolution. Previous studies of PVA- Acrylamide photopolymer as a recording media show that it has high efficiency but its storage life and shelf life is poor. The present work describes the incorporation of silver nanoparticles into methylene blue sensitized poly vinyl alcohol-acrylamide photopolymer and the efficiency is studied. The gratings are recorded on the films with different concentrations of nanoparticle solutions. For PVA-Acrylamide photopolymer diffraction efficiency decreases from 9.89% to 4.03% after 2.5 months, but when silver nanoparticle incorporated in PVA-Acrylamide Photopolymer the reduction in diffraction efficiency is only from 10.91% to 9.14 % after 2.5 months. For gratings recorded on PVA-Acryl Amide Photopolymer after 2.5 months of its preparation shows diffraction efficiency of 2.59%, but silver nanoparticle incorporated PVA-Acryl Amide photo polymer shows diffraction efficiency of 10.34% after 2.5 months of its preparation. The nanoparticle incorporated recording media show stable diffraction efficiency, storage life and shelf life than films without nanoparticles. Further, the proposed recording medium shows better performancecompared to the PVA-Acryl Amide photopolymer rendering it to be potential candidate for holographic recording.

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PP 27

Controlling the Oxidation States of Transition Metal Ion Dopants in ZnS Quantum Dots: A Focus on Vanadium

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Keywords: Quantum Dots, Aqueous Synthesis, Vanadium doping

Incorporation of transition metal ions into semiconductor nanocrystals (quantum dots) can dramatically modify the properties of quantum dots.[1,2,3] Among the different strategies forthe synthesis and doping of quantum dots, the one using aqueous medium is generally challenging, especially in the case of sulphides and selenides.[4] Here, we have developed an aqueous based synthetic strategy, where different oxidation states of a given dopant transition metal ion could be stabilized in a controlled manner and incorporated into ZnS quantum dots. The general procedure begins with the reaction between zinc metal powder and an acid to generate Zn ions and hydrogen. The transition metal ion in the highest possible oxidation state is then introduced into the reaction mixture, which will subsequently get reduced in presence of hydrogen. Finally, the sulphide source is added to facilitate the formation of quantum dots. As an illustration of this general procedure, doping of ZnS with different oxidation states of vanadium will be discussed. The obtained vanadium doped ZnS quantum dots are characterized using powder x-ray diffraction, Field Emission-SEM-EDAX, and XPS.

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PP 28

A Comparative Study on the Antibacterial Properties of Zinc Oxide Nanoparticles Synthesised through Chemical and Biological Route.

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Keyword: Green synthesis, Chemical route, Zinc Oxide Nanoparticle.

In the recent decades, nanotechnology has become an important research field of modern materials science. Green synthesized nanoparticles have gained wide interest due to its features like rapidity, eco-friendly and cost effectiveness. This study is a comparison between the chemically synthesized and green synthesized zinc oxide nanoparticles and its antibacterial properties. In green synthesis the leaf extract of ixora coccinea is used as the main biological agent while in case of chemical route, Zinc acetate dehydrate and Triethanolamine were used as the precursor. The X-ray diffraction and UV Visible analysis are done. In addition to the purely synthesized zinc oxide nanoparticles, silver doped ZnO NPs were also synthesized and studied. Interestingly, the results of the study showed variation in the inhibition zone of different bacteria created in both samples.

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PP 29

Fe^{3+} Induced Antibacterial Efficacy of Spherical Flower-like CuO Nanoparticles with Enhanced Structural and Optical Properties

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Keywords: Hydrothermal route, Copper oxide, Fe doping, Antibacterial activity, Escherichia coli

Advancements in antibacterial fields are growing, since the demand for an efficient antibacteral nanomaterial is increased in order to resist the pathogenic bacterias, againt which the current antibiotics are failing. Herein, we synthesied and characterised pure and Fe doped CuO nanostructures using conventional hydrothermal route and investigated its ability to become a potential member in pathogenic bacterial treatment. XRD studies revealed the formation of highly crystalline monoclinic CuO nanostructures with no secondary or impurity peaks. The successful incorporation of dopant in to host crystal structure were clearly indicated by the shift in (-111) peak.[1] Blue shift in the major peak position in the Raman spectraupon doping advocates the generation of oxygen vacancies in the crystal.[2] Morphological investigations showed the transformation of spherical CuO microflowers to clustered nature composed of nanoflakes of width in range of 700-900 nm with tiny sugar-like nano-cubes spreaded over them as the doping percentage increases. The reduction of band gap value on doping propose the additional energy level creation by Fe^{3+} ions on CuO band structure.[3] The antibacterial acitivity assay of pure and Fe doped CuO nanostructures were conducted by well diffusion method. Importantly, the Fe-doped CuO nanoparticles showed potential antibacterial ability, significantly inhibiting the growth of both E.coli. and Pseudomonas bacterias compared with that observed in pristine CuO. This study suggests that the Fe-doped CuO nanostructures are have the capacity to become a promising antibacterial material.

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PP 30

X-Band Electromagnetic Interference Shielding Application of PVA-MWCNT-$BaTiO_3$ Metacomposites with Tuned Negative Permittivity

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Keywords: Metamaterial, Metacomposites, MWCNT, Negative Permittivity, $BaTiO_3$, Electromagnetic Interference Shielding

Negative permittivity has garnered more attention recently due to the creation of novel metamaterials made of periodic array structures. However, in view of low-cost production, it is imperative to generate negative permittivity behaviour based on inherent features of the material rather than artificially periodic patterns. Due to their affordability, flexibility, and controllable negative permittivity, polymer-based percolated metacomposites have drawn a lot of interest and are appealing for a variety of applications. In this study, metacomposites are fabricated through die-casting with polyvinyl alcohol (PVA) as a flexible, low-cost, green polymer matrix and multiwalled carbon nanotube (MWCNT) as the filler. Interestingly, electrical percolation caused the PVA-MWCNT metacomposites to exhibit conductivity switching (from hopping to metal-like conduction), permittivity shifting (from positive to negative), and capacitive to inductive transition. This was accomplished by varying the concentration of MWCNT. The PVA-MWCNT metacomposites is observed to follow the Drude- Lorentz model[3] as they exhibited a weakly negative permittivity at kHz-MHz frequencies. Then, $BaTiO_3$ is added to the above metacomposites for tuning of permittivity. Interestingly, negative permittivity value increased on the order of hundred. The electromagnetic interference shielding performance of the sample was also analysed and shows good absorption efficiency of -54 dB at 10.1 GHz and also shows shielding efficiency of above 10 dB in the whole x-band region[4]. These PVA-MWCNT-$BaTiO_3$ sample is suitable for electromagnetic interference shielding application.

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PP 31

Ti-N-C bonded close coupled TiO_2/g-C_3N_4 for rapid degradation of cationic dyes from multi-dye system by persulfate activation

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Keywords: Binary dye mixture, derivative spectrometry, graphitic carbon nitride, persulfate activation, Z-Scheme photocatalyst

A novel Z-Scheme photocatalyst (TCN) was prepared with TiO2 and GCN and was utilized to study the degradation efficiency of a binary dye mixture consisting of 5 ppm Rhodamine B and 5 ppm Crystal violet solutions by persulfate activation. Derivative spectrometric analysis was adopted to find the degradation efficiencies of the individual dyes in the mixture. The results indicate that in the presence of persulfate ions 0.6 TCN gives 100 % degradation in 60 min and 30 min for Rh B and CV respectively. Hydroxyl radicals, superoxide radicals and sulfate radicals are found to be the active species involved in photocatalytic degradation. From the results of radical scavenging experiments and band potentials of the semiconductors, a plausible mechanism of photocatalytic degradation of the model pollutants is proposed.

PP 32

Catalytic Reduction of Methylene Blue using Poly-o-phenylenediamine-Silver Nanoparticle Composite

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Keywords: Conjugated polymer, Silver nanoparticle, catalytic reduction

Poly-o-phenylenediamine was synthesized by chemical oxidative polymerization using ferric chloride as an oxidizing agent in aqueous medium. [1] POPD has intense yellow fluorescence in water, and its fluorescence emission was quenched upon oxidation with $AgNO_3$. Similarly, $AgNO_3$ reduced to Ag (0). The synthesis of poly-o-phenylenediamine was also carried out using silver nitrate as oxidizing agent in aqueous medium. Powder XRD studies revealed the formation of silver nanoparticles along with the POPD polymer. The POPD-silver nanoparticle composite was effectively used as a catalyst for the reduction of methylene blue (MB) using sodium borohydride (see Figure 1). The catalytic reduction kinetics were measured using UV-Visible absorption spectroscopy. The rate constants and activity factors were also determined.[2]

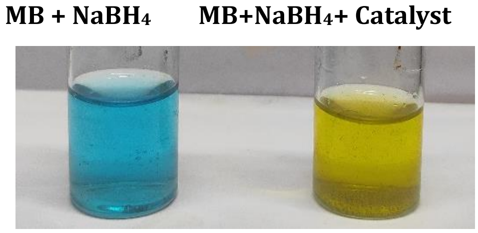

***Figure 1**: Photographs of reduction in methylene blue in the presence of POPD-silver catalyst.*

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PP 33

Enhanced Thermoelectric Performance of Cu_2Se/ZnSe Composites Through Band Convergence and Carrier Optimization

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Keywords: Copper selenide, Thermoelectricity, Band convergence, Powerfactor

Thermoelectricity (TE) stands out as a promising method for harvesting energy, offering potential renewable sources that can efficiently transform a thermal gradient into usable electrical energy and vice versa, all without the need for moving components and without contributing to greenhouse gas emissions. [1,2] Achieving high conversion efficiency in TE devices for commercial applications necessitates the development of materials with superior TE properties. Unfortunately, the current low efficiency of these materials results from the interdependence of transport parameters, limiting their widespread application. The focus of research should be on improving the TE properties of these materials by employing various strategies capable of decoupling these transport parameters in a favourable manner in order to achieve high conversion efficiency.[3] In this study, we present the improved thermoelectric performance of Cu_2Se by incorporating ZnSe into the system through ball milling. The introduction of ZnSe can induce pronounced band convergence within the electronic structure of Cu_2Se, potentially resulting in an enhancement in TE properties. Notably, the electrical conductivity simultaneously improved with the Seebeck coefficient, attributed to an increase in carrier concentration and the effective mass of the density of states, respectively. This improvement, in turn, enhanced the thermoelectric properties of Cu_2Se/ZnSe composites, resulting in the attainment of a maximum power factor of 736 $\mu W/mK^2$ at 573K for the sample incorporating 5wt % of ZnSe, which is five times higher than that of pristine Cu_2Se.

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PP 34

Electrical and Optical Characterization of CuZnS Thin Films Prepared by Chemical Bath Deposition Method

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Keywords: Electrical, Optical, Characterization, CBD ,CuZnS thin film

Here we report the electrical and optical studies of the CuZnS thin film prepared by the process of the Chemical Bath Deposition method. The methodologies adopted for the studies were UV-Vis Spectrophotometry[JASCO V-670 UV-Vis NIR Spectrophotometer] and Hall effect measurement system [Ecopia HMS 3000s]. The parameters extracted from the electrical studies include Mobility, Sheet resistance, Resistivity, Conductivity, Hall coefficient, etc where the sheet resistance value is set only for the corresponding thickness of the thin film.[1,2] The thickness measurement for the film was done by using Profilometer. The resistivity and Conductivity of the samples lie in the benchmark values of Semiconductors. The hall coefficient obtained indicates the nature of the prepared sample be a p-type semiconductor. From the optical characterization of the thin film, we found that the direct bandgap was 2.6146eV.

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PP 35

Structural and Optical Properties of Y-Doped ZnS Nanoparticles

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Keywords: Y doped ZnS NPs, structural properties, Optical properties

Y-doped ZnS nanoparticles with doping percentages of 0.5%, 1%, 2.5%, and 5% were created using the hydrothermal technique. TEM pictures confirmed the phase change from cubic to hexagonal structure suggested by XRD and Raman investigations[1,2]. Studies using SEM and TEM showed structural alterations. Diffused reflectance studies showed the band gap, which ranged from 3.33 eV to 3.45 eV for various doping doses. The study of photoluminescence revealed defect states exhibiting peaks at 362 nm, 383 nm, and 390 nm. Peak intensity increased up to 1% with Y doping; at higher percentages, concentration quenching was noted[3]. EDAX verified that Y integration was successful.

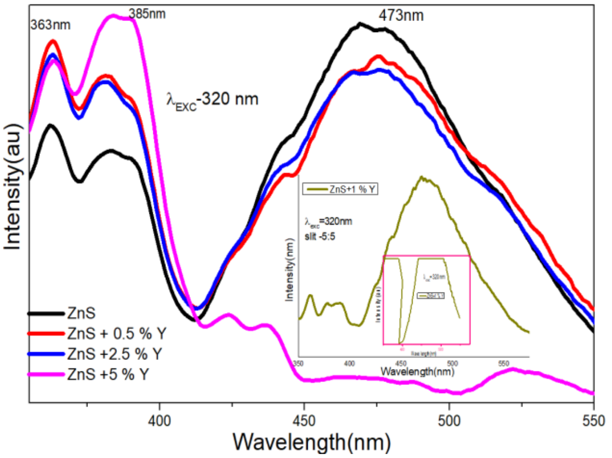

***Figure 1**: PL Spectra of ZnS and Y doped ZnS nano structures*

Visible light photocatalytic activity first increased and then decreased with doping concentration; the best degradation efficiency of 93% was observed at 1% doping. This work innovatively synthesized hexagonal ZnS at low temperatures, avoiding high temperatures and advanced apparatus, providing insights into doping-dependent luminescence and photocatalytic behaviour.

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PP 36

Growth, Characterization and Dielectric Investigation on Crystalline Zinc Mandelate

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Keywords: Zinc mandelate, dielectric, metal organic frameworks

Metal ions are coupled to organic linkers to form metal-organic framework (MOF) complexes. This class of compounds has several uses in the areas of sensing, catalysis, gas adsorption, non-linear optics, etc. owing to its distinctive markings[1,2]. In the present study a MOF - Zinc Mandelate crystals were grown by gel encapsulation technique for the first time. The crystalline nature of the grown sample is evident from the Powder XRD data. The existence of the various functional groups in the sample was confirmed by the FTIR and Raman spectra. CHNS analysis confirmed the molecular formula of the compound. From the UV Vis studies it is demonstrated that the sample shows zero absorbance throughout the entire visible spectrum. This qualifies the sample as a prospective nonlinear application candidate. The computed lower cut off wavelength was 267 nm. The optical bandgap of the material is predicted to be 4.45 eV. The TGA curve suggests that Zinc Mandelate crystals are thermally stable up to 280^{o}C. The produced crystals exhibit typical dielectric behavior and it is investigated how the dielectric loss and dielectric constant of the sample vary with applied field frequency. With an increase in applied field frequency, it is discovered that both the dielectric constant and dielectric loss decrease. For an applied frequency range of 0.01Hz - 10MHz, the dielectric constant ranges from 12.80 to 6.39.

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PP 37

Spectroscopic Properties of $Sr_{1.0}Ca_{2.0}B_6O_{12}$:0.5$Sm^{3+}$

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Keywords: Borate Phosphor, Samarium, Luminescence

This research endeavors to gain a comprehensive understanding of the spectroscopic properties of Sm^{3+} -doped strontium calcium borate phosphor, synthesized through the widely adopted solid-state reaction method, a common choice for various phosphor types, including borate-based variants. The primary objective is to identify high quantum efficiency luminescent materials activated by samarium ions. Elemental composition analysis was conducted using Energy Dispersive X-ray spectroscopy (EDS), which revealed the presence of specific elements through distinct peaks in the EDS spectrum. Absorption spectra, which featured peaks in the UV-Vis and NIR regions, offered valuable insights into the energy band gap determined from the Urbach edge. The band gap values were determined for both direct (E_g = 5.4 eV) and indirect (E_g = 4.7 eV) transitions. Moreover, the nephelauxetic ratio, derived from the absorption spectrum, indicated a combination of ionic and covalent bonding in the phosphor. The photoluminescence spectrum, observed under 403 nm excitation, demonstrated emission transitions spanning from blue to red, a phenomenon supported by the energy level diagram of Sm^{3+} ions. Colorimetric analysis further confirmed the phosphor's ability to emit white light, rendering it a valuable candidate for White Light Emitting Devices (W-LEDs). The synthesis method yielded a material with multiple visible wavelength emission channels, making it applicable in a wide array of technological applications, including LED technology, tunable lasers, optical communication devices, and display technologies. The exceptional spectroscopic properties of Sm^{3+} -doped strontium calcium borate phosphor significantly enhance its suitability for display lighting applications.

PP 38

Dielectric and Conductivity Investigations on Sodium Zeolite Incorporated Polymer-Nanocomposites

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Keywords: Nanocomposite, PVA/PVP blend, dielectric spectroscopy

Nanocomposite polymer films (NPFs) have garnered significant attention due to their vast potential applications in rechargeable batteries, separation membranes, gas sensors, etc.[1-3] This study focuses on the preparation, characterization, dielectric, and conductivity studies of zeolite sodium nanoparticles (ZNPs) incorporated poly (vinyl alcohol) (PVA)/poly (vinyl pyrrolidone) (PVP) blend. NPFs were synthesized by blending PVA with PVP in 1:1 ratio and incorporating of ZNPs with varying concentrations (1 wt% - 4 wt%) as the filler. This was achieved through ultrasonic dispersion of the filler in PVA/PVP blend solution, followed by the solvent casting method.[4]

The prepared polymer films were undergone characterization using FTIR, XRD, TGA, FESEM, and broadband dielectric spectroscopy (BDS). FTIR revealed characteristic peaks corresponding to vibrational groups in the fabricated samples, with the major vibrational peaks of the ZNPs clearly present in the polymer blend, confirming a strong interaction with blend molecules. The FESEM images explored a uniform morphology, indicating well-dispersed ZNPs in the polymer blend. The XRD pattern of ZNPs exhibited a crystalline nature and its incorporated polymer composite. The amorphous nature of the composite decreases with an increase in the concentration of zeolite. TGA study indicated that the blend nanocomposites exhibited improved thermal stability over a wide temperature. Alternating current (AC) electrical conductivity and dielectric properties were analyzed through BDS measurements.[3,4] The concentration of zeolite nano filler was observed to enhance the dielectric constant and AC conductivity. The introduction of these nanoparticles into the polymer blend contributed to superior crystallinity, thermal stability, dielectric properties, and AC conductivity, making them a promising material for applications in energy storage devices, including serving as an intermediate layer in supercapacitors and batteries.

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PP 39

Device Grade Spray-Coated Transparent Conducting Thin-Films

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Keywords: FTO Thin films, Transmittance, Photovoltaic applications

Fluorine-doped tin oxide (FTO) is a transparent conducting oxide material commonly used in consumer electronics like display devices, solar cells, etc. The critical doping of tin oxide (SnO_2) with fluorine (F) leads to transparent conducting oxide thin films with high electrical conductivity and optical transparency, making it suitable for optoelectronic applications requiring transparent conducting layers. In this paper, we report on the development of a process recipe for growing fluorine-doped tin oxide-coated glass slides using an in-house spray pyrolysis technique. XRD analysis of the film reveals that the spray pyrolyzed flourine-doped SnO_2 thin film is tetragonally crystallized without any impurity phases. The film thickness was calculated by the gravimetry method and confirmed by the optical transmittance method. The optical transmittance of the thin films is found to decrease as the volume increases. We have optimized the process recipe which enables us to grow transparent conducting films whose sheet resistance can be tuned as per device requirement from $100\Omega/cm^{2,}$ to as low as $14\ \Omega/cm^2$.

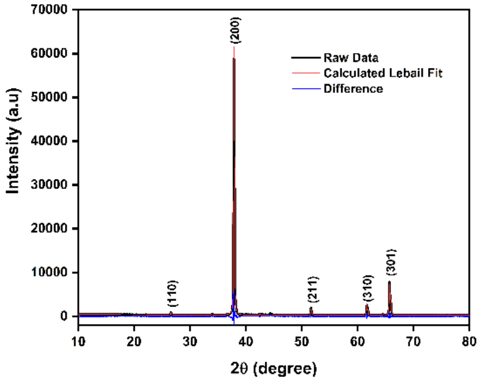

Figure 1: *Lebail-fitted XRD data of the optimized FTO Thin Films*

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PP 40

Enhanced Thermoelctric Power Factor of Nickel Ferrite Incorporated Zinc Oxide for Waste Heat Retrieval

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Key words: High Temperature Thermoelectricity, Energy filtering, Oxide Semiconductor Composites, Ferrites, Magnetic properties

Thermoelectric (TE) devices have emerged as a potential solution to mitigating global warming, as they allow for the conversion of waste heat into usable electrical energy. Achieving optimal performance in these devices often relies on dual-phase materials that possess a unique energy filtering mechanism. This mechanism allows for the control of certain properties, such as electrical conductivity and Seebeck coefficient, in relation to carrier concentration and carrier mobility. In this study, we focus on the preparation of NF@ZnO samples from Nickel Ferrite (NF) and ZnO as the precursors. The stoichiometric weight ratio between NF and ZnO was varied to investigate its influence on the thermoelectric properties. For our investigation, we analyzed the NF1.25 sample, which exhibited the highest values of carrier mobility and a moderate carrier concentration. The involvement of carrier energy filtering results the highest power factor value 1189 $\mu W m^{-1} K^{-2}$ and improved electrical conductivity value 17434 $S m^{-1}$ at a temperature of 953 K. These values were found to be 5.6 times higher for the power factor and 22.7 times higher for electrical conductivity compared to pristine ZnO. The findings of this study offer a promising and efficient material for high-temperature thermoelectric applications.

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PP 41

Evaluation of Optical, Thermal, Electrical and Gas Sensing Properties of Poly(pyrrole-co-indole)/Copper Alumina Nanocomposites

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Keywords: Poly(aniline-co-indole), nanocomposites, temperature-dependent conductivity, dielectric parameters, DC conductivity modelling

PANI-co-PIN)/Cu-Al_2O_3 with excellent AC conductivity, dielectric traits, and ammonia gas sensing properties were synthesized by benign in-situ chemical oxidation polymerization. The presence of Cu-O bonding vibration and shift of some characteristic peaks in the FT-IR spectrum revealed the efficient encapsulation of Cu-Al_2O_3 nanomaterial within the macromolecule. The π– π * transitions and n– π * transitions are observed in the UV spectra of copolymer and nanocomposites. The optical bandgap energy of PANI-co-PIN, calculated from Tauc plot was observed to decrease with reinforcement of Cu-Al_2O_3. Comparing the XRD of PANI-co-PIN and (PANI-co-PIN)/ Cu-Al_2O_3, crystallinity was enhanced with filler content. This manifests the interaction between filler particles and copolymer. The HR-TEM images confirmed the reinforcement of inorganic moiety in the copolymer. From TGA it was quite perceptible that thermal resistance of (PANI-co-PIN) was enhanced with the inclusion of Cu-Al_2O_3 nanomaterial. The room temperature and high temperature alternate current (AC) conductivity properties of nanocomposites were higher than pure PANI-co-PIN.[2] The DC conductivity of copolymer was enhanced with encapsulation of Cu–Al_2O_3 nanoparticles and the change in conductivity was in compromise with McCullough models. The match in theoretical and experimental conductivity values was advocating the presence of an efficient conductive pathway[4]. The gas sensing properties of synthesized copolymer nanocomposites showed excellent sensitivity and response towards ammonia gas at room temperature. Maximum gas sensing traits was observed for (PANI-co-PIN)/5wt.%Cu-Al_2O_3 nanocomposite. The magnificent AC conductivity, dielectric properties and gas sensing traits of (PANI-co-PIN)/ Cu-Al_2O_3) could well be exploited in developing electrochemical sensing devices.

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PP 42

Selective Detection of Biologically Relevant Ions and Molecules by Pillar[5]arene Derivatives in Water Milieu

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Keyword: Supramolecular Chemistry, Pillar[n]arenes, Metal Ions, Amino Acids

Transition metal ions of copper and iron play a vital role in biological processes owing to its involvement in oxido-reductace processes, electron transfer, etc. In addition to cations, amino acids are involved in several biological processes and they are part of several cellular functions. However, the excess intake and deficiency of metal ions and amino acids lead to several disorders in humans. Hence, the detection of metal ions and amino acids by various synthetic receptors using spectral techniques is an emerging area of research. Supramolecular systems functionalized with multiple binding cores and fluorophores are good candidates for sensing ions and molecules due to their unique characteristics such as ease of synthesis and functionalization, preorganized binding core, electron-rich cavity, tunable solubility either in organic or aqueous medium, etc. In this perspective, we have synthesized a water-soluble pillar[5]arene (**PAA**) bearing a triazole and carboxylic acid group for the detection of ions and molecules. The pillar[5]arene derivative, **PAA** is found to be selective for Fe^{3+} and Cu^{2+} among 11 biologically relevant ions with a minimum detection limit of 2.09×10^{-6} and 5.89×10^{-6} M respectively based on fluorescence spectroscopy. Further, the secondary sensing abilities of the *in-situ* prepared Fe^{3+} and Cu^{2+} complexes of **PAA**, viz.; **FePAA** and **CuPAA** were tested for amino acid sensing. The **FePAA** detects Arg, Cys, and Lys among 18 amino acids while the **CuPAA** detects His among 18 proteinogenic amino acids by fluorescence spectroscopy. The interaction of **PAA** with cations and the metal complexes of **PAA** with amino acids were further supported by UV-visible spectroscopy.

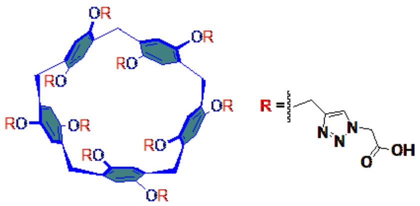

***Figure 1:** Structure of PAA*

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PP 43

Exploring Phase Transition-Driven Self-assembly of Poly(aryl ether) Dendron Derivatives for Sustainable Materials

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Keywords: Liquid crystal, dendron, spherulite, supramolecular gel

Electronic devices based on organic semiconductors have gained increasing attention in nanotechnology, especially in the area of field-effect transistors and photovoltaics. Discotic liquid crystals, comprising disc-shaped molecules forming one-dimensional columnar superstructures through aromatic unit interactions, emerge as promising materials in this domain.[1] Investigation into red, green, or blue-coloured small organic molecules has been extensive for the advancement of organic light-emitting diodes (OLEDs).[2] Notably, among the blue emitters, anthracene derivatives exhibit superior photoluminescence and electroluminescence properties. Strategies involving the integration of long alkyl chains or steroidal groups into discotic structures have been explored to achieve highly ordered assembly.[3] However, these additions can often remain inert and undesired for the optoelectronic characteristics of the system. Given previous findings indicating self-assembly in discotic fashion in gel phases with poly(aryl ether) dendron derivatives, our study aims to investigate the impact of phase transitions on this self-assembly. The resulting spherulites from poly(aryl ether) dendron derivatives exhibited high anisotropy, indicative of coherent long-range order, suggesting spontaneous self-assembly of the dendron derivatives over extensive distances, observed specifically in AB_3 type dendrons. This exploration aligns with the pursuit of sustainable materials for electronics, showcasing the potential for self-assembly in these organic systems. Understanding phase transition impacts on assembly behaviours in eco-friendly materials like dendron derivatives contributes to the development of sustainable electronic devices with tailored properties and reduced environmental impact.

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PP 44

Facile synthesis of Fe_3O_4 nanoflake array on iron foil for supercapacitor application

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Keywords: Hydrothermal synthesis, Nanoflakes, Phase transformation

This research introduces a novel approach for the hydrothermal synthesis of nanoflakes on iron oxide films. The iron oxide films were initially prepared through a high-temperature annealing process, followed by a meticulous hydrothermal treatment to induce the unique nanoflake morphology. The synthesis process was systematically characterized to elucidate the growth mechanism and optimize the formation of the desired nanostructures.[1]

Comprehensive ultraviolet (UV) studies were conducted to analyze the band gap properties of the synthesized materials. The phase transition from hematite to magnetite was observed, shedding light on the structural modifications resulting from the hydrothermal synthesis subsequent to the annealing process.[2] Various characterization techniques were employed to provide a detailed understanding of the phase changes throughout the synthesis.

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PP 45

Hydrogen Gas Sensors Based on Nano Pt Functionalized Endoped Carbon Nanofibers with Induced Mesoporosity

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Keywords: Hydrogen Sensors, Mesoporous Carbon Nanofibers, Electrospinning

One of the most significant reducing gases is hydrogen, an odourless, colourless gas that is exceedingly buoyant and combustible at concentrations between 4 and 75% (by volume) when combined with air. Therefore, as hydrogen is flammable or explosive if not handled properly, its manufacture, storage, and transportation may be dangerous. Moreover, hydrogen (H_2) is a reliable clean energy carrier that can be produced from a variety of renewable energy sources and it is used in numerous chemical processes and a wide range of industries. Recently, interest in the use of hydrogen in fuel cells for power generation and transportation has increased. In this regard, researchers have directed their efforts towards the formulation of novel materials. In this scenario, room-temperature H_2 gas detection can be significantly useful for hydrogen safety and leakage applications. Towards realization of room temperature gas sensors, carbon-based nanostructures can be potential candidates because of their huge surface area and high electrical conductivity. Carbon nanofibers (CNFs) based sensors are also typically more sensitive to a wider variety of gases at ambient temperature.[1] However, due to poor selectivity, CNFs-based sensors are not as widely used in gas sensing applications. Integration of Catalytic metals to CNFs can be used to solve such selectivity issues, and they may operate exceptionally well towards hydrogen gas. So that Pt catalysts have been demonstrated due to its outstanding efficacy. It is suggested that Pt can be functionalized on mesoporous carbon nanofibers (pCNF) to increase the selectivity towards hydrogen.[2,3] Here, we demonstrate the evolution of a hydrogen sensor using electrospun mesoporous carbon nanofibers. In order to detect hydrogen gas at the trace level, gas sensing characteristics were methodically studied.

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PP 46

Imidazole based Highly Selective “Turn-Off” Fluorescent Chemosensor or Iron(III) Ions Detection and Biological Applications

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Keywords: Imidazole, Chemosensor, Fe^{3+} ion, Fluorescence quenching, Bioimaging, A549 cells

Two imidazole based fluorescent chemosensor**1** (2-(2-(4-(2-(4,5-c-2-yl)naphthalene-3-yloxy)butoxy)naphthalene-1-yl)-4,5-diphenyl-1*H*-imidazole) and chemosensor **2** (2-(2-(4-(4-methyl-2-(4,5-diphenyl-1*H*-imidazole-2-yl)phenoxy)butoxy)-5-methylphenyl)-4,5-diphenyl-1H-imidazole) were synthesized and characterized by FT-IR, ^{1}H,^{13}CNMR, ESI mass spectroscopy and single crystal X-ray diffraction analysis. The chemosensor **1** crystallizes in monoclinic, space group *C 2/c.* The chemosensors **1** and **2** displayed a selective fluorescence quenching response towards Fe^{3+} ions at 435 nm and 390 nm, respectively, in DMF solutions among other tested cations due to the well-known mechanism of chelating quenched fluorescence (CHQF). The binding constant to form the **1**+Fe^{3+} and **2**+Fe^{3+} complexes were calculated using the modified Benesi-Hildebrand equation, which were about 2.2×10^{3} M^{-1} and 1.3×10^{4} M^{-1},respectively. The calculated average fluorescence lifetimes of **1** and **1**+Fe^{3+} were 2.51 ns and 1.17 ns and for **2** &**2**+Fe^{3+} were 1.13 and 0.63 ns, respectively. Furthermore, chemosensors **1** and **2** could be utilized to detect the presence of Fe^{3+} ions in live cells and showed negligible cell toxicity.

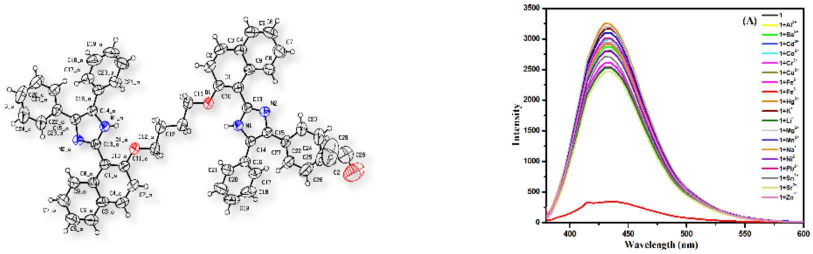

Figure 1*: ORTEP diagram of 1 (50% probability) and Fluorescence emission spectra of chemosensor*[1]

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PP 47

Oxalamide-Based Sensor for Detection of Cu^{2+}/Fe^{3+} ions and its Application in Live Cell Imaging

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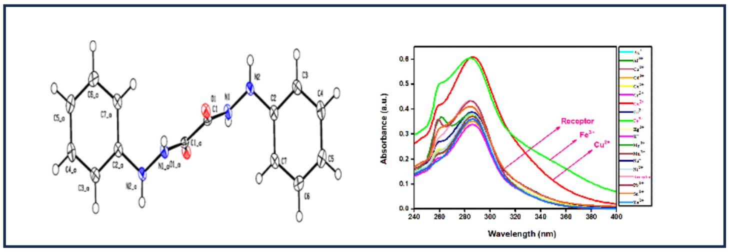
Keywords: Oxalohydrazide, Single crystal X-ray diffraction, Copper (II) ion, Iron (III) ion, DFT, and MDA-MB-231 cell line



The *N*^{1},*N*^{2}-diphenyloxalohydrazide $OX(HA)_2$ chemosensor was synthesized and used as a colorimetric and fluorescent receptor to detect Cu^{2+} and Fe^{3+} ions in the presence of other metal ions. A range of physicochemical approaches were utilized to characterize the symmetrical oxalohydrazide-based receptor, including FT-IR, ^1H and ^{13}C NMR, TGA, and mass spectrometry. According to single crystal X-ray diffraction investigation, $OX(HA)_2$ crystallizes in monoclinic with space group *C2/c*. UV-vis and fluorescence spectroscopy were used to thoroughly explore $OX(HA)_2$'s sensing capabilities towards diverse cations. Using measurements of fluorescence intensity, the binding constant for $OX(HA)_2$ with Cu^{2+}/Fe^{3+} ions was calculated to be 2.78×10^3 M^{-1} and 1.12×10^3 M^{-1} with the lower detection limit of 0.43 µM and 0.2 µM respectively. With a 1:1 binding mechanism validated by density functional theory. The average fluorescence lifetimes of $OX(HA)_2$, $OX(HA)_2+Cu^{2+}$, and $OX(HA)_2+Fe^{3+}$ were calculated to be 2.19 ns, 1.73 ns, and 1.26 ns, respectively. This fluorescence lifetime measurement results strongly support the complexation of Cu^{2+} and Fe^{3+}. When Cu^{2+} and Fe^{3+} ions bind with $OX(HA)_2$, they induce the 'Turn-Off' signal. Then, fluorescence imaging of the $OX(HA)_2$ receptor in MDA-MB-231 demonstrated that the receptor holds a lot of promise for usage in bioimaging. Furthermore, fluorescent probe for detecting Cu^{2+} and Fe^{3+} ions in living cells, making it potentially helpful as an anticancer medication.

PP 48

Multi-stimuli-responsive Chromogenic Systems for Smart Applications

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Keywords: Chromogenic, Multi-responsive, Smart materials

Stimuli-responsive materials are of immense interest these days because of their ability to undergo adjustment of their properties in response to their environment. The properties of such materials can be tuned by subtle changes in temperature, voltage, light, and so on. Various reactions to these stimuli include changes in colour, shape, volume, etc.[1,2] Among such smart materials, chromogenic systems are notable where the property being changed is their colour. Colour alteration indicates change in their optical properties which make these intelligent systems notable for energy efficient applications. Moreover, addition of multi-responsive feature to such chromic materials greatly enhances their applicability.

In our present work, we focus upon multi-stimuli-responsive chromogenic materials where their properties can be tuned via more than one stimulus. The designed systems are simple electro-thermoresponsive metal complexes which reversibly switch their colour between variable colour states upon optimum changes in voltage and temperature. The electrochromic behaviour is attributed to the variation in the redox properties of the metal ion and the thermal liability of the ligand in the presence of a coordinating solvent is responsible for the thermochromic behaviour. This dual responsiveness has been explored using different characterisation techniques and these systems are expected to be used for several smart applications such as in smart windows, anti-counterfeiting, sensing etc.

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PP 49

Analyte Selective Oxidative Fluorescence Sensing in Poly-N-phenylanthranilicacid-co-poly-o-phenylenediamine Copolymers

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Keywords: Fluorescence sensor, copolymers, polymer blends, conjugated polymer

Conjugated polymers possess many functional applications in optoelectronic devices.[1] Their optical and electronic properties can be tuned to maximum extents in copolymers than homopolymers.[2] Analyte selective oxidation strategies were adopted in poly-N-phenyl anthranilic acid-co-Poly-o-phenylenediamine copolymers for fluorescence sensing. Copolymers of N-phenyl anthranilic acid (NPA) and o-phenylenediamine (OPD) were synthesized by chemical oxidative polymerization and compared with homopolymer blends of poly-N-phenyl anthranilic acid (PNPA) and poly-o-phenylenediamine (POPD). The structural differences between copolymers and blends were evident from methods such as ^{1}HNMR, FTIR, and PXRD. The higher reactivity of the NPA monomer in P(NPA-co-OPD) copolymer was confirmed from spectroscopic analysis and using the Fineman-Ross method.[3] The emission tuning of the homopolymer blend (PNPA-b-POPD 25:75) at different pH resulted in fluorescent colors like blue, violet, yellow, green, and cyan. In copolymers, the blue emission was dominated except for P(NPA-co-OPD) 10:90, which has yellow emission. The change in the fluorescence of copolymer P(NPA-co-OPD) 10:90 from yellow to blue was obtained by adding $AgNO_3$, and subsequently, a blue to colorless was obtained by adding acidified $KMnO_4$, indicating the semi-oxidation of POPD fragments and complete oxidation of both POPD and PNPA fragments respectively (figure 1).

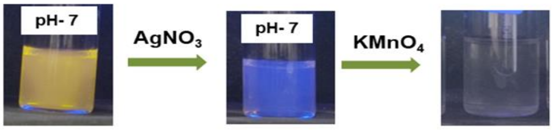

Figure 1: *Analyte Selective Oxidative Fluorescence Sensing*

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PP 50

Synthesis, Structural Characterization, and NLO Studies of Metal-Complexed Iminium Phosphoryl Groups

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Keywords: Metal complex, iminium phosphoryl, NLO

The objective of this research work is an investigation of the synthesis, structural characterization, and study of the NLO and biological properties of metal-complexed iminium phosphoryl groups. A number of transition metal complexes of the type $[M(CO)_xCl_yL]$ have been predicted to exhibit non-linear optical (NLO) properties based on Density Functional Theory calculation. The isolated iminium phosphoryl molecules to selected platinum group metals and other late transition metals, with designed ancillary ligand systems, to afford air-stable complexes that can be spectroscopically and structurally characterized. These transition metal complexes will then be investigated for non-linear optical and its biological properties.

PP 51

Black Color Electrochromism in Terpyridine-based Metallosupramolecular Assemblies

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Keywords: Black color electrochromism, Terpyridine MSPs, Solvent dependent electrochromism

The reversible optical changes associated with transparency and absorption occurring in a system under external bias due to the presence of redox-active units is called electrochromism.[1] Coordination-driven self-assembled metallo supramolecular polymers (MSPs) are a promising class of electrochromic materials, due to the presence of electrochemically active metals and ligands.[2] The quest for achieving black or neutral shades in electrochromic material has been prevalent since its introduction. However, developing such systems are not straight forward and are still in its infancy. The use of a combination of conducting polymers, different device architectures including blends, laminates, multilayered devices, etc. have provided initial advancements in this field.[3] We have developed a few terpyridine-based metallosupramolecular materials and their assemblies, whose optical response can be tuned by the use of different solvents and exhibit multicolor electrochromism, including black color in their neutral or redox states. These assemblies in their film and device configurations exhibit fast switching response and are stable for multiple cycles of operation.[4]

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PP 52

Successive Detection of Zn^{2+} and PA Using a Schiff Based Fluorescent Sensor Derived from 2-Hydroxy-1-Naphthaldehyde

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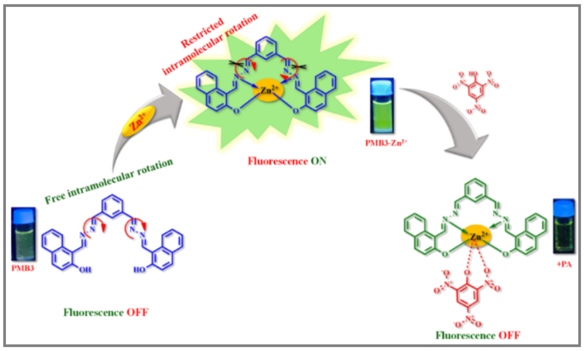
Keywords: Fluorescent sensor, femtomolar, picric acid

A novel fluorescent Schiff based sensor PMB3 derived from 2-hydroxy-1-naphthaldehyde was designed, synthesized, and characterized by different spectroscopic methods. PMB3 displays a highly selective, sensitive, and rapid response to Zn^{2+} with fluorescence changes. The sensor PMB3 binds with Zn^{2+} to form a complex in a 1:1 ratio which resulted in the significant fluorescence enhancement upon gradual addition while there is no significant effect on emission intensity even in presence of other metal ions. The limit of detection of zinc was found to be 11.12×10^{-7}M. The PMB3-Zn^{2+} complex ensemble was found to be highly selective for femtomolar detection of highly explosive picric acid(PA), over other aromatic explosives in the aqueous medium. The detection limit for picric acid found by using the *in-situ* formed zinc complex [PMB3-Zn^{2+}] ensemble was 42.40×10^{-15}M. Hence the newly developed sensor complex ensemble is highly efficient for the detection of PA aqueous medium[1].



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PP53

Theoretical Screening Into Urea-Based Receptor As A Promising Toxic Gas Sensor Upon SO_2, NH_3 And H_2S

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Keywords: urea-based receptor; Density functional theory; QTAIM; EEF; PDOS

The adsorption of toxic gases such as NH_3, SO_2, H_2S, on 1,3 bis (4-nitrophenyl) urea (BNPU) was investigated via the M062X/6-311++ g (d, p) level of theory to evaluate the utility of BNPU-based gas sensors[1]. For each gas molecule, the most stable configuration was determined and the adsorption energies were calculated. The trend of adsorption stability of complexes is observed as, SO_2@BNPU≈NH_3@BNPU>H_2S@BNPU. Further, electronic properties such as orbital analysis, natural bond orbital analysis, and density of states were investigated to understand the mechanism of sensing[2]. The HOMO-LUMO gap was lowered upon adsorption with these gases. The QTAIM analysis was carried out to sketch the nature of the hydrogen bond. Also, short recovery time was found for all three toxic gases, which is a crucial discovery since it establishes the value of a sensing material's recyclable nature[3]. An external electric field (EF) of intensity -0.15 V/Å up to +0.15 V/Å was used to further improve the toxic gas-sensing properties of the BNPU[4]. Furthermore, the presence of the EF has a significant effect on the dipole moment and the HOMO-LUMO energy gap.

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PP 54

Metal-Organic Coordination Compound: Probing Electrical and Geometrical Properties through Spectroscopic Analysis

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Keywords: Metal-organic crystal, XRD, DFT, Vibrational studies, NBO, UV-Vis

The quantum mechanical investigations on the structure, electronic, and vibrational spectra of hexachlorobis(μ-1λ5-pyridine-1-olato)-di-copper are done in this study. Computational quantum chemistry, uses many approximation methods, including Density Functional Theory. DFT is used in this work to obtain necessary information about the many-electron system under study.[1] The metal-organic crystal was synthesized and single crystals were grown by slow evaporation technique.[2] The crystal structure was reinvestigated by X-ray diffraction analysis and DFT software package. DFT was used to obtain the theoretical calculations using the Gaussian G09 program package. BLYP/cc-PVTZ/LANL2DZ level of theory was used to obtain the geometrical optimization of the compound. The electron transport mechanism and hydrogen bonding interactions in hexachlorobis(μ-1λ5-pyridine-1-olato)-di-copper have been studied using Natural Bond Analysis. The vibrational spectral investigations of the compound have been carried out using experimental and computational FT-IR. The UV absorption spectrum of the studied compound was recorded in the region of 550 nm. The optical band gaps obtained from the tauc plot, HOMO-LUMO, and PL was found to be nearly equal values such as 2.35 eV, 2.19 eV, and 2.318 eV respectively. The full-width half maximum of PL was found to be 14.373 eV which shows the broadening of the PL peak and suggests the impurity effect of the crystal[3].

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PP 55

Predictive Modeling of MAO-B Inhibitory Compounds: A Machine Learning-Enhanced QSAR Analysis

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Keywords: Monoamine oxidase B, QSAR, machine learning, regression, chemical space

Monoamine oxidase B (MAO-B) is a critical enzyme involved in the catabolism of various biogenic amines, including dopamine and serotonin. Dysregulation of MAO-B activity has been implicated in various neurodegenerative disorders, making it an attractive target for drug discovery and development. In this study, we present a machine learning regression model developed to predict the inhibitory activity of compounds against MAO-B using data sourced from the ChEMBL-33 database. We generated both PaDEL molecular descriptors and Lipinski's Rule of Five descriptors to capture key structural and physicochemical properties of the compounds. A quantitative assessment of compound efficiency is derived through the application of a Quantitative Structure-Activity Relationship (Regression) model, developed using the meticulously prepared dataset. We conducted a comparative analysis of the MAO-B inhibitors' regression model using Python's Lazy Predict library, assessing its performance against various alternative models based on R-squared error metrics and computational time measures. The comparisons were visualized using two Lipinski descriptors, Logp and MW, that analyze active and inactive classes of chemicals. It was found that the two bioactivity classes occupy similar chemical regions.

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PP 56

A Theoretical Exploration of the Antioxidant Activity of Hibiscetin Using DFT, NCI, AND QTAIM

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Keywords: Hibiscetin, DFT, QTAIM, antioxidant

The present work focuses on the structural and antioxidant ability of the naturally occurring flavonol Hibiscetin investigated in gas, water, and benzene media using M06-2X functional level of density functional theory (DFT) with 6-311+G(d, p) basis set. The quantum theory of atoms in molecules (QTAIM) is used to study the strength of intramolecular hydrogen bonding[1] and non-covalent interactions (NCI), which are critical for the antioxidant action of polyphenols. Thermodynamic factors associated with the three primary antiradical mechanisms of polyphenols have been investigated[2]. The favorable radical scavenging mechanisms in gas, polar, and non-polar solvents are identified. The reactivity of the molecule is confirmed by the examination of Frontier molecular orbitals (FMO) and global descriptive characteristics. According to the study, radical attacks prefer to occur at the 8-OH position. The FMO and electrostatic potential (ESP) map confirm the location of the active site[3].

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PP 57

Investigations on Phenylisothiocyanate by FT-IR, FT-Raman, NMR, UV-Vis Spectroscopy, HOMO-LUMO, MEP, and NLO Properties Using Density Function Theory Analysis: A Potent Antimicrobial Compound

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Keywords: Density Functional Theory, HOMO_LUMO orbital, Mulliken Charge, Hyper Polarizability

Phenyl Isothiocyanate (PITC) is a phytochemical derived from the cruciferous vegetable that shows antimicrobial as well as anti-cancerous activity.[1] The Fourier transform infrared (FTIR), Fourier transform Raman (FT-RAMAN), nuclear magnetic resonance (NMR), and ultraviolet-visible (UV vis) spectra of Phenyl isothiocyanate have all been studied in great detail using quantum chemical calculations. Density functional theory (DFT) 6–31G(d,p) basis sets were utilized to aid in the interpretation of the molecular structure, fundamental vibrational frequencies, and intensities of the vibrational bands.[2] The charge transfer within the molecule is indicated by the predicted HOMO-LUMO energies,[3] which were determined to be -6.31eV and -1.24 eV respectively. Additionally, calculations of Mulliken charge, global descriptive parameters, thermal properties, and first-order hyperpolarizability were performed. The large value of hyperpolarizability indicates PITC interact well with electromagnetic radiation.

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PP58

A Theoretical Analysis of Ti based 2D-MXenes as HER Catalyst

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Keywords: HER, electrocatalysts, Mxenes

Hydrogen has emerged as an optimistic remedy as the world continues to grapple with the challenges of green energy storage and conversion, fulfilling the eco-consciousness. Along with high energy density, Hydrogen serves several positive aspects like recycling, zero pollution emissions, no greenhouse gas emissions, and many more. It is feasible to produce Hydrogen in various ways, like fossil fuel burning and biomass fermentation. However, the water-splitting-based Hydrogen Evolution Reaction (HER) is both cost-effective and eco-friendly [1]. The electrocatalyst plays a pivotal role in hydrogen production in the HER. Precious metal-based electrocatalysts, such as Pt and Ru, demonstrate high efficiency and stability. However, constrained resources and mounting expenses have hindered the ever-increasing demand for precious metal-based electrocatalysts. Therefore, it has been an imminent issue [2, 3, 4] to advance highly efficient non-precious metal (NPM) based HER electrocatalysts for preparing hydrogen. In our work we focus on MXenes which has emerged as a potential catalyst for HER, since its first discovery in 2011. MXenes appears in a graphene-like structure usually containing non-toxic elements such as Ti, C, and N and various functional groups on its surface along with its intriguing electrical, optical, and thermal properties, good hydrophilicity, redox capability [5]. In this particular study we have tried to cover Ti-based MXenes and the effect of metal doping on those in the field of HER catalyst.

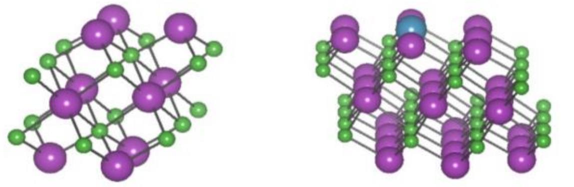

***Figure 1**: Monolayer structure of Ti_3C_2 and monolayer structure of $(Ti_{0.97}Zr_{0.03})_3C_2$ respectively*

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PP 59

Jackfruit Pectin-Chitosan Polyelectrolyte Coated Microcapsules

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Keywords: Pectin, jackfruit, microcapsules, polyelectrolytes

Pectin is mostly produced commercially from citrus peels and apple pomace. However, since the uses for pectin have been growing throughout time, continuous research is currently being done to investigate and examine more botanical sources of extraction. Jackfruit is a seasonal fruit that is usually grown in tropical and subtropical regions. Jackfruit cultivation is limited in commercial settings due to a higher percentage of inedible components such as the internal core, inner perigones, and prickly rind make up around 60% of the entire jackfruit., which increases waste production. This situation can be avoided by producing value-added compounds from jackfruit waste. Microencapsulation is used as an approach aiming to preserve substances from the environment through a thin layer. One of the various strategies for encasing active substances is the formation of polyelectrolyte complexes based on the beneficial interaction between polymers with opposing charges. The aim of this study was to, first, extract pectin from Jackfruit waste[1] and investigate the film-forming potentials of jackfruit pectin by forming a polyelectrolyte complex with Chitosan, an antibacterial agent. Finally, to provide evidence of the possible applicability of the novel jackfruit pectin- Chitosan polyelectrolyte complex in the formation of microparticles and capsules suitable for active agent encapsulation. It was observed that about 30% of pectin yield is obtained from jackfruit waste parts. The ATR-FTIR spectra of jackfruit pectin shown to be identical to those of commercial pectin. Multilayer build-up process between jackfruit pectin - chitosan were monitored using ATR-FTIR and FE-SEM. The results from ATR-FTIR spectra reveal that pectin and chitosan gets loaded to the multilayer system at all the studied pH and the FE-SEM data agrees with the ATR-FTIR spectrum findings. For the continuous ultrathin film formation lower pH was found to be more suitable. Hence the polyelectrolytes multilayer film formation on the $CaCo_3$ substrate[2,3] was carried out by using lower pH. From the FE-SEM images of jackfruit pectin-chitosan coated microparticles and capsules show smoothest thin layer formation indicates greater adsorption by cover up all the pores on the $CaCo_3$ substrate surface.

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PP60

Synthesis, Characterization, and Photophysical Analysis of Meso-Aryl Substituted Porphyrins: Unveiling Potent Antibacterial Photodynamic Activity

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Keywords: Metalloporphyrin, Photodynamic therapy, Antibacterial, Meso-aryl substituted porphyrin

The objective of this research is to synthesize and characterize *Meso*-tetrakis(4-methyl-5-hydroxyphenyl)porphyrin (1) and 5,10-(4-trifluoromethyl phenyl)10,20-(4-hydroxyphenyl) porphyrin (2) and their Zn complexes. Both of these porphyrins and their complexes had exceptional yields. The synthesized porphyrin and zinc complexes were careful characterized using a variety of spectroscopic methods, including mass analysis, nuclear magnetic resonance (NMR), and ultraviolet-visible (UV-Vis) spectroscopy. As a result of the powerful antibacterial qualities that they possess, porphyrins have significant ligand potential for antibacterial activities by virtue of their features. The fact that the porphyrins that were replaced with meso-aryl shown a significant antibacterial efficiency is something that should be taken into consideration. The purpose of this study is to investigate the production of one-of-a-kind photosensitizer complexes, despite the inherent challenges that are associated with the solubility and selectivity of these macrocycles. The research makes important additions to our knowledge of the many uses of meso-aryl substituted porphyrins, with a particular emphasis on the potential of these porphyrins to be viable competitors in the field of antibacterial photodynamic treatment.

PP 61

Production and Spectroscopic Investigation on Nucleation of Metal Oxide Nano Crystals and their Response in the Production of Anthraquinones in *In-vitro* Cultures of *Rubia Cordifolia L.*

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Keywords: Anthraquinone, Green nanotechnology, Raman spectroscopy

Green nanotechnology, or the creation of nanoparticles (nps) using biological processes, notably plant extracts, is a developing field of study. Today, combining nanosystems with plant tissue culture is essential for bioactive component manufacturing, genetic engineering, crop improvement, and mass reproduction.[1] Here we have created ZnO and CuO nps using stem extract of *Rubia cordifolia L*. and their structural features have been confirmed using the methods of UV-Vis, FT-IR, Raman spectroscopy, DTG, XRD, SEM-EDX, and TEM.[2] The green synthesised nps were applied in tissue culture media of *R. cordifolia L*. The plants were harvested after 60 days of growth. The percolation of ZnO and CuO nps from the tissue culture medium to the roots of the plant was demonstrated by Raman spectroscopy. Moreover, the reduction of CuO to Cu_2O inside the plant system was also indicated by Raman spectroscopy. The carotenoids, and chlorophyll contents as well as the anthraquinone pigments (Alizarin and purpurin), in the plant samples treated with nps showed enhanced bands when compared to control samples, however anthocyanin content was repressed. The present study points out the importance of green synthesised nps ZnO and CuO in enhancing the production of the natural dye-producing components alizarin and purpurin on a commercial scale in *in vitro* cultured *R. cordifolia,* thus avoiding the overexploitation of this endemic plant. [3,4]

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PP 62

Structural and Thermal Characaterisation of Bacterial Cellulose Produced by *Novacetimonas Hansenii* in Static Culture Condition

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Keywords: Biopolymer, Bacterial Cellulose, *Novacetimonas hansenii*

With the advances in nanotechnology, there is increasing demand for nanocellulose as the packaging material, film for various implants, paints, coatings, and electronic sensors. At the biomedical level, nanocellulose has immense application as a scaffold for tissue engineering and wound healing as it mimics the extracellular matrix. Here comes the importance of bacterial cellulose (BC), the nano cellulose synthesized by microorganisms.The cellulose obtained by bacteria comprises repeated D-glucose units linked by β (1-4) linkage and is free of other complex polymers such as lignin and hemicelluloses. The Gram-negative *Komagataeibacter xylinus* is one of the most exploited organisms for BC production. Recently, four different species of *Komagataeibacter*were reclassified to be novel members of the genus *Novacetimonas.*[1] This work has been designed to isolate cellulose-producing bacteria from rotten fruits such as apples, oranges, pomegranates, and grapes. Among the various bacteria screened, the isolate P3 purified from the rotten pomegranate sample demonstrated the cellulose-producing property. Upon 16S rDNA sequencing-based molecular identification, the P3 was identified as a strain of *Novacetimonas hansenii (*GenBank Acc. No. OM883845). This was the first report on isolating cellulose-producing *Novacetimonas hansenii* from rotten pomegranate.[2] The BC synthesized has also been characterized in detail by Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (XRD), and Thermo Gravimetric Analysis (TGA). The cellulose film was demonstrated to have mainly the cellulose I structure with a high relative crystallinity index and stable up to 300˚C.

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PP63

Extraction and Characterization of Cellulose Derived from Peanut Shell

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Keywords: Extraction of cellulose, Peanut shell, Alkali treatment, Bleaching

Repurposing peanut shells as agricultural waste for cellulose production to reinforce polymers involves a detailed process explored in this study. Through alkali treatment and bleaching, cellulose was efficiently extracted from peanut shells, yielding an impressive 50% of cellulose. Infrared spectroscopy revealed the removal of lignin and hemicellulose post-bleaching, confirming successful cellulose extraction. X- ray diffraction showed enhanced cellulose peaks and increased crystallinity from 37% to 60% after alkali and bleaching treatments. Surface morphology analysis demonstrated the removal of hemicellulose and lignin, highlighting the transformation of peanut shell waste into versatile cellulose for polymer reinforcement. This study emphasizes the potential of peanut shells as a valuable resource for sustainable material production.

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PP 64

Poly-N-phenylanthranilicacid Fluorescent Polymer Dye for Cell Imaging and Secret Writing Applications

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Keywords: Conjugated polymer, secret ink, fluorescent dye, cell imaging

Poly-N-phenyl anthranilic acid based UV active fluorescent dye was developed to stain different non-emissive hydrophilic substrates for multifunctional applications.[1] The stability of fluorescence emission of PNPA-H in an acidic, neutral, basic medium made them suitable for various applications (see figure 1). The invisible character of PNPA-H was utilized for secret writing as an anti-counterfeiting tool. The biocompatibility and staining ability of protonated N-phenyl anthranilic acid monomer and poly-N-phenyl anthranilic acid polymer enabled us to perform cell imaging studies.[2] Cell uptake of monomer NPA-H and polymer PNPA-H were compared using normal cell line L929 and papillary thyroid cancer cell line MDA-T32. The nuclear staining ability of NPA-H and PNPA-H was evident from the bright blue fluorescence from the nucleus of the cells. The nuclear staining of NPA-H and PNPA-H toward cancer cells was more effective compared to normal cells, which indicates the selectivity of NPA-H and PNPA-H toward cancer cells. A fluorescent conjugated polymer, suitable for both nucleus-targeted staining and invisible ink applications, was not yet reported. In short, poly-N-phenyl anthranilic acid is a suitable candidate in both anticounterfieting areas and in bioimaging fields.

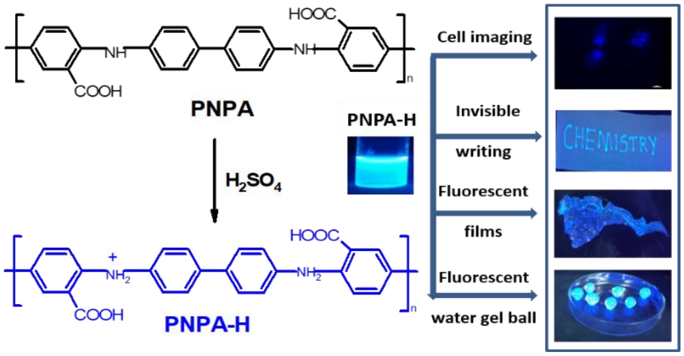

***Figure 1**: Schematic representation of Protonation in PNPA and its applications.*

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PP 65

Tuning Luminescence, Mechanical Flexibility, and Transport Properties in Single Crystals of Thiazolothzaole Derivatives

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Keywords: Molecular Crystal, Interaction Engineering, Luminescence, Mechanical Flexibility

Organic π-conjugated materials have demonstrated remarkable potential as active materials in optoelectronic devices due to its ease of synthesis, tunable properties and processibility. As the market moves towards flexible, adaptive, and wearable electronic systems, organic semiconductors are promising candidates, owing to their inherent capability to sustain mechanical stress and their ability to harmoniously fulfill the fundamental requirements of optoelectronic properties such as charge transport and luminescence. Optoelectronic properties of organic molecules can be substantially different to its bulk and depending upon interaction and relative orientation of molecules. Controlling the intermolecular interactions and molecular packing is therefore very crucial in tailoring the mechanical as well as the optoelectronic properties of organic conjugated molecules. We are interested into elucidating the molecular structure-packing-property relationship in a series of thiazolothiazole derivatives and utilize this understanding to develop novel materials with enhanced performance. In the poster we attempt to depict our efforts to understand the photophysical properties, charge transport and mechanical properties in simple thiazolothiazole derivatives by introducing functional groups. Co-crystal formation was employed as a strategy to fine-tune the photophysical and mechanical properties of these material.[1,2]

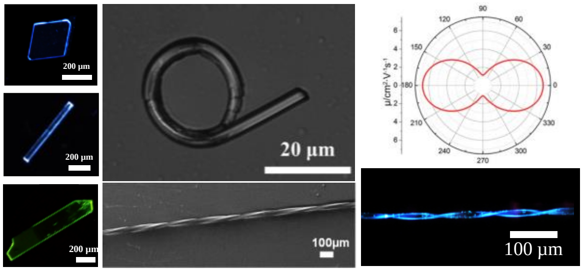

Figure 1: *Representative images of the crystalline polymorphs, mechanical flexibility, twist crystals and the polar plot for charge transport mobility.*

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PP 66

Mitigation of Mild Steel Corrosion in HCl Media Using the Leaf Extract of a Common Perennial Leguminous Plant

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Keywords: Pueraria phaseoloides, EIS, Polarisation, Maltoxazine

The potential of Pueraria phaseoloides (PP), a member of the Fabaceae family considered detrimental to forestry, was explored for its ability to mitigate mild steel corrosion in HCl media. Analysis of the water extract via LCMS identified corrosion-resistant phytochemicals, while GCMS analysis of the alcohol extract provided a list of bioactive ingredients in PP leaves. Gravimetric study of the sample showed that the PP water extract have better inhibition efficiency (94%) than the PP alcohol extract (85%). With this background corrosion mitigation studies of PP water extract was explored. The optimum inhibitor concentration in acid media is shown to be 3%(v/v) aqueous PP extract, as shown by the higher R_{ct} (495.6) value obtained through electrochemical impedance spectroscopy (EIS). The degree of inhibition was investigated by polarisation test (PDP) through a 7-hour immersion period. An inhibition efficiency of 95% was obtained using 3% aqueous extract through PDP data. The adsorption mechanism of maltoxazine inhibitor molecule on mild steel is explained through Biovia material studio software.[1]

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PP 67

Synthetic Access to 1,3-Butadiynes via Electro-redox Cuprous Catalyzed Dehydrogenative C_{sp}-C_{sp} Homocoupling of Terminal Acetylenes

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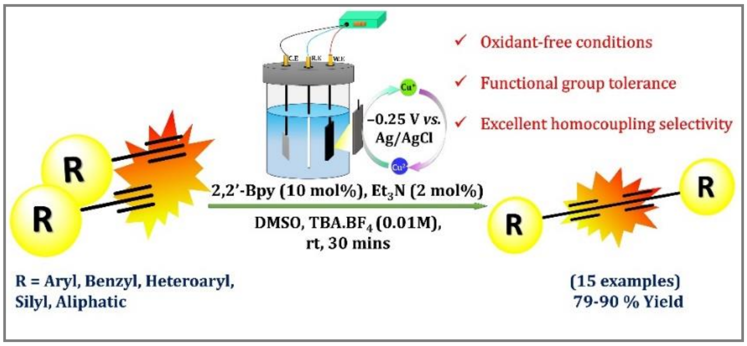
Keywords: Electro-redox chemistry, Cuprous catalysis, Glaser-Hay coupling, Homo-selectivity, 1,3-Butadiyne products

We have disclosed the oxidative homocoupling of terminal alkynes under electrochemically generated cuprous catalysis. The scope of this protocol is established by preparing an array of structurally and electronically different 1,3-butadiyne derivatives. Good synthetic yields, functional group tolerance, oxidant-free conditions and no cross-selectivity are some of the intrinsic advantages of this methodology. The developed chemistry features the electro-redox formation of copper-acetylide, an intermediate appropriate for the Csp-Csp coupling step. The chemical state of copper in the acetylide intermediate was found be Cu(I) as confirmed by click-trapping experiments, CV, EPR and XPS. Competition reaction to determine the reactivity of electronically dissimilar acetylenes revealed that the product ratio is rather dependent on the electronic nature of alkynyl substituents. To highlight the synthetic value of the products, selected diynes were subjected to chemical diversification.



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PP 68

CO_2-induced Glassification as a Green Method for the Preparation of Sustained Release Drug-Excipient Composites

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Keywords: Sustained release, supercritical CO_2, glassification

Sustained-release drugs are sought after due to reduced side effects and improved patient compliance. Earlier, it was reported from our group that supercritical CO_2 ($scCO_2$) processing results in glass formation in sucrose octaacetate (SOA), a CO_2-philic, FDA-approved excipient.[1] This hydrophobic glassy matrix immobilizes the drug, resulting in a slower release. Here, $scCO_2$ has been used as a green alternative solvent owing to its non-toxicity, low processing conditions (T_c = 31. 1̊ C, P_c = 73.8 bar), and ease of complete removal. Herein, we report the preparation, morphology (Figure 1,2), and drug release studies (Figure 3) of the composites of Ibuprofen (IBU) in SOA. The stability of the drug-excipient composite has also been investigated using structural (Figure 4), morphological (Figure 5), and release kinetic studies (Figure 6).

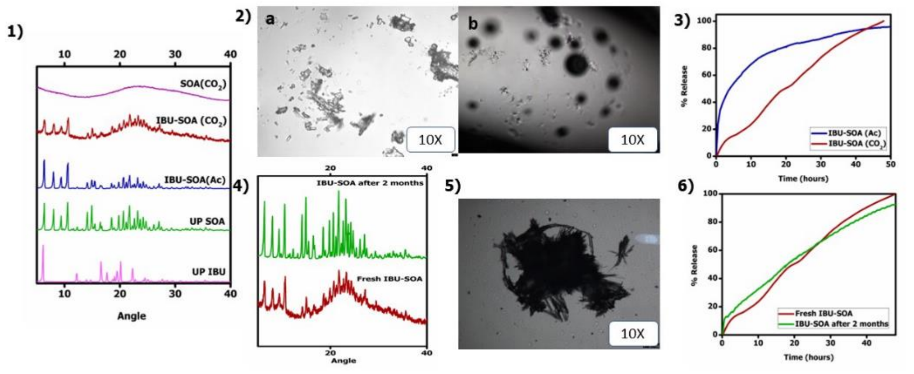

Figure 1: *XRD patterns of unprocessed IBU, unprocessed SOA, acetone processed IBU-SOA (1-20), $scCO_2$ processed IBU-SOA (1-20) and $scCO_2$ processed SOA;* ***Figure 2:*** *System microscopic images of IBU-SOA processed in a) acetone and b) $scCO_2$.* ***Figure 3:*** *Comparison of release patterns of IBU-SOA processed in acetone and $scCO_2$ using water as the medium; Fig 4: XRD patterns of fresh and two-month-old samples of $scCO_2$-processed IBU-SOA;* ***Figure 5:*** *System microscopic image of IBU-SOA after two months of being processed in $scCO_2$;* ***Figure 6:*** *Comparison of release patterns of fresh sample and sample kept for two months.*

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PP 69

Synthesis and Characterization of Ytterbium Molybdate Nanoparticle Modified Glassy Carbon Electrode for the Electrochemical Determination of Theophylline

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Keywords: Ytterbium Molybdate, nanoparticle, co-precipitation approach, theophylline and sensor

The synthesized Ytterbium Molybdate nanoparticle modified GCE for the electrochemical determination of theophylline via simple co-precipitation approach.[1] Various Analytical techniques such as FE-SEM, XPS, TEM were confirmed the formation of Ytterbium Molybdate nanoparticle. Subsequently the applicable electrochemical studies were followed and reported the considerable enhancement of electro catalytic activity of a Ytterbium Molybdate nanoparticle.[2] The proposed Ytterbium Molybdate nanoparticle was developed as an electro catalyst for the sensitive determination of theophylline. The electrochemical studies reveal that the Ytterbium Molybdate nanoparticle has a good linear dependence and high sensitivity towards theophylline. It also produces good practical availability. The proposed electrochemical sensor showed relatively low detection of 2 nM. It is expected that Ytterbium Molybdate/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of theophylline.

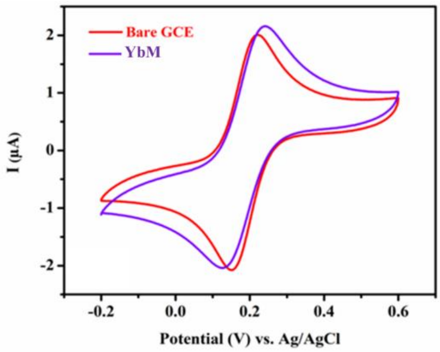

Figure 1. *CV responses of the bare GCE and Ytterbium Molybdate modified GCE in 1mM* $[Fe(CN)_6]^{3-/4-}$ *containing 0.1M KCl at scan rate of 50 mVs*$^{-1}$.

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PP 70

Fluorescent Trigonal Selenium Quantum Dots for Optical Sensing of Artificial Food Colorant

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Keywords: Selenium, quantum dots, sensing.

Luminescent nanomaterials especially quantum dots (QDs) have always attracted attention for their application in sensors, light emitting devices (LEDs) and other solid-state electronics. Trigonal Se quantum dots entrapped in a porous silica was synthesized via solvothermal assisted sol-gel route[1]. Morphology and structural validation of the dots was observed from Transmission Electron Microscopy (TEM) images, X-ray Diffraction (XRD) and RAMAN spectra. The dots exhibit a strong blue emission at 434 nm upon ultra-violet excitation wavelength at 350 nm which was successfully used for the optical sensing of artificial food colorant sunset yellow (E110)[2]. The emission spectrum of trigonal Se nanodots overlaps with the absorption spectra of sunset yellow facilitating a photon transfer between the probe and the analyte. Experimental evidences towards t-Se quenching behaviours are validated using extend of spectral overlap, steady state absorption spectra of the composite and time resolved fluorescence lifetime decay measurements. A linear response is established by plotting the ratio of fluorescence intensities (I_{616}/I_{434}) against the concentration of the quencher. Monitoring the amount of such colorants in consumed foods and cosmetics can therefore be achieved.

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PP 71

Enhanced Adsorption of Ciprofloxacin Antibiotic using Graphene Oxide Activated Carbon Composite: Synthesis, Characterization, and Performance Evaluation

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Keywords: Adsorption, Antibiotic, Ciprofloxacin, Graphene Oxide, Activated Carbon

In this study centered on adsorption application, a composite of graphene oxide activated carbon (GOAC) was formulated to counteract the agglomeration tendency of graphene oxide (GO) in water, which otherwise results in a decrease in its surface area. The GOAC composite, designed to enhance the adsorption capacity of GO, was thoroughly characterized using X-ray diffraction (XRD), Raman spectroscopy, and field emission scanning electron microscopy (FESEM) analyses. These analyses confirmed the successful incorporation of activated carbon (AC) into the GO matrix while retaining the distinctive properties of individual materials.

The introduction of AC into the GO structure proved effective in preventing agglomeration, as AC particles infiltrated the spaces between GO layers. This unique configuration not only mitigated agglomeration issues but also optimized the available surface area for enhanced adsorption performance. The study determined that the graphene oxide activated carbon (GOAC) composite has an impressive adsorption capacity of 120 mg/g for the antibiotic ciprofloxacin in aqueous solutions. Using only 0.01g of the composite, 99% of a 10ppm ciprofloxacin solution was removed within 35 minutes, highlighting its efficient contaminant removal capabilities.

Furthermore, the adsorption process was found to follow pseudo-second-order kinetics, providing valuable insights into the reaction dynamics. This research highlights the significance of a carefully designed composite approach to overcome inherent limitations and enhance the overall adsorption capabilities. This approach offers promising implications for water treatment applications.

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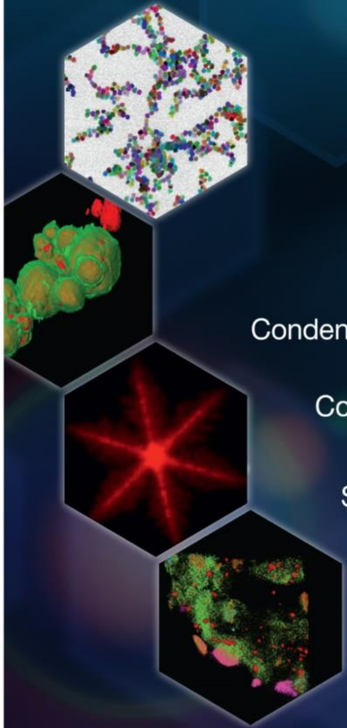

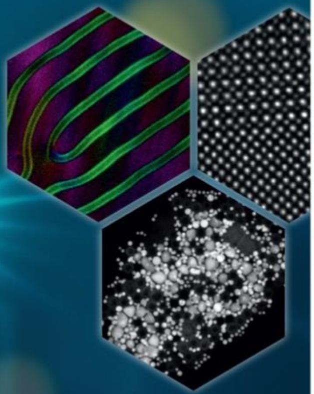

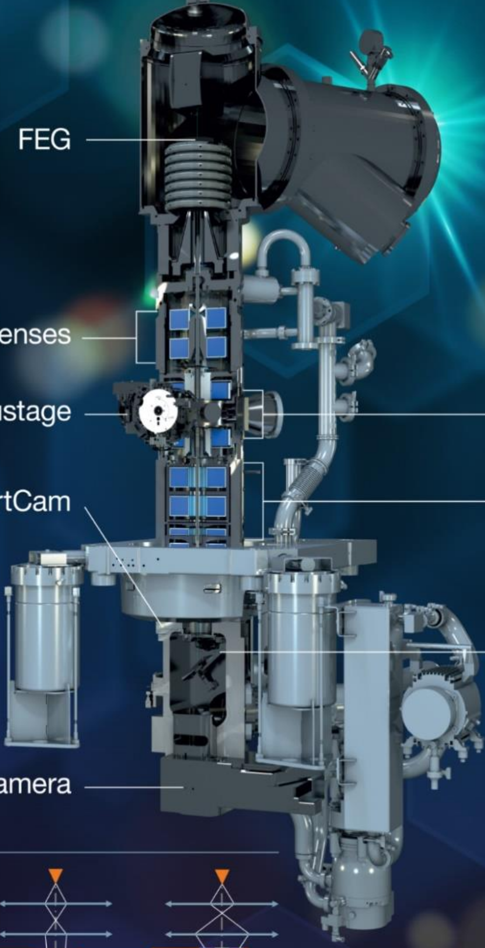

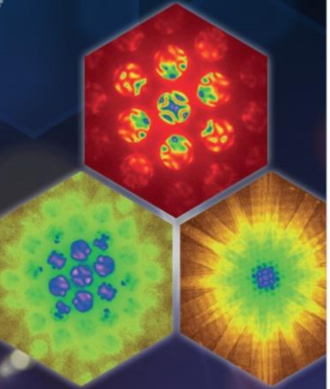

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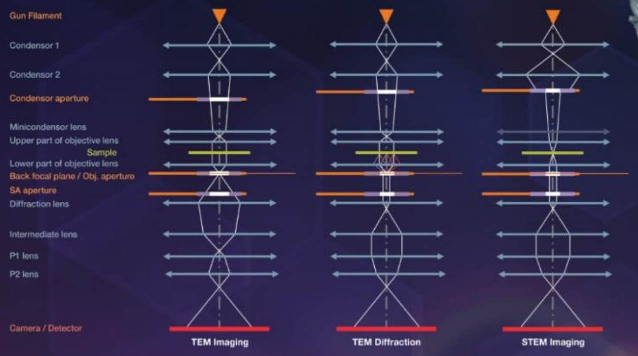

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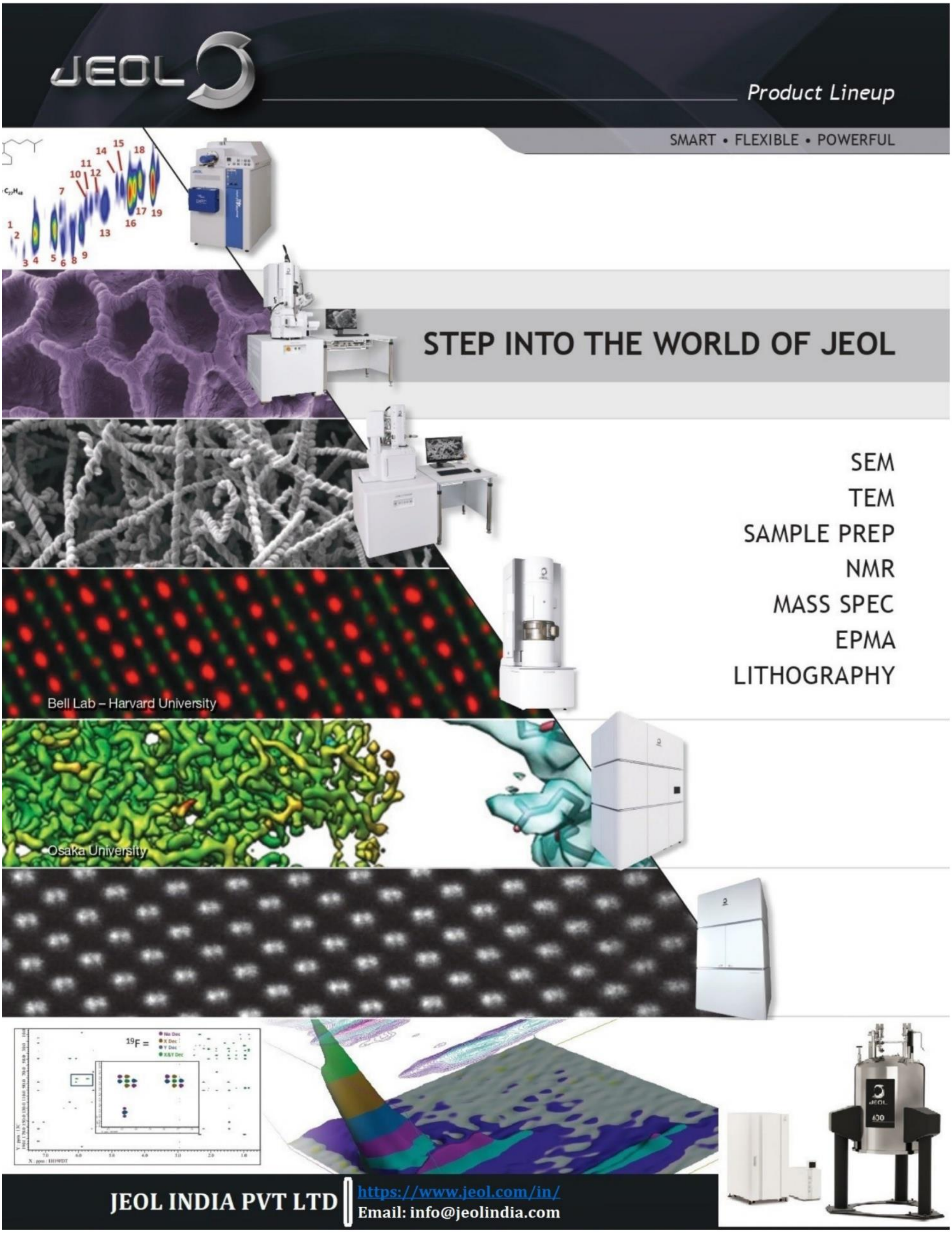

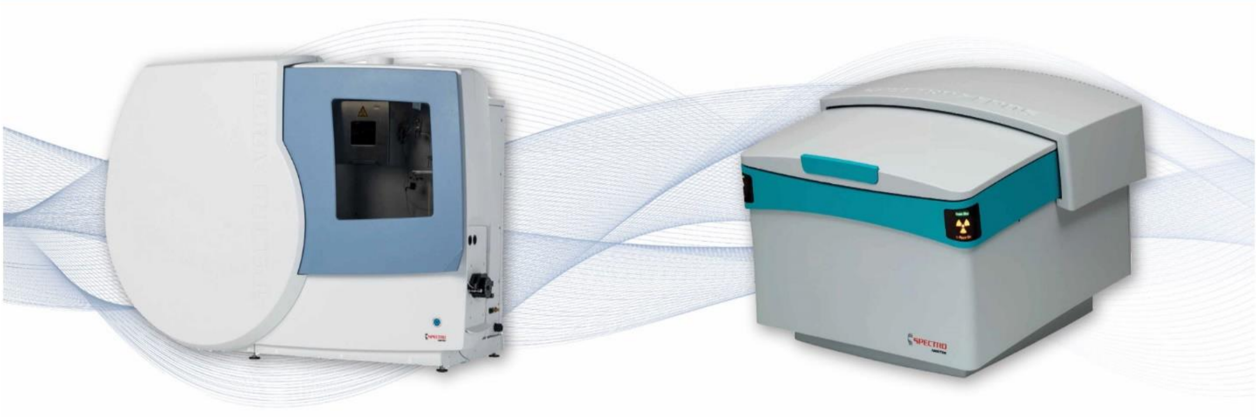


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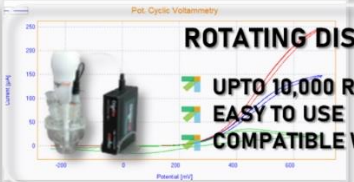
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