FCS 2025

National Seminar

FRONTIERS IN CHEMICAL SCIENCES

February 3-5, 2025

BOOK OF ABSTRACTS

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FCS 2025

Book of Abstracts

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Foreword

Chemical Sciences, although popularly conceived as a system of knowledge, has become interwoven into human life with a strong influence. It has birthed large industries, and has grown into a pillar that supports human civilisation. Thus, advancements in various fields of Chemical Sciences, in addition to their academic importance, assume great relevance to society. Recognising this academic importance and social relevance, the Department of Chemistry at University of Calicut regularly gathers leading experts of the science to set a stage to announce new developments, exchange ideas and mark the advancing frontiers of Chemical Sciences. The National Seminar series, is therefore titled **"Frontiers in Chemical Sciences (FCS)."** In its previous editions, FCS has seen announcements of important discoveries, birth of successful collaborations and young researchers being inspired to take up a career in Chemistry. The Department proudly continues this cherished tradition in the form of FCS-2025 on February 3-5,2025.

The Editorial team and the Department of Chemistry is happy to present to you the contributions to FCS-2025 in the form of this ***Book of Abstracts***. The abstracts of 18 invited lectures, 5 short presentations, 14 oral presentations and 38 poster presentations can be found in this volume. They address advancements in various sub- realms of Chemical Sciences. A lot of planning and coordinated effort from abstract committee members, editorial board members, other faculty members, research scholars and staff of the department have made the collection, compilation and publishing of this book of abstracts possible. I am honoured to place on record, deep sense of gratitude and high appreciation for all who worked tirelessly for releasing this ***Book of Abstracts***. I hope that it will find a permanent place in your memory and bookshelf.

Prof. Rajeev S. Menon
Head of the Department
Department of Chemistry, University of Calicut

Preface

True to the tradition, the Department of Chemistry, University of Calicut, is organising the 2025 edition of the National Seminar series ‘Frontiers in Chemical Sciences’ (FCS-25) during Feb. 3-5. The Department is proud and honoured to welcome all the participants to the campus. The Department of Chemistry, was founded in 1968 along with the University. Since then, it has been contributing significantly in various realms of chemical education and research catering mainly to the northern regions of Kerala. Along with developing skilled professionals in the core areas of chemistry, the department has been involved in the organization of events focussing on the latest developments in chemical sciences and allied fields. Frontiers in Chemical Sciences (FCS) is one such venture which brings together the leaders of various sub-domains of Chemical Sciences. New directions, change of trends and important breakthroughs in Chemical Sciences are presented by eminent researchers for the benefit of the partcipants, especially the younger members of the community. Over the years, FCS has set a platform for exchange of ideas, exchange of personnel for research and initiation of collaborations. It is hoped that such exchanges and interactions will also enrich this years FCS too.

We are pleased that 120 participants from various reputed institutions in India and abroad are attending FCS-25. The ***Book of Abstracts*** of FCS-25 features 1 keynote address, 18 invited lectures, 5 short invited lectures, 14 oral presentations and 38 poster presentations. Dedicated and elaborate team work of all abstract committee members, editorial board members, other faculty members, research scholars and staff of the department were instrumental in the production of the book of abstracts. We extend our gratitude to university, anrf and all the other industrial sponsors, whose generous support made this venture possible. We wish you all a pleasant and memorable stay at University of Calicut during FCS-25

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KEYNOTE ADDRESS

Biomimetic Sensing-Actuation Multifunctionalities from The Electrochemistry of Conducting Polymers

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Life functions are based on electro-chemical reactions involving as reactants macromolecular (protein) motors, ions and water. Most of their organs are multifunctional: motors and (simultaneously) thermal, chemical and mechanical sensors. Only two neurons include, at any time, the full information package that, treated by brain, originates proprioception. Here an artificial approach to such a multifunctionality will be presented using conducting polymers. During electrochemical reactions each chain becomes a macromolecular motor, exchanging ions and water with the electrolyte for charge and osmotic balance and sensing any chemical, mechanical or electrical perturbation. Actuating (current and charge) and sensing (potential and energy) signals are present, at any reaction time, in the two connecting wires. The way is open to develop proprioceptive tools and robots.

INVITED LECTURES

IL 01

Albumin Hitchhiking and Antibody Production by Tumor-Associated Carbohydrate Antigens

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Tumor-associated carbohydrate residues are present on the cell-surface glycoproteins of immune-compromised cancer cells. Due to the lack of immunological potencies, the proliferation of antibodies is restricted in these cells, leading to the disease progression. Carbohydrate antigens possess mono-, di- and oligosaccharide constitutions. In order to activate the cellular machinery to elicit antibodies, administration of antigens is developed as an approach involving an orchestrated method of antigen presentation to the cells. In an approach, we undertook to establish the potential of serum albumin as a method to deliver antigen to the sites of antibody production. Albumin possesses few binding pockets for complexation with hydrophobic segments in a ligand-receptor binding mode. Exploiting this binding mode, our investigations identify conjugation of the tumor-associated carbohydrate antigen to lipid modules. These synthetic glycolipids bind circulating serum albumin and in the event, the antigens are taken up at the lymph nodes where antibody biosynthesis occurs. Upon chemical synthesis, biophysical and biochemical studies, the synthetic glycolipids were utilized as antigens and the corresponding antibody production were evaluated *in vivo* in mice. Time course analysis shows a robust antibody production against the antigen involved chemical and biological studies show that synthetic glycolipids are potent antigens to raise antibodies against the tumor cells. The presentation will cover aspects of synthesis and subsequent studies on the tumor-associated carbohydrate antigens.[1]

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IL 02

Soft Actuators Based on Conducting Polymers: From Microactuators to Textile Wearables

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Conducting polymers (CP), such as polypyrrole and PEDOT, can be used as soft actuators from micrometre-sized robots and mechanostimulation devices for single cells to textile actuators for macroscopic wearables. They are driven at low potentials (1<V), biocompatible, and can be operated in any aqueous electrolyte, including salt solutions, full blood and cell culture medium, which makes them interesting for biomedical devices. We are developing CP-actuators for bionic devicess, such as single cell mechanostimulation, and for medical applications. Traditional microfabrication technology, including photolithography, and novel additive manufacturing methods such as 3D printing are used to create new soft microrobots comprising conducting polymer microactuators to drive the microrobots. We have developed new biohybrid materials based on gels and Plasma Membrane Nanofragments that induced bone formation is soft actuators. By combining these new biohybrid materials with the CP microactuators we have created microrobotic devices that create their own bone. The same conducting polymers, now shaped as fibres or yarns are used to make macroscopic textile actuators, by merging advanced textile technology with conducting polymer processing. Using knitting and weaving, we are developing soft textile actuators ("Knitted Muscles") for use in wearable devices such as haptic communication garments and textile exoskeletons.

IL 03

Aptamers - The Rising Stars in Theranostics

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Aptamers are synthetic RNAs and DNAs (recently peptides) originating from in vitro selection experiments, SELEX (Systematic Evolution of Ligands by Exponential Enrichment). The strategy involves isolation of rare nucleic acid molecules binding with high affinity to given ligand, from a pool of random nucleic acids with subsequent repeated rounds of selection and amplification. Aptamers can be isolated against a number of target molecules, such as nucleic acid binding proteins, non-nucleic acid binding proteins, certain small molecules, haptens, drugs, toxins and food related large structures and cells. Hence, they are suitable tools for health sciences and eco & food diagnostics. Since, aptamers possess the ability to target molecules and proteins for which antibodies are not well suited with equally high specificity and affinity, these have enormous application potential. Aptamers can be used as synthetic antibodies.

Aptamers are small in size and non-immunogenic. They can be tagged with various functional groups. Aptamers have been shown as a valuable alternative to protein antibodies. The strong target affinity/selectivity, cost-effectivity, chemical versatility, long shelf-life and safety of aptamers are superior to traditional therapeutics. Aptamers provide a novel class of pharmaceuticals with diagnostic and therapeutic potential. These are the next generation of biomarkers, diagnostic tools and drug delivery systems for therapeutic purposes. Because of their stability, low cost, short development duration and facile manipulation, aptamers are emerging as rising stars in theranostics. A brief overview of aptamers and their theranostic potential will be presented.

IL 04

Better biomaterials through synthetic chemistry-Challenges in Translation

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Even though ceramic materials, mainly inorganic compounds, have a close association with mankind since pre-historic times, some of them find innovative uses as implantable materials for a variety of clinical applications for the last fifty years. This has made an impact on the quality of human health. A host of specialty ceramics have been developed during the past decades for the health care industry through advanced chemical synthesis methods. Several ceramic products are being marketed for medical and dental applications - like eye glasses, diagnostic instruments, chemical ware, thermometers, tissue culture flasks, fiber optics for endoscopy, carriers for enzymes and antibodies, dental restorative materials, gold porcelain crowns, glass filled ionomer cements, dentures etc. Apart from developing medical and dental products, scientists and technologists had been exploring the possibility of ceramics to be used as permanent implants inside the body, especially for skeletal repair. Many ceramics have been tested for the application, but only a few qualified for clinical use. These materials termed as BIOCERAMICS, have drastically enhanced the survivability of man against hard tissue disease and damage. Bioceramic products based on alumina, calcium phosphates and calcium- phosphate-silica systems are now widely used for skeletal repair. This talk reviews the experience of a dedicated laboratory, which has been exploring the various synthetic chemical approaches and made them for specialty clinical applications.

IL 05

Recent Progress in Zeolite-Based Composite Catalysts as Potential Catalysts in Fine Chemicals Biomass Component Transformations

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Keywords: Zeolite, ITQ-2, SAPO-37, Nickel-oxy-hydroxide, Hydrotreating

The depletion of fossil fuels and rising pollutants pose significant threats to future generations. To address this, renewable energy sources must be utilized for sustainable social and environmental growth. Biomass, analogous to petrochemical feedstock, offers potential for producing fine chemicals and fuels. Effective valorization of biomass-derived platform molecules requires catalysts with multifunctionality, stability, reactivity, and accessible active species. Consequently, researchers have focused on developing composite materials like meso-micro hybrids, metal-metal oxides, and metal carbide-metal oxides. Zeolite and SAPO-based materials, known for flexible porosity, hydrothermal stability, tunable Brönsted acidity, and redox properties, are ideal for biomass transformations.[1-5]

This study explores composite materials such as delaminated zeolite-metal oxyhydroxide, zeolite-zirconia, and zeolite-metal-oxy-carbide. Techniques including Powder XRD, FTIR, FESEM, TEM, N_2 sorption, and chemisorption analyses were used to assess composite nature and active species interactions. The catalysts were tested for hydrogenation, hydrotreating, and biomass component conversions.

A 5 wt% ruthenium-loaded zeolite-β efficiently hydrotreated *m*-cresol to fully hydrogenated products.[1] Ruthenium-incorporated SAPO-11 yielded ring-hydrogenated products like methyl cyclohexanol and methyl cyclohexanone.[2] NiO(OH)-decorated ITQ-2 demonstrated efficient hydrodeoxygenation of *m*-cresol to methylcyclohexane.[3] A SAPO-37 composite with molybdenum-oxy-carbide synthesized via TPR achieved an 83% yield for MTBE.[4] Similarly, SAPO-37-zirconia composites produced ethyl levulinate from furfuryl alcohol with a 99% yield.[5] Thus, zeolites and SAPOs incorporating metals, oxides, or carbides as composites show promise as future catalysts for converting biomass to fuel additives and value-added chemicals.

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IL 06

Biological and Environmental Degradation for Two-Dimensional Materials

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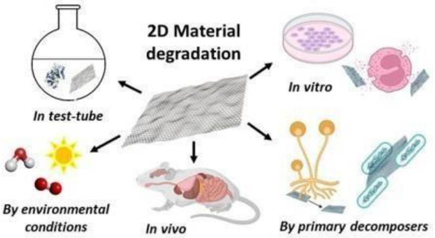
Keywords: Two-dimensional materials, biodegradability of GFMs, nanoparticle doping

As the use of two-dimensional materials (2DMs) continues to grow and expand their range of industrial and biomedical applications, understanding their long-term in the organisms and environment is still in its infancy. However, the biodegradability of 2DMs in organisms by immune cells has shown to be significant, especially by the peroxidase enzymes present in the neutrophils and macrophages. In addition, it is also necessary to thoroughly investigate their metabolite formation by the degradation of 2DMs. Herein, the biodegradability of graphene family materials such as rGO, GO, and CNOs, Sb sheets including graphitic carbon nitride (g-C3N4) by treating them with human myeloperoxidase (hMPO) isolated from the neutrophils plant peroxidase (HRP) and the photo-Fenton (PF) reaction mimicking the physiological environment during the tumour progression. In addition, we investigated the impact of chemical functionalization on the biodegradability of GFMs and the impact of nanoparticle doping, such as iron oxide nanoparticles (IONPs), ZnS nanoparticles, etc. High- resolution electron microscopy (HRTEM), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and mass spectrometry (MS) were employed to understand the biodegradation of GFMs and their by-products.[1-6] However, these results indicate that the oxidized (functionalized) graphitic materials can undergo faster biodegradation than the pristine ones. The possible by-products of biodegradation of graphene materials were characterized using mass spectrometry.



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IL 07

Polymeric Composites for EMI Shielding

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Keywords: Electromagnetic interference, electromagnetic pollution, polymer composites

Electromagnetic interference is a kind of electromagnetic pollution that can harm sensitive electronic sensors and devices. With a huge rise in demand for advanced devices for communication, diagnostic medical devices, household electronic entertainment equipments etc., the level of pollution inches towards the life-threatening stage. With frequency of operation ranging from kHz to several tens of GHz, the electromagnetic pollution poses challenges to prepare suitable shields to prevent or reduce the level of pollution. As the pollution damages the high-frequency electronic devices through interference, these shields are generally called ElectroMagnetic Interference (EMI) shields.

The conventional EMI shields utilize metal structure which are bulky and heavy. With increase in the number of portable electronic devices, these shields have to be made of materials to reduce the weight, enhanced flexibility, and offer advanced functionalities. Moreover, the shielding does not only stop the external interference but also avoids the internally generated interference sources within the instrument. This modifies the requirement of shielding nature from reflection to absorption. With increase in such functionalities, the choice of materials shifts away from metal structure to composite materials.

Polymer composites offer flexibility in material properties depending on the combination of the fillers in the base polymers. In this talk, basic background about the theory of shielding and the choice of materials that can be used to prepare the polymer composites would be provided. The talk primarily covers the shielding in the microwave frequency range between 8 and 18 GHz.

IL 08

Fluorescent Probes for Cellular Imaging and Theranostic Applications

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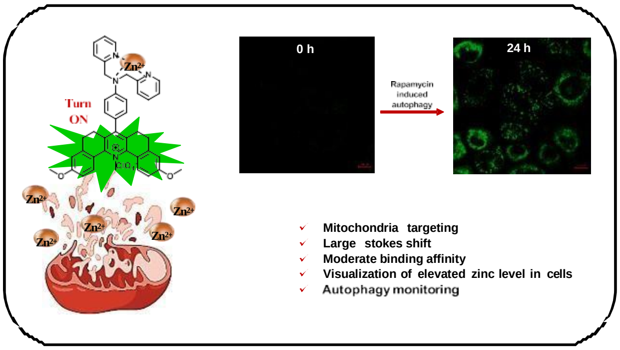
Molecular probes for sensing, imaging, and theranostic applications play a crucial role in clinical diagnostics and disease management. Given the low inherent fluorescence of biological entities, current fluorescence techniques heavily depend on fluorescent dyes. Small molecule-based probes are especially favored due to their compact size, ease of chemical modification, reproducibility, and compatibility with biological systems. Traditional chromophores such as coumarin, pyrene, 1,8-naphthalimide, xanthenes, boron dipyrromethene difluoride (BODIPY), and diketopyrrolopyrrole have been widely employed across various fields, including sensing, enzyme analysis, cellular imaging, and therapy. Each dye presents unique photophysical and physicochemical properties, along with its own set of advantages and limitations. Therefore, the development of new fluorescent probes with superior optical properties, biocompatibility, targeting abilities, and low toxicity is highly valuable for medicinal and biological applications. In our lab, we focus on designing novel fluorescent molecules that can monitor cellular microenvironments by selectively detecting specific analytes, such as Zn^{2+}, OCl^-, and SO_3^{2-}. For instance, we developed a pentacyclic pyridinium-based probe, PYD-PA, equipped with a pendant N,N-di(pyridin-2-ylmethyl)amine (DPA), for detecting Zn^{2+} in the cellular environment, which was further used to monitor autophagy. Additionally, we investigated dinuclear Ir(III) complexes as imaging probes and photodynamic therapy (PDT) agents for cancer treatment. PDT is a non-invasive therapy that utilizes light to activate a photosensitizer (PS) in the presence of molecular oxygen, producing cytotoxic reactive oxygen species (ROS) that destroy cancer cells. In this regard, we designed a 2-(2,4-difluorophenyl)pyridine-based dinuclear Ir(III) photosensitizer for imaging and PDT applications. Our research efforts in developing new, brightness-optimized fluorophores for cellular sensing and imaging will be discussed during the talk.



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IL 09

Reigniting Natural Product Chemistry: Bridging Biodiversity, Tradition, and Modern Science for Health and Innovation

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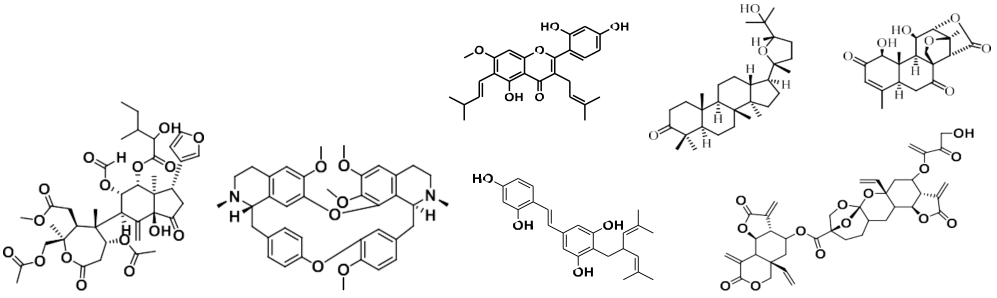
In the realm of pharmaceuticals, chemistry, and biology, the fusion of ancient wisdom with modern science holds transformative potential. Despite India's unparalleled biodiversity, the field of natural product chemistry—once a cornerstone of innovation—is waning. Vital plant species anchoring India's health and food biodiversity remain critically understudied, while smallholder farms and wild fields housing invaluable resources are neglected. A revival is imperative. By uniting botanists, social scientists, agricultural experts, chemists, and biochemists, this interdisciplinary effort aims to uncover the untapped potential of India's biodiversity. Collaborating with local communities, the goal is to harness traditional knowledge and advance food and health security while addressing global health challenges. This exploration highlights the phytochemical profiles of medicinal plants and the development of potent molecules combating multi-drug-resistant *S. aureus* and SAS oral cancer. Revitalizing natural product chemistry is not just about rediscovery—it is about securing a sustainable, healthier future while preserving a rich scientific legacy.



IL 10

Phenol/Thiol–Nitrite Interactions at First-row Late Transition Metal Sites

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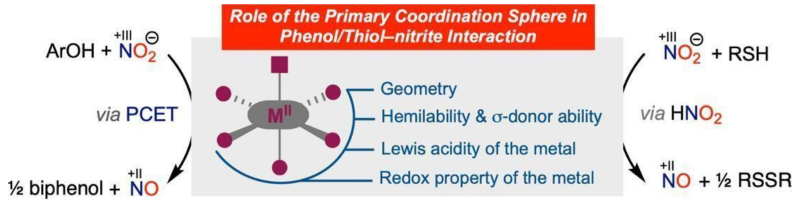
Keywords: Nitric oxide, Nitrous acid, Reaction mechanism.

Redox transformations of nitrogen oxides (NO_x) mediated by metalloenzyme active sites precisely regulate the flux of nitric oxide (NO) in the biological milieu.[1] While the variable redox states of the Fe/Cu-based metalloenzymes are directly involved in the transformations of NO_x,[2] sacrificial redox cofactors featuring thiol and phenol functional groups may play a pivotal role in dictating these redox transformations. This talk aims to showcase the role of phenol/thiol as a sacrificial reductant in nitrite reduction at first-row late transition metal (M = Cu/Zn) sites.[3,4] The tuning of the primary coordination sphere of several structurally characterized M(II)–nitrite complexes reveal that the properties of the ancillary ligands (such as hemilability and ⍰-donor ability) as well as the metal site (such as Lewis acidity and redox behavior) govern the underlying mechanism for the generation of NO from phenol/thiol–nitrite interactions.



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IL 11

Understanding the Electrochemistry of Conjugated Polymers to Boost the Development of their Applications

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Understanding the basic principles of any kind of materials is key to develop working and reliable devices by using such materials. Most of the devices nowadays are constructed using materials which composition is constant while working, that is, they do not change their composition during their function. That is also the case of conjugated (or conducting) polymers. There, applications such as flexible and softer electronics, or solar energy conversion emerge and are being already in use nowadays. However, they also can change their composition reversibly through electrochemical reactions. Such changes in the composition originate changes in their properties (such as volume, colour, porosity, surface properties,…) that can be adjusted on demand, giving the possibility to develop devices based on these changes. This results in a paradigm change where materials without a constant composition are used in devices, posing new challenges and many unknowns for their use in applications for the real-life, outside research labs. Thus, even though the fundamental working principles have been stablished, it is still needed to understand all their behaviours in full, which will be very helpful for the development of present and new applications. Examples of applications and how the basic working principles affect their development will be presented, ending with the discussion of future possibilities.

IL 12

Discovery of MDV6058 (PF-06952229), A Selective and Potent Tgfβr1 Inhibitor: Design, Synthesis and Optimization

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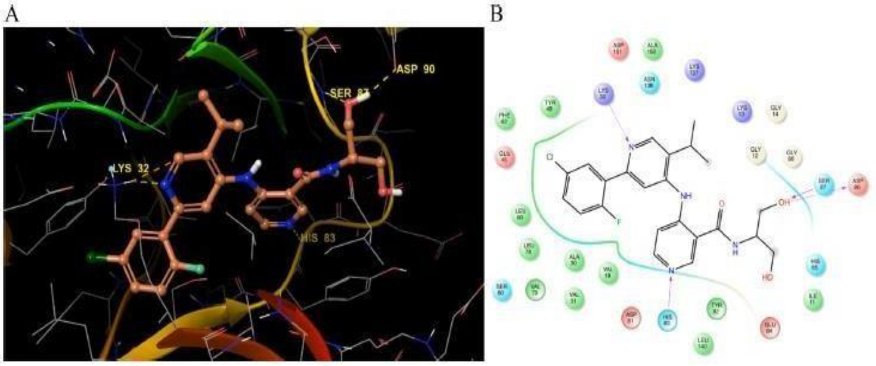
Keywords: TGFβ inhibitors, 4-aminopyridine derivatives, cell-based assay

TGFβ dysregulation has been implicated in carcinogenesis, especially in late stages of cancer, where TGFβ exhibits tumor-promoting effects, increasing tumor invasiveness and metastasis. Inhibitors of TGFβ have progressed to clinical trials. TGFβ is also key to immune suppression in the tumor microenvironment. TGFβ ligand levels are higher in many cancer patients and increased ligand levels are also correlated with poor prognosis and severity of disease. Additionally, inhibitors of the TGFβ intracellular signaling pathway are recognized as being useful for the treatment of fibroproliferative diseases.

We have identified a novel scaffold from which to develop selective TGFβR1 inhibitors leading to the discovery of a 4-aminopyridine-containing compound with low nanomolar ALK5 IC50. Despite good biochemical and cellular potency, this required optimization to improve pharmacokinetic properties. Our research efforts focused on optimization of biochemical potency (inhibition of human ALK5 kinase phosphorylation), followed by a cell-based assay (MDA-MB-231 cells) to measure the efficacy of inhibition of TGFβ-dependent phosphorylation of SMAD2 (p-SMAD2). Our lead compounds were then selected for optimal *in vivo* pharmacokinetics in mice. Herein we report our efforts to optimize our initial hit, which led to the discovery of **MDV6058** (**2**), a selective ALK5 inhibitor which can potentially be used in cancer as well as in fibroproliferative diseases. **MDV6058 (PF- 06952229)** was selected for testing in Phase I clinical trials.



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IL 13

When Protein Sings the Phonic Song – The Sequence Matters!!

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Keywords: Protein, Structural hierarchy, computational quantum mechanical methods

Amino acids serve as the fundamental units of proteins, akin to letters in words. The sequence of amino acids dictates the protein's structural and functional properties, much like the order of letters determines a word's pronunciation and meaning. Diverse amino acid sequences can yield proteins with analogous structures and functions, similar to how different letter combinations produce the same sounds. Proteins exhibit structural hierarchy from primary to quaternary levels, akin to letters forming words and sentences. Detailed structural insights, grounded in chemistry, reveal the interactions and bonds at the atomic level, that are crucial for understanding biological functions. By elucidating how specific structural features enable diverse protein functions, we bridge the gap between chemistry and biology, unveiling the molecular mechanisms that sustain life. This relationship will be discussed through computational quantum mechanical, molecular mechanical, and hybrid methods, particularly in ion channels and immunoproteins, highlighting the complexity and versatility of protein structural biology.

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IL 14

Organic Chemistry – Excitements and Opportunities

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Organic chemistry is a fairly extensive discipline and can span out over development of organic synthetic methodology and targets, medicinal chemistry, functional organic materials, natural products and characterization of synthetic products. Organic chemists are often interested in using existing synthetic methodologies to create promising compounds with practical utility. The latter is an interdisciplinary approach which has led to the emergence of several functional materials like ionic liquids, metal organic frameworks, drug delivery vehicles, specialized polymers, catalysts, chemosensors and so on and so forth.

Our explorations in the broad area of organic chemistry have resulted in development of new synthetic pathways using reactive species like nitrones and nitrile imines; spiropyrrolidine molecules with appreciable anticancer activities and spirotryptanthrins with substantial antibacterial activities. The fluorescence property associated with some of our molecules, were exploited for developing chemosensors for sensing of specific metal ions, aniline and picric acid as well. The first part of the present talk will be discussing the evolution of organic chemistry over the years, emphasizing the need for research in basic sciences and the second part will give an overview of the research happening in our lab and the future prospects.

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IL 15

Structure-Property Engineering in Hybrid Metal Halides for Optoelectronic Applications

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Hybrid metal halides have emerged as a promising class of semiconducting materials for next-generation optoelectronic applications due to their solution processability, tunable properties, and unique electronic structure. Recent advances in the molecular design of bismuth, tin and copper-based systems have established them as environmentally friendly alternatives to lead halides. The strategic engineering of organic cations and controlled structural dimensionality has been demonstrated to effectively tune the optoelectronic properties of these materials. Through systematic investigations, fundamental correlations between quantum confinement, dielectric effects, band alignment, and charge carrier dynamics have been established. The incorporation of functional organic cations has been shown to modulate electronic structure, photoluminescence, and charge transport characteristics. Notably, novel approaches to control dielectric confinement through organic spacer cations have led to materials with enhanced visible light absorption and improved photoconductivity. These findings provide critical design principles for developing new hybrid metal halide materials with optimized properties for photodetection and light emission applications.

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IL 16

Titania Nanotube and gC3N4-based 1D and 2D Materials for Energy and Environmental Applications

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The development of 1-D (one-dimensional) and 2-D (two-dimensional) nanomaterials has garnered significant attention due to their unique physical, chemical, and mechanical properties, making them highly effective for energy and environmental applications. These nanomaterials, including nanowires, nanotubes, graphene, and transition metal dichalcogenides, offer enhanced surface areas, tunable electronic properties, and superior conductivity, which are essential for improving the efficiency and sustainability of various devices. In energy applications, 1-D and 2-D nanomaterials have shown promise in solar cells, energy storage systems (such as batteries and supercapacitors), and fuel cells, offering improved performance, faster charge/discharge cycles, and better energy conversion efficiencies. For environmental applications, these nanomaterials are explored for water purification, air filtration, and pollutant removal due to their high surface reactivity and adsorption capacity. The talk provides a comprehensive detail of titania nanotube and g-C_3N_4 based 1D and 2D material, highlighting their current and potential roles in addressing global energy demands and environmental challenges. The integration of these materials into real-world applications holds the potential for a transformative impact on energy sustainability and environmental protection.

IL 17

Can Molecules Perform Photosynthesis Beyond Green Plants? Exploring CO_2 Reduction Coupled with Water Oxidation under Visible Light

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Despite significant recent advancements, there are still critical challenges in the molecular catalyst (MC) approach to artificial photosynthesis.[1] One of the primary issues is the "photon-flux-density problem," which stems from the limited intensity of sunlight. In particular, the four-electron oxidation of water to produce oxygen requires the molecular catalyst to wait for successive photon arrival over a relatively long period (~one second), which is far longer than its inherent reaction timescale. During this waiting period, MCs often decompose or transform as they try to reach higher oxidation states. To address this, we have developed a one-photon, two-electron oxidation of water to hydrogen peroxide, catalyzed by various metalloporphyrins.[2] Recently, we have also explored the integration of durable molecular Ru-based photocathodes with photoanodes, utilizing two-electron oxidation of water via metalloporphyrins as the key step. Under visible light irradiation, these integrated photoelectrodes simultaneously produce H_2O_2 at the anode and CO, HCOOH, as the reduction production in the cathode, achieving high Faradaic efficiencies in purely aqueous conditions, all without requiring any external bias, and relying solely on two-electron redox reactions.[3,4]

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IL 18

Exciton and Biexciton Dynamics in Semiconductor Nanocrystals

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Developing semiconductor systems for light energy harvesting and optoelectronic applications require an in-depth understanding of exciton and biexciton dynamics, as well as charge delocalization of photogenerated carriers. Compared to binary (II–VI and III–V) semiconductor nanocrystals (NCs), lead halide perovskite nanocrystals (PNCs) offer several notable advantages due to their defect tolerance. The first part of the talk will explore the dynamics of bound charge carriers in both binary semiconductor NCs and lead halide PNCs using time-resolved emission spectroscopy. Our findings reveal that trap depth plays a vital role in exciton dynamics in semiconductor quantum dots whereas the biexciton quantum efficiency in cesium lead bromide PNCs is influenced by the number of facets. As progressing from cube to rhombic dodecahedron, and further to rhombicuboctahedron PNCs, the biexciton quantum efficiency increases. This enhancement is primarily attributed to the increase in surface polarity as the number of facets increases, which reduces Coulombic interactions between charge carriers and suppresses Auger recombination. In the second part of the talk, I will present strategies to enhance electron delocalization in semiconductor heterostructures and vertex-oriented cube assemblies of perovskites.

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INVITED SHORT LECTURES

SL 01

Rationale Design and Synthesis of Macromolecules with Structural Tuneability for Environmental and Biological Application: A Custom-Made Approach

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Structural diversity and tuneable properties achieved in synthetic macromolecules uniquely qualify them for a wide array of applications in material/biomedical sciences. However, having an efficient 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. We developed two new classes of macromolecules: (i) non-conventional synthetic polymer, named as Sequence-Defined Polymer (SDP) and (ii) functionally tuneable Organic Polymer (OP) and explored their applications for environmental remediation and biological sciences. An unique functional group, dithiocarbamate(DTC), was strategically incorporated in both the cases, as DTC is known to be a potential functional group for material/biomedical applications. DTC-based-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 was found to be highly efficient in removing several classes 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 are developing low-cost multi- purpose macromolecules for environmental remediation and biological applications.

SL 02

Unravelling the Molecular Mysteries of EGCG, the Major Green Tea Polyphenol through Chemical Biology

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Keywords: Natural polyphenols, Structure-activity relationship (SAR), Anti-bacterial, Anti-cancer, Chemical proteomics, Mito-targeting

Tea is the most popular beverage consumed worldwide, only next to water. It is enriched with multiple polyphenols and exhibits a wide variety of beneficial health effects including antibacterial, antiviral, antioxidative, hypocholesterolemic, hypoglycaemic, anticancer and chemopreventive, etc. Epigallocatechin-*3*-gallate (EGCG) is the major polyphenol in green tea and is attributed to most of its biological properties. We began with a very basic query: *Why is EGCG still not a recognized prescription drug, given how important it is as a therapeutic molecule?* To address this, we realized that the precise mode of action and molecular target of EGCG (or green tea in general) are unknown. This has been a major setback for the translational aspects of EGCG. Another bottleneck in the therapeutic journey of EGCG has been its poor stability and dramatically low bioavailability which does not exceed 1%. In this talk, I will shed light onto the chemical proteomics platform that we developed to understand the mechanism of action of EGCG and identify its molecular targets with the help of bio- orthogonal Click chemistry. In addition, I will share our efforts on making various EGCG derivatives along it with their nano-formulation that showed superior stability and much improved activity as an anticancer (targeting EGFR, DHHC, etc.), antibacterial and antidiabetic agents. Overall, the talk will focus on the chemistry and biology of EGCG and how we can take it further to use it as a potent natural product-based drug molecule.

SL 03

Mechanochromism and Aggregation-Induced Emission in a Fluorene-Fumaronitrile-based Molecular System: The Influence of Supramolecular Control on Donor-Acceptor Interactions

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Keywords: Stimuli-responsive materials, Donor-acceptor systems, Supramolecular chemistry, Nanoparticles, Solid-state luminescence.

Effective control and reversible switching of solid-state luminescence in organic molecules are crucial for optoelectronic applications. A novel molecular system based on fluorene-diphenylfumaronitrile-fluorene (FDF), which exhibits mechanochromism and aggregation-induced emission (AIE) was studied. Significant mechanochromic properties were observed, in which mechanical stress induces a reversible shift from greenish-yellow to red emission due to alterations in molecular packing and hydrogen bonding. Additionally, FDF exhibits pronounced AIE behavior in DMF/water mixtures, transitioning from non-emissive in DMF to highly fluorescent upon nanoparticle formation. The investigation reveals that the control over donor-acceptor interactions is critical in modulating these luminescent properties, offering potential applications in stress sensing, bioimaging, and optoelectronic devices.

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SL 04

Theoretical Insights on Critical Factors that Influence the Performance of Organic Solar Cells

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Keywords: Organic Solar Cells, Non-fullerene acceptors, Density Functional theory.

The design and development of several new high-performing non-fullerene acceptors (NFAs) improved the power of conversion efficiency of organic solar cells. However, the photovoltaic performance is still lower than the commercial inorganic solar cells. In this presentation, we show how the current architecture of NFA limits the performance of organic solar cells. Our results indicate design and choosing the right combination of functional units in NFAs would be an effective way further to improve the power conversion efficiencies of organic solar cells.

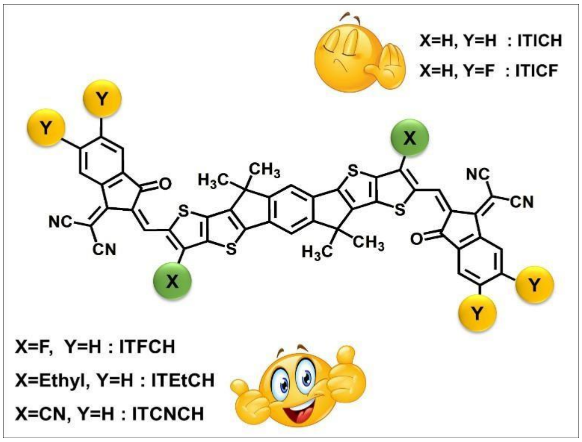

Fig. 1: Chemical structures of ITICH and its derivatives ITICF, ITFCH, ITEtCH, and ITCNCH.

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SL 05

Understanding Thermodynamic and Kinetic Properties of Complex Biomolecular Systems Employing Molecular Dynamics Simulation

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Understanding functionalities and mechanistic behavior of biomolecular systems such as protein – ligand and protein – DNA are highly desirable due to implication in basic biology as well as various diseases. Often, experimental techniques can be useful in measuring various thermodynamic quantities, but they cannot, at least directly, provide microscopic details and kinetics, pathways etc. Employing state of the art, classical all-atom molecular dynamics (MD) simulation and integrating with biased sampling techniques, we explore thermodynamics and kinetics of such complex systems. In this talk I will discuss a few of these methods and our efforts in understanding the stability, thermodynamics, and kinetics for different protein – ligand systems.

ORAL PRESENTATIONS

OP 01

Improved Corrosion Protection of Mild Steel in Acidic and Saline Media Using Phytogenic MnO_2 - Stearic Acid Composites

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Keywords: Anti-corrosive coatings, phytogenic MnO_2, green synthesis

Globally, corrosion is still asignificant concern, whichhas led to large investments in preventative techniques. The application of inhibitors, coatings that contain organic compounds and nanoparticles (often in combination), are some of the successful strategies that have been followed. These methods work together to safeguard infrastructure, save maintenance costs, and limit the harmful consequences of corrosion. Research on green chemical pathways that achieve anti-corrosive properties with fewer harmful ingredients has recently peaked. This study uses an ethanolic extract of Hibiscus rosa-sinensis flowers to synthesize benign phytogenic MnO_2 nanoparticles. The bioactive ingredients in this natural extract make it a viable and sustainable alternative to traditional chemical processes. The size, shape, and morphology of synthesized nano metal oxides can be precisely controlled by using phytochemicals, which usually serve as stabilizing and reducing agents. The particle morphology, size, and shape are fine- tuned under sono-chemical conditions. The synthesized MnO_2 nanoparticles were incorporated into stearic acid and the composite was dip-coated on to mild steel with the help of epoxy resin. The materials were characterized using FT-IR, SEM, TEM, XRD, TGA, XPS and the mild steel coated samples was characterized by SEM, AFM and water contact angle measurement techniques. Potentiodynamic polarization and electrochemical impedance spectroscopy were used to examine the coupons toprovide corrosion resistance and barrier performance. The 0.2wt% coated material showed increased resistance to corrosion in 0.5M HCl media and in 3.5% saline media with η value of 95.55% and 98.76% respectively. From PDP studies the coated samples showed decreased I_{corr} value of 0.0158 mA/cm^2 in 0.5 M HCl and 0.0019 mA/cm^2 in 3.5 % NaCl when compared to blank. Therefore, this epoxy-based coating can be used in the future to protect mild steel from corrosion in a way that is environmentally friendly.

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OP 02

Green Synthesis of Silver Nanoparticles from *Artocarpus Heterophyllus* Lam. Inflorescence: Synergistic Effect with Noni Leaves; Cytotoxicity and Antimicrobial Studies

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Keywords: Antimicrobial Drug Resistance, Reducing agent, Capping agent, Stabilising agent, Disc Diffusion Assay

Antimicrobial drug resistance is one of the greatest threats faced by health sector all over the world. Scientists are constantly trying to resolve this disaster with the help of metal nanoparticles. In this study, we biosynthesised novel silver nanoparticles from *Arthocarpus heterophyllus* (AH) female and male inflorescence and spathe separately. Most of us misunderstood AH inflorescence to be AH fruits itself and the biomolecules inside inflorescence remained unexplored. Here we are exploring the potential of such bioactive compounds within AH inflorescence. Besides we studied the synergestic effect of Noni leaves on AH inflorescence by synthesising silver nanoparticles from their combined extract.

We followed a methodology which is a combination of magnetic stirring and ultrasonication for this study. We preferred biosynthesis over chemical syntheses of silver nanoparticles, since it ensures minimal use of chemicals as well as minimum cytotoxicity. Plant extract itself act as stabilising agent, reducing agent and capping agent in biosynthesis unlike chemical synthesis where we require separate chemicals as reducing, stabilizing and capping agents. Various characterisations such as UV Visible spectroscopy, XRD, FTIR, DLS Zeta particle size, SEM and TEM are done as part of this study. Besides, cytotoxicity studies on human embryonic kidney cells (HEK293) using MTT assay and antimicrobial studies on E-coli and S. aureus using Disc diffusion assay, are performed on AH flower silver nanoparticles.

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OP 03

Eco-Friendly Synthesis, Characterization, and Properties of Copper Oxide Nanoparticles in Cashew Gum/Polypyrrole Blend for Energy Storage Applications

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Keywords: Cashew gum, Polypyrrole, Copper oxide nanoparticles, Thermal properties, AC conductivity

Conducting biopolymer blend nanocomposites of cashew gum (CG) and polypyrrole (PPy), with varying concentrations of copper oxide (CuO) nanoparticles were synthesized through an in-situ polymerization method using water as a sustainable solvent. The formation of blend nanocomposites was characterized using UV–visible (UV–vis) spectroscopy, Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and field emission scanning electron microscopy (FE-SEM). UV spectroscopy revealed a significant reduction in absorption intensity with adding CuO, indicating enhanced optical properties. FT-IR and XRD analysis confirmed the successful incorporation of CuO into the CG/PPy blend. FE-SEM images revealed the uniform distribution of nanoparticles throughout the biopolymer blend, particularly in the 7 wt% sample. TGA and DSC results demonstrated a significant enhancement in thermal stability, increasing from 352 ◦ C to 412 ◦ C, and a rise in the glass transition temperature from 89° C to 106° C in the blend nanocomposites. The dielectric constant, dielectric loss, and electrical conductivity were extensively examined at different temperatures and frequencies. The dielectric constant of the CG/PPy blend increased from 2720 to 92,950 with the addition of 7 wt% CuO, measured at 100 Hz. The improved glass transition temperature, thermal stability, and superior electrical properties imply potential usage of the developed nanocomposite in nanoelectronics and energy storage applications.

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OP 04

Fe-Hnt@Pvp/Pei Membranes: Development and Enhancement for Effective Dye Elimination and Water Purification

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Keywords: Fe-doped halloysite nanotubes, PVP/PEI membranes, Adsorption, Cationic and anionic dye, Water treatment, Membrane porosity

This study envisages the improvement in adsorption efficiency of polyetherimide (PEI) membranes by integrating Fe-doped halloysite nanotubes (Fe-HNTs) into polyvinylpyrrolidone (PVP)-modified PEI matrices for reducing water contamination caused by dyes, which are known for their harmful impact on aquatic life. Fe-HNTs were synthesized via Co-precipitation method and incorporated into PEI/PVP membranes at 1% and 2% concentrations by utilising simple, non-destructive phase inversion technique. The modification of polyetherimide matrix by PVP/ Fe-HNTs brought significant structural alterations, improved hydrophilicity, and morphological changes in the membranes. These changes were witnessed through techniques including Fourier Transform Infra-Red, X-Ray diffraction, Xray Photoelectron Spectroscopy, contact angle measurements, Scanning Electron Microscopy and Atomic Force Microscopy. The 2%-Fe-HNTs@PVP/PEI membrane demonstrated superior adsorption capacity for methylene blue (MB) dye, with significantly enhanced removal efficiency compared to the unmodified PVP/PEI membrane. Kinetic studies revealed a fast adsorption rate, fitting with pseudo-first-order and Langmuir isotherm models. The membrane also exhibited excellent reusability, maintaining its efficacy over multiple cycles. In textile effluent treatment trials, the modified membrane achieved an impressive 85% removal of dye pollutants within 300 min, underscoring its appropriateness for environmental remediation and purification of water.

OP 05

A Trinuclear Zinc (II) Complex with A Tetradentate Schiff Base Ligand Containing Phenolate Donor Group

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Keywords: Trinuclear complex, self-assembly, X-ray diffraction

Trinuclear zinc (II) complexes are important in inorganic and bioinorganic chemistry for their roles in catalysis, biological functions, and optical properties.[1] A novel trinuclear Zinc (II) complex [$Zn_3(\mu\text{-}L)_3$.3 DMF] (**1**) that contains an N, O, S- donor Schiff base ligand N4-cyclohexyl-2-(2-hydroxy-3,5-diiodobenzylidene hydrazine carbothioamide (H_2L) has been designed and synthesized by self-assembly. The trinuclear Zn (II) complex was fully characterized and confirmed *via* single crystal X-ray crystallography. The unique structure of the trinuclear Zinc (II) complex, crystallized in a monoclinic crystal system with $P2_1/n$ space group, reveals distorted trigonal bipyramidal coordination geometry around each Zn (II) ion (Figure 1). The X-ray diffraction analysis establish the existence of a new kind of trinuclear metal system containing thiosemicarbazone ligand. Hirshfeld surfaces (HSs) and 2D fingerprint plots (FPs) have been analyzed to study and quantify the intermolecular interactions.

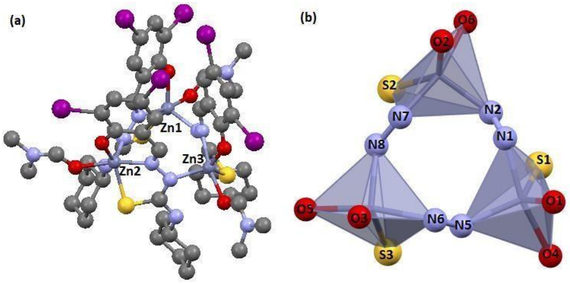

Figure 1.: (a) Molecular structure of trinuclear complex [$Zn_3(\mu\text{-}L)_3$.3DMF] (**1**). (b) The coordination polyhedra around Zn (II) centers of complex **1.**

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OP 06

Multifunctional Pillar[5]Arene Carboxylate Derivative for the Selective Sensing of Metal Ions, Amino Acids, and Organic Dye Molecules

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Keywords: Pillar[5]arene, metal ions, methylene blue, amino acids, and host-guest interactions.

This study explores the versatile sensing capabilities of a water-soluble pillar[5]arene derivative (PAA) functionalized with triazole and carboxylic acid groups towards biologically relevant ions, amino acids, and methylene blue. The PAA sensor exhibits high selectivity and sensitivity for Fe^{3+} and Cu^{2+} among 11 biologically significant cations with detection limits of 2.09×10^{-6} M and 5.89×10^{-6} M, respectively, based on fluorescence spectroscopy. Secondary sensing capabilities of the *in-situ* prepared Fe^{3+} and Cu^{2+} complexes of PAA (FePAA and CuPAA) reveal selective detection of amino acids: FePAA interacts with Arg, Cys, and Lys, while CuPAA selectively detects His among 18 proteinogenic amino acids. The detection limits of CuPAA with His was found to be 2.9×10^{-6} M, while the detection limits were 7.7×10^{-8} M, 8.5×10^{-8} M, and 1.6×10^{-7} M for FePAA with His, Arg, Cys, and Lys respectively. In another study, PAA exhibits remarkable host- guest interactions with methylene blue (MB), and shows a 90-fold enhancement in fluorescence response and a low detection limit of 2.43×10^{-6} M, with minimal response towards other dyes in water milieu. The interaction mechanisms and binding properties are supported by UV-visible, and fluorescence spectroscopy. These findings highlight the multifunctionality of PAA as a robust supramolecular receptor for the selective sensing of ions, amino acids, and dyes, showcasing its potential applications in biological and industrial fields.

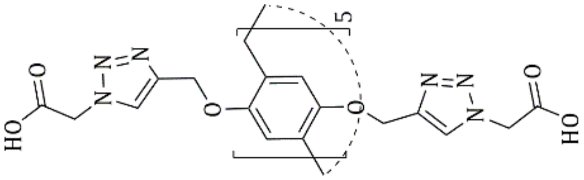

Figure 1. Structure of PAA.

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OP 07

Effect of Surface Modification in Pl Tuning in Sensing Characteristics of Carbon Nanodots

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Keywords: Carbon nanodots, photoluminescence, sensor, surface modification

Nanoparticles are vital in sensing applications due to their unique properties and high surface-to-volume ratio, which enhance analyte interactions and boost sensitivity. Carbon nanodots (CNDs), zero dimensional nano particles, are ideal for sensing due to their strong Photoluminescence(PL), biocompatibility, and tunable properties, enabling sensitive, selective, and real-time detection for diagnostics, monitoring, and safety. The emission properties of CNDs can be fine-tuned by surface modification[1]. In addition to PL tuning, surface modification also tunes the PL response of CNDs to the external environment. The functional groups on the surface of CNDs play a crucial role in their response towards specific analytes [2].

Here we have developed a methionine-derived blue luminescent CND system (MCD) using water as the reaction medium[3]. Which shows nill response towards nitroaromatic compound. Changing the medium to sulphuric acid in the synthesis step shifted the luminescence colour to bluish green, and the CNDs (SMCDs) show commendable response towards one of the nitroaromatic compounds, picric acid (PA). The picric acid-induced quenching of SMCDs showed high specificity, allowing selective detection of picric acid among 11 nitroaromatic compounds with a limit of detection (LOD) of 3.54 μM, highlighting the importance of surface functionalization in tuning the response to external environments. SMCDs also showed high reliability in real-water sample analyses, with an error margin below 3%. Solid-phase detection using test strips provided a solvent-free and contamination-resistant method, improving practical utility

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OP 08

Exploring the Photophysical Properties of Self-Assembled Phenylalanine: Aggregation-Induced Emission, Fluorescent Hydrogel Formation and Selective Interaction with Hemin

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Keywords: Self-assembly, FE-SEM, Hemin, Quenching, AIE

The aggregation of amino acids has garnered significant attention due to its involvement in various health disorders. In this study, we investigated the self-assembly of unmodified L-phenylalanine (Phe) monomers into unique fluorescence-enhanced assemblies while grasping the time-dependent structural transformations, using fluorescence spectroscopy and FE-SEM. Phe, a weak fluorophore, demonstrates remarkable enhancement in fluorescence intensity upon self-assembly, with a shift in emission maximum from 290 nm (λ_{ex} = 240 nm) for the monomer to 490 nm (λ_{ex} = 410 nm) for the assembly, accompanied by a nearly tenfold increase in quantum yield (ϕ = 0.207) compared to monomers (ϕ = 0.022)[1, 2,] which can be attributed to aggregation-induced emission (AIE). FE-SEM revealed stacked sheet-like structures, distinct from the typical fibrillar assemblies, highlighting a unique self-assembly driven by π-π stacking and hydrogen bonding interactions. The fluorescence intensity of these Phe-assemblies can be selectively quenched by hemin. The interaction mechanism, involving both static and dynamic quenching, was elucidated through Stern-Volmer analysis, revealing a detection limit as low as 50 pM for hemin. Additionally, the Phe- assemblies form a fluorescent hygroscopic gel, paving way for moisture absorption, environmental remediation and biomedical applications. The Phe-assemblies' remarkable selectivity and sensitivity for heme and heme-containing proteins, coupled with their potential for various biomedical and environmental applications, make them a promising material for fluorescence-based sensing and gel technologies.

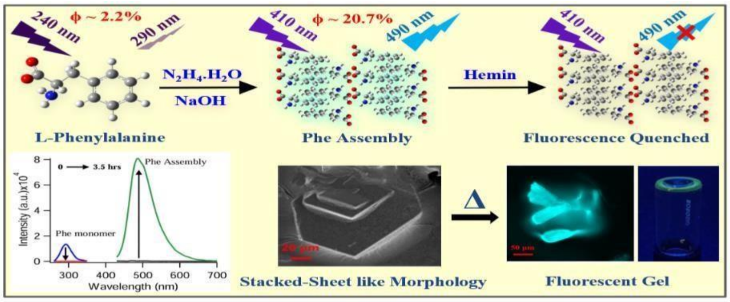

Figure 1: Schematic representation of the L-Phe assembly formation

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OP 09

An Intramolecular Charge Transfer and Stimuli-Responsive Emission in Cholesterol-Appended Phenothiazine–Cyanostyryl-Based Donor–Acceptor Systems

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Keywords: Organic LEDs, Phenothiazine, Cyanostyrylbenzene, Mechanochromic Luminescence, Electronic Excitation

Organic fluorescent molecules are highly valued for their versatile applications in optoelectronics. This study presents two cholesterol-functionalized cyanostyrene-phenothiazine-based donor–π–acceptor (D–π–A) systems, **PTCS-1** and **PTCS-2**, (see figure) which fluoresce in solution and solid states. These compounds differ in the *N*-alkylation of phenothiazine with octyl and hexyl chains, respectively. **PTCS-1** and **PTCS-2** exhibit strong fluorescence and high quantum yields in nonpolar solvents due to twisted intramolecular charge transfer (TICT). In their solid state, the molecules display aggregation-induced emission. The flexible alkyl chains in the phenothiazine and cholesterol groups enable mechanochromic luminescence switching, where emission changes occur under external shear stress and are reversible upon methanol vapor exposure. Powder X-ray diffraction reveals this behavior stems from a reversible transformation between crystalline and amorphous states triggered by external stimuli. These results underscore the potential of **PTCS-1** and **PTCS-2** for developing advanced luminescent materials, and optoelectronic devices.

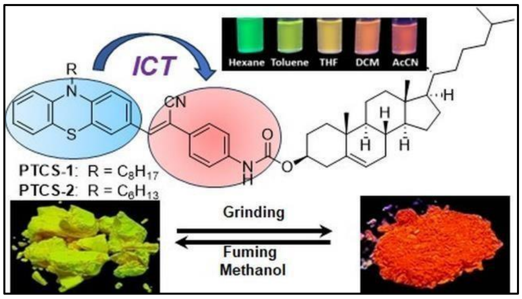

Figure: Graphical representation of stimuli-responsive emission in **PTCS-1** and **PTCS-2**

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OP 10

Organic Donor-Acceptor π-Conjugated Compounds: Twisted Intramolecular Charge Transfer and Stimuli-Responsive Fluorescence Switching

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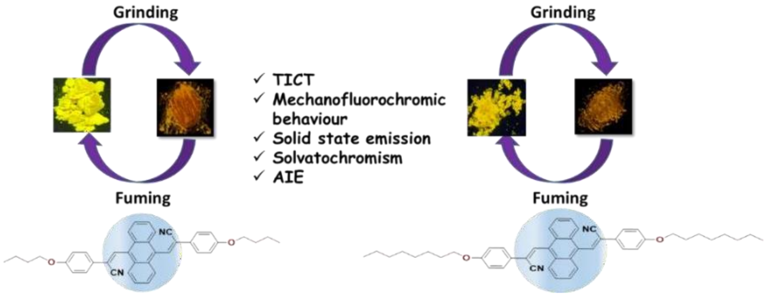
Keywords: Solvatochromism, Mechanochromism, Intramolecular charge transfer (ICT), Twisted intramolecular charge transfer (TICT).

Design and synthesis of donor-acceptor-based molecular design embrace great promises to afford bright emissive solid-state materials with tunability. Among various π-conjugated materials cyanostilbene-based organic fluorophores have drawn interest due to their extraordinary emissive properties resulting from their rigid and twisted geometry along with the tendency to form emissive aggregate in the solid state.[1,2,3] So molecular designs with the possibility for TICT are ideal designs for achieving strong emission in both solution and solid state. In this work, we report a series of donor-acceptor systems of cyanostilbene moiety (**2a**, **2b**, **3a**, and **3b**) with varying conjugation as well as the alkyl group at the terminal position. The study explores the photophysical properties of the luminogens both in solution as well as in the solid state. And the comprehensive understanding of structural dependence on photophysical properties. The findings open up the door for the creation of cutting-edge materials with remarkable thermal stabilities and adjustable emission characteristics. They may be used in a variety of optoelectronics, which is a promising development area.



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OP 11

Sulphur-Doped MoO_3 Integrated with Holey Graphene as Anode Material in Asymmetric Supercapacitors

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Keywords: Sulphur-Doped MoO_3, Holey Graphene, Asymmetric Supercapacitors, Anode Material

A green and cost-effective approach is presented for synthesizing a supercapacitor (SC) electrode material, sulphur-doped MoO_3 incorporated into a holey graphene (S-MoO_3/HG) nanostructure. The holey architecture of graphene forms upon the incorporation of sulphur-doped MoO_3, and structural analyses confirm that sulphur doping induces oxygen vacancies in the MoO_3 lattice, enhancing ionic diffusion and improving rate performance. The synergistic effects of graphene's high electrical conductivity, large ion-accessible surface area, the pseudocapacitive behaviour of MoO_3, and the enhanced redox activity due to sulphur doping result in remarkable energy storage performance. The material achieves a high specific capacitance, with excellent cycling stability in a three-electrode configuration. Additionally, an asymmetric supercapacitor fabricated with S-MoO_3/HG as the anode and MoS_2 as the cathode demonstrates high energy and power densities, along with stable cycling performance. The results highlight the potential of S-MoO_3/HG as a promising material for high-performance supercapacitors.

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OP 12

A Comparative Study of Structural, Spectral and NLO Response of Fomecin A and Fomecin B Using Density Functional Theory

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Keywords: Density Functional Theory; HOMO-LUMO; Spectral analysis; NLO, UV spectrum

The present work focuses on revealing the NLO properties of two drug molecules, Fomecin A and Fomecin B, derived from the polypore Pyrofomes demidoffii using computational techniques. This is the first attempt to explore the properties of Fomecin A and Fomecin B using Density Functional Theory.[1] Using Density Functional Theory (DFT), we performed a detailed computational analysis of Fomecin A and B with Gaussian '09 software and the B3LYP/6-31+G(d,p) basis set.[2] We optimized their geometries to identify minimum energy on the potential energy surface and conducted spectral analyses, including vibrational frequencies, Raman activities, and UV absorption. Frontier Molecular Orbital (FMO) theory provided insights into reaction mechanisms, focusing on HOMO-LUMO interactions and the energy gap's influence on stability, reactivity, and electronic transitions. Mulliken population analysis and electrostatic potential maps (MEP surfaces) helped identify electronic charge distribution and reactive sites.[3] We also explored global descriptors and thermal properties to predict chemical reactivity. Additionally, we assessed the potential of Fomecin A and B as nonlinear optical (NLO) materials, underscoring their applications in laser technology, optical communication, and high-density optical storage.[4]

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OP 13

Identification of HLA-DR Associated Peptides Involved in Beryllium Hypersensitivity

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Keywords: HLA protein, hypersensitivity, binding energy

Beryllium exposure leads to beryllium sensitization and Chronic beryllium disease (CBD) which is a granulomatous lung disease caused by accumulation of Be-responsive CD4$^+$ T-cells in the lower respiratory tract.[1] Beryllium hypersensitivity and CBD is mainly associated with HLA-DP alleles having glutamate residue at 69th position of chain.[2,3] In HLA-DPGlu69 negative individuals, HLA-DRPhe47 is the susceptible marker of beryllium hypersensitivity.[4] However, the potential Be^{2+} binding site on the HLA-DR allele is unknown because the natural presenting peptide is unknown. Hence, molecular dynamics (MD) simulations were carried out to identify the appropriate peptide-Be^{2+} ion combinations that can bind to HLA-DR protein and to explore the potential binding site of Be^{2+} ion on the protein-peptide complexes [Figure 1a]. The Be^{2+} ion binds with HLA-DR protein and peptide simultaneously. Further, the peptide has a significant role in maintaining the structural stability of the Be^{2+}-HLA-DR system. The binding free energies between HLA-DR protein and peptides show that Pep5 is the most suitable peptide that could bind with Be^{2+} and HLA-DR protein [Figure 1b].

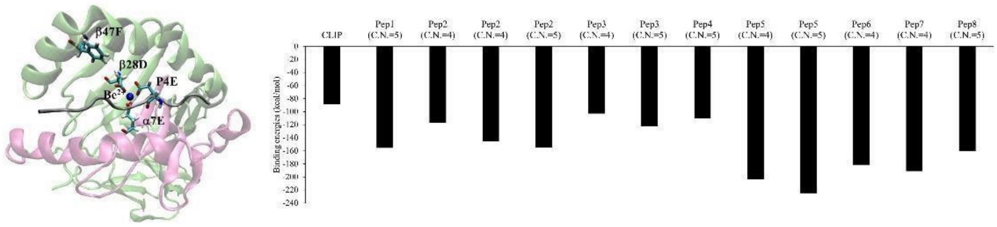

Figure 1. (a) Representative snapshot from MD simulation of HLA-DR3_peptide_Be^{2+} complex. (b) Binding energies between protein and peptides without and with Be^{2+} ion

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OP 14

Exploring The Inhibitory Potential Of Flavonols Against SARS-Cov-2 M Pro: A Computational Molecular Docking And Simulation Approach

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Keywords: SARS-CoV-2; M Pro; molecular docking; Molecular Dynamics (MD) simulations; ADMET

In the battle against infectious diseases, COVID 19 has been a tough opponent. COVID-19, also known as Coronavirus Disease 2019, is a highly contagious respiratory illness caused by the SARS-CoV-2 virus, initially identified in Wuhan, China in late 2019. A promising approach to combat the SARS-CoV-2 pandemic involves the development of novel, targeted medications that inhibit essential viral proteins. Computer-aided drug design is a game-changer for researchers looking to develop new COVID-19 treatments, offering a faster and more efficient alternative to traditional methods. The M Pro enzyme, essential for SARS-CoV-2 replication, has been identified as a key target for the design of COVID-19 inhibitors. Inhibition of M Pro's proteolytic activity presents an optimal therapeutic approach to impede the replication of SARS-CoV-2 within host cells. Plant-derived polyphenols, renowned for their prophylactic properties against various diseases, including viral infections, have been identified as potent inhibitors of SARS-CoV-2 M Pro, exhibiting promise as antiviral agents. Flavonoids with a ketone group called flavanols exhibits a broad spectrum of health benefits. In this study, we undertook a comprehensive investigation to assess the inhibitory potential of 15 flavonols against M Pro, employing a multi-faceted approach that integrated molecular docking studies, Molecular Dynamics (MD) simulations, MM-GBSA analysis, and ADMET analysis. This investigation presents kaempferol as a highly potent inhibitor of M Pro, surpassing the efficacy of Paxlovid. Additionally, kaempferol demonstrated a superior safety profile, marked by minimal toxicity and maximal biocompatibility.

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POSTER PRESENTATIONS

PP 01

High-Performance PAAm-Pectin Double-Network Organogels for Transparent Electronics Applications

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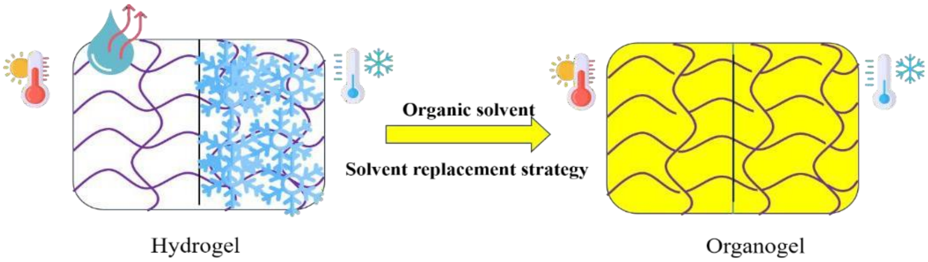
Keywords: Hydrogel, Organogel, Anti-freezing, Anti-drying, Ionic conductive



The demand for advanced materials in transparent electronics has driven the development of innovative hydrogels that combine mechanical robustness, flexibility, and environmental resilience. This study introduces a high-performance PAAm-pectin double-network organogel, engineered through ionic crosslinking of pectin and covalent crosslinking of polyacrylamide (PAAm). By employing a solvent replacement strategy with ethylene glycol and water, the resulting organogels demonstrate exceptional anti-freezing and anti-drying properties, maintaining structural integrity and ionic conductivity at temperatures as low as -40°C. Comprehensive characterization, including FTIR, SEM, and mechanical testing, reveals a highly porous microstructure and enhanced mechanical properties, with tunable transparency and flexibility. These features position the PAAm-pectin organogels as ideal candidates for transparent electronic applications, such as wearable optoelectronic devices, and transparent sensors. The sustained ionic conductivity of the organogels under extreme environmental conditions ensures their reliability in real-world applications, while their renewable and biocompatible components support sustainable material innovation. This work represents a significant advancement in the design of multifunctional organogels, paving the way for their integration into next- generation transparent electronic devices.

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PP 02

Optimizing the Structural, Thermal, Gas Sensing and Electrical Properties of In-Situ Polymerized Poly (Thiophene-Co-Indole)/Silicon Carbide Nanocomposites for Energy Storage Applications

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Keywords: Poly (thiophene-co-indole); Copolymer nanocomposites; Thermal properties; Dielectric constant; Ammonia sensing

Conducting copolymer nanocomposites of thiophene and indole incorporated with silicon carbide nanoparticles [poly (thiophene-co-indole-SiC) (PPSiC)] were synthesised via in-situ copolymerization and characterized using different analytical techniques. The FTIR peak at 865 cm^{-1} signifies the successful incorporation of SiC nanoparticles in the copolymer matrix.[1] Enhanced optical properties were evident in UV-Vis spectra, where PPSiC7 exhibited the highest absorbance, correlating with its low optical bandgap (3.032 eV) and high refractive index (2.388). XRD revealed the consistent positioning of sharp and distinct crystalline peaks of SiC in the copolymer.[2] SEM and HR-TEM imaging revealed a well-dispersed nanostructure with uniformly distributed spherical-shaped particles SiC nanoparticles in 7wt% nanocomposite. Thermal stability was greatly improved, as demonstrated by TGA and DSC, positioning these nanocomposites as resilient materials for high-temperature applications. AC conductivity and dielectric propeties showed a frequency and temperature dependent increase, with PPSiC7 achieving the highest conductivity, lowest activation energy and enhaced dielectric storage. Most notably, the excellent ammonia gas-sensing capabilities at ambient temperature highlight its potential in environmental monitoring.[3] With superior electrical, optical, and thermal properties, PPSiC7 emerges as a multifunctional material which can be exploited in developing optoelectronic materials, energy storage devices and gas sensors.

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PP 03

Six-Membered Sulfonated Polyimide Decorated with Metal-Organic Framework as Proton Exchange Membrane for Fuel Cells

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Keywords: Fuel cell; proton exchange membrane; sulfonated polyimide; acid-base composites; ionic conductivity.

Fuel cells are electrochemical devices that employ a redox process to convert chemical energy into electrical energy. Proton Exchange Membrane Fuel Cells (PEMFC), one of the many fuel cell types, have been used in several fixed and mobile applications because of their benefits, which include strong ionic conductivity, durability, flexibility in installation, and low cost. The proton exchange membrane is the heart of PEMFC operation. Aromatic polyimides act as an electrolyte material which has a remarkable significance owing to their excellent mechanical stability, chemical resistance, thermal stability, and notable film-forming ability. A new six-membered sulfonated polyimide (sPI) was prepared by the chemical imidization method that shows the maximum proton conductivity of 0.032 S/cm at 80°C. Amino-functionalized Ni-MOF (Ni-NH2-BDC) was impregnated into the pristine matrix to improve the performance of the virgin polymer. The incorporation of MOF into the polymer was confirmed structurally by FTIR, NMR, SEM, and XRD analyses. The acid-base interaction between the -NH2 and -SO3H group of the MOF and polymer increases the mechanical strength of the composites. The water uptake of the composite membranes was found in the range between 10.26 and 17.91%. Composite membrane embedded with 3 wt. % MOF showed a maximum power density of 145.7 mW/cm^2 at 60°C which is two-fold higher than that of the pristine. This improved performance could be due to the conduction path channels created by the Grotthus and Vehicle mechanics. Overall, the findings showed that the sPI/Ni-NH2-BDC membrane is a good option for PEMFC uses.

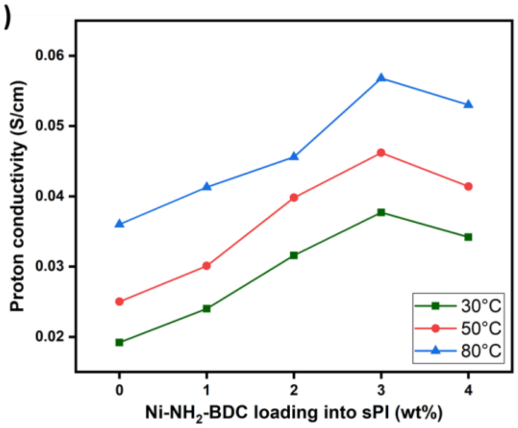

Figure1: Proton conductivity of sPI and composites at varied temperature

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PP 04

Petal-Inspired Zinc Cobaltite with Cubic Spinel Structure: Surface-Modified Tremella Flower for High-Efficiency Hybrid Energy Storage

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Keywords: Co_3O_4 (H1-C), ZnO (H2-Z) and $ZnCo_2O_4$ (H3-ZC), Tremella-like microsphere, Electrode material.

In this investigation, modulating the morphological structure of oxide metals strategically has consistently directly impacted the electrochemical characteristics of redox reactions in energy storage applications[1]. Microstructures that are hollow and porous are very intriguing materials for energy storage devices, especially supercapacitors, and enhance the properties of their applications[2].The unique tremella-like hierarchical microsphere of $ZnCo_2O_4$ (H3-ZC) has successfully synthesized morphological variation with porous and higher surface area. The same method is followed by an ultrathin hierarchical nanosheet of Co_3O_4 (H1-C) and nanorod with hexagonal bodies of ZnO (H2-Z). Crystal structure, packing factor calculation, and electrochemical investigations have been verified for the synthesized nanomaterials. The H3-ZC exhibited improved electrochemical performance without the addition of impurities. It has superior specific capacitance and cycling stability, achieving a specific capacitance of 1232 $F\ g^{-1}$ in 1 M KOH at a current density of 1 $A\ g^{-1}$. It exhibited excellent cycling stability, retaining 93% of its capacitance after 5,000 cycles, with a low charge resistance of 0.8 Ω. This result indicates that the tremella flower-like microsphere exhibits greater supercapacitor performance.

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PP 05

Metalloporphyrin Decorated NiO/*Poly-Pyrrole*-RuCAT Interfaces for Photoelectrochemical CO_2 Reduction

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Keywords: Photoelectrochemistry, CO_2 Reduction, Sustainable Energy

Socio-economic impacts of global warming and allied climate related disasters are existing as one of the stumbling blocks against the sustainable development of the country. Combustion of fossil fuels for both energy sector and transportation emit vast majority of CO_2 into the environment, and which is driving the global warming to a dangerous level. Technologies for direct capturing and conversion of greenhouse gases like CO_2 will lead to lower the atmospheric CO_2 level and thus furnish a solution for environmental concerns like global warming. Functional molecular catalysts give clear idea on the mechanistic aspects, tunability, high metal atom economy and selectivity for catalytic cycles.[1] Photoelectrodes for the selective conversion of CO_2 into reduced fuels such as CO and HCOOH by using water as the reductant and visible light as the only energy input has been reported recently.[2,3] Herein, we are reporting a scalable methodology for the fabrication of the photocathode by choosing a $Ru(CO)_2Cl_2$ (RuCAT) modified NiO electrode by using a poly-pyrrole linked free bipyridine linkages as the host material (NiO/*PolyPyr* RuCAT). Different metalloporphyrins as light harvesting units has been immobilized on the host material by using both covalent and ionic binding (NiO/*PolyPyr* RuCAT/MP). The metalloporphyrin incorporated photocathodes exhibited photocurrent density upto ~ 125 $\mu A.cm^{-2}$ in aqueous solutions clearly suggests the applicability of the photocathodes in molecular solar fuel systems. Optimization of anchoring modes, redox tailoring of sensitizer units suggests ionic binding of Porphyrin units exhibits maximum photocurrent densities towards CO_2 reduction.

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PP 06

Investigation of Nb_2AlC Max Phase Integrated With 2D GCN (Nb-MX/GCN) as a Bifunctional Electrocatalyst for Water Splitting Reaction

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Keywords: Carbon nitride, Energy conversion, Hydrogen evolution reaction, Max phase (Nb_2AlC), Oxygen evolution reaction

Noble metal-based electrocatalysts are impractical for large-scale manufacture due to their high cost, limited availability, and poor long-term stability in performing several functions. Hence, an alternative is the need of the hour that emphasizes blending metals and ceramic property materials with compelling electroconductivity. In this research, we synthesized two bare materials, Nb_2AlC MAX (Nb-MX) phase and graphitic carbon nitride (GCN) sheets using the calcination method which is then converted into a composite (Nb-MX/GCN) material through wet impregnation technique. The electrochemical investigations were conducted to assess the catalytic efficacy of the composite material. The synthesized Nb-MX/GCN electrocatalyst exhibited outstanding electrocatalytic efficiency for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in an alkaline environment. The catalyst exhibits a significantly low overpotential of just 66mV and 450mV for the HER and OER performance, respectively, at a current density of 10 mA cm^{-2} in a 1.0 M KOH solution. In addition, the catalytic activity exhibited no change over 24 h which indicated the excellent stability of the material. This performance surpassed the previously reported electrocatalysts.

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PP 07

The Synthesis of Gold Nanoparticles Using Nitrogen-Doped Carbon Dots

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Keywords: Carbon dots, Reduction, Gold nanoparticles

Metal nanoparticles are widely recognized for their distinctive physical and chemical properties, which differ significantly from those of bulk materials or individual atoms. These unique characteristics arise from the quantum size effect that shapes their specific electronic structures. Gold nanoparticles (AuNPs) stand out as an elegant among the metal nanoparticle family. They have garnered significant attention due to their potential applications across diverse fields, including catalysis, biology and optics.[1] Metal nanoparticles are typically synthesized through the reduction of metal salt solutions, a process that requires reducing agents like sodium borohydride or citrate under stringent reaction conditions. Additionally, capping agents are essential for the formation of these nanoparticles, with organic ligands containing amine or thiol groups and various surfactants commonly used for stabilization.[2,3] Recently, carbon dots (CDs) have been recognized for their reducing properties, especially for the synthesis of metal nanoparticles from metal salt precursors. In the present work, CDs are synthesized using citric acid as carbon source and orthophenylene diamine as nitrogen dopant by hydrothermal method. The system is characterized using Transmission Electron Microscope analysis, X-Ray Diffraction analysis, Fourier Transform Infrared spectroscopy, UV–VIS Spectroscopy, X-ray photoelectron spectroscopy and Fluorescence spectroscopy. The synthesized CDs are used for the reduction of Chloroauric acid to produce AuNPs. Formation of AuNPs are confirmed by UV-Vis spectroscopy and FT-IR spectroscopy. Previous methods on AuNPs synthesis have limitations, such as the necessity for high reaction temperatures and lengthy procedures and reliance on additional supporting chemicals, which can be challenging in certain cases. However, these drawbacks are absent in the current reduction method, where carbon particles serve a dual function as both reducing and stabilizing agents.

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PP 08

Fossicking *Pueraria Phaseoloides* Leaf-Derived N-Doped Carbon Dot Nanofillers Engrafted Anticorrosive Epoxy Coatings for Mild Steel in Saline Environments

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Keywords: *Pueraria phaseoloides,* N-doped carbon dot, Epoxy polymer, Nanocomposite, Mild steel, Amorphous silica, Impedance.

Leveraging the 'seed to weed' paradigm, a novel azure fluorescent *Pueraria phaseoloides* (Pp) leaf-derived nitrogen-doped carbon dots (PNCD) with an abundant phytochemical profile was synthesized for marine corrosion abatement. These PNCDs were integrated onto amorphous silica nanoparticles to yield solid silica-loaded PNCD (SPNCD), which were subsequently incorporated into epoxy to produce an enhanced anticorrosive coating.[1] Structural, optical, and morphological assessments substantiated the synthesis and effective adsorption of PNCDs onto nanoscale silica adsorbents. The rate of uniform corrosion on coated mild steel (MS) investigated by gravimetric method. Corrosion performance for MS in saline conditions was evaluated through continuous immersion tests over durations ranging from one hour to sixty days, revealing that the epoxy coating containing 0.4% SPNCD exhibited exceptional protective efficiency (99%).[2] Surface studies were carried out using SEM and AFM before and after corrosion studies which shows that the nanofiller particles can block the diffusion of chloride ions to reduce the corrosion rate.

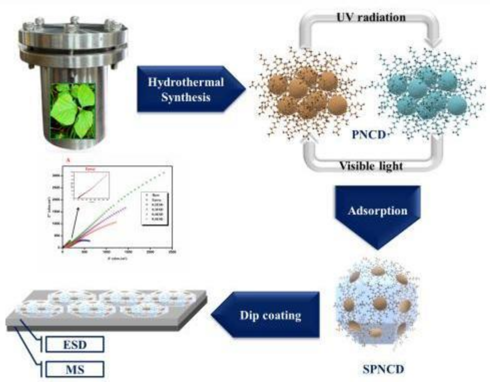

Figure 1: Schematic representation of the synthesis and application of ESD coating.

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PP 09

Development of Nano-Crystalline Nickel Containing-Laalo3 Perovskite as a Promising Catalyst for Hydrogenation of Biomass Component

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Keywords: Cinnamaldehyde, Hydrocinnamylalchol, Hydrogenation, Nickel, Perovskite oxide

Perovskite is an interesting group of mixed metal oxides-based materials with the general formula ABO_3 and enormous potential as ferromagnetic, energy storage, and catalytic materials. Partial substitution of appropriate cations at the A or B sites produces multi-component perovskites ($A_{1-y}A'_yB_{1-x}B'_xO_3$) with variable structures and properties compared to its pristine oxides.[1] Lanthanum aluminate ($LaAlO_3$) is an important family of mixed metal oxide with a perovskite structure, which exhibits a broad spectrum of structural, electronic, thermal, phonon, and optical properties under different applied conditions.[2]The doping of different transition metals on B sites of $LaAlO_3$ broadens the scope of lanthanum-based perovskite and offering applications in various fields such as catalysts, nano-adsorbents, sensors, and microwave dielectric resonators etc. Incorporation of nickel ions into the perovskite oxide structure, thereby tuning the redox or acid- base properties of the system and exploring it as catalytic materials for biomass, and CO_2 transformation, is the area of recent research interest.[3] The present work focused on the synthesis of Ni-doped $LaAlO_3$ ($LaAl_{1-x}Ni_xO_{3-\delta}$) with x = 0, 0.1, 0.2, 0.3, 0.4,0.5, 0.6, and 0.75 (LANx)by the combustion method, followed by an annealing treatment. The resulting LANx materials crystallized in the cubic structure by the Pm-3m (221) space group. The XPS studies showed that nickel was present in the +2 and +3 oxidation states. The resultant materials were explored for hydrogenation of Cinnamaldehyde (CAL) under ambient conditions to produce hydro- cinnamylalcohol (HCOL). The highest catalytic activity (CAL conversion of 98% with 96.5% HCOL selectivity) was obtained in the presence of the LAN7 catalyst at 150°C for 6 h using 10 bar H_2 pressure.

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PP 10

Photocatalytic and Adsorption-Based Removal of Methylene Blue Dye Pollutant Using Tungsten Trioxide Nanoparticles

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Keywords: Tungsten trioxide, Photocatalysis, Degradation, Adsorption

Photocatalytic and adsorption-based removal of organic pollutants offers a promising approach to mitigate environmental pollution. In this study, tungsten trioxide materials were synthesized using a combination of precipitation and hydrothermal methods. The synthesized materials were characterized by various techniques to assess their structural and functional properties. Key experimental parameters, such as pollutant concentration, pH, contact time, and material dosage, were optimized to enhance the removal effectiveness for both adsorption and degradation processes. The results demonstrated that the materials exhibited good selectivity, reusability, and adsorption capacity, following typical adsorption models and kinetic behaviors. Photocatalytic testing showed significant degradation of organic pollutants under light exposure, indicating the materials' strong photocatalytic performance (Fig. 1). Overall, the study highlights the potential of tungsten trioxide-based materials in environmental cleanup applications.

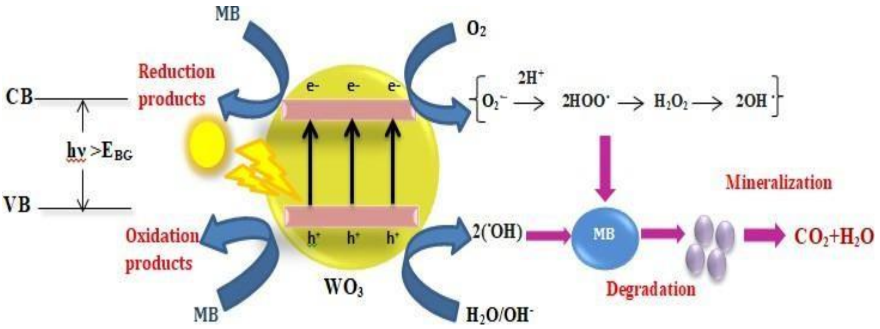

Figure 1: Mechanism of the photocatalytic degradation

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PP 11

Decarboxylation of Fatty Acids to Value-Added Hydrocarbons via a Facile Route over MWW Zeolite Framework

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Keywords: Decarboxylation, Zeolite, MWW, lauric acid, hydrogenation

The depletion of various non-renewable sources of energy has resulted in the urgent development of catalytic technologies for processing renewable energy sources, viz., biomass. The platform chemicals derived after the pyrolysis of biomass include components such as phenolic compounds, C5- C6 carbohydrates, and fatty acids, which are further upgraded to fine chemicals and fuels. Fatty acid triglycerides are an ideal source of low-cost, abundant, renewable feedstock typically containing around 50% lauryl derivatives, such as lauric acid and its esters. The decarboxylation of these components is performed using conventional molybdenum disulphide (CoMo, NiMo) catalysts that require harsh operating conditions (>300 °C).[1] Recent studies reflect the development of layered zeolites with interparticle mesoporosity in addition to uniform micropores, which improves accessibility, reduces diffusion limitations and facilitates reaction under milder conditions. Accordingly, the MWW zeolite framework, a known layered zeolite[2] with a topology consisting of two independent pore systems, is well suited for decarboxylation reactions. In addition, group VIII metals (Ru, Ni, Pd) are well known for their role in deoxygenation reactions[3], among which Ru facilitate excellent hydrogen spillover.

The current study focuses on the selective decarboxylation of biomass- derived fatty acid, viz., lauric acid, to gasoline additives by utilizing a ruthenium-dispersed MWW zeolite framework. Ru dispersed within the medium pore channels, and 12-membered external pockets of the MCM-22 framework was prepared by the incipient wetness method. Powder X-ray diffraction (XRD) confirmed that the synthesized materials exhibited high crystallinity. The *in-situ* formation of metallic Ru under reaction conditions (3 MPa H_2, 190 °C), along with hydrogen spillover and acidic centres, contributed to the excellent catalytic activity for lauric acid decarboxylation. Catalytic studies revealed that the reaction followed two distinctive pathways: decarboxylation (DCO) and hydrodeoxygenation (HDO), yielding *n*-undecane (54%) and *n*-dodecane (31%), respectively.

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PP 12

Tert-Butyl Nitrite (Tbn) Mediated Acid-Free Direct Nitration of Carbazoles

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Keywords: Nitration, TBN, 3-nitrocarbazole

Nitro compounds are an intermediates in synthetic chemistry as well as drug designing. Due to its essential in various fields the interest for the synthesis of nitro compounds were gradually increasing. The traditional nitration mixture (Sulfuric acid + Nitric acid) creates a serious problems like pollution and selectivity. While considering a metal nitrates and nitrogen oxides as nitrating agents, the reaction condition are harsh to get a selectivity. In addition, toxic reagents will limit the further applications. In this context, development of acid free nitration reactions taken into the consideration, due to their availability, easy handling specifically their environmental concern. This work presents a mild, metal-free, and acid-free method for the direct nitration of carbazoles using tert-butyl nitrite (TBN) as the nitrating agent. This approach selectively nitrates carbazoles at the C1 position, even when the C3 and C6 positions are blocked, without needing a directing group.

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PP 13

Synthesis of Indoloquinolines via Pictet-Spengler Reaction Using *p*-TSA

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Keywords: Indoloquinolines, Pictet-Spengler cyclization, Aerobic oxidation.

Indoloquinoline, fused indole and quinoline rings, represents a promising scaffold for drug design. Indoloquinoline alkaloids such as cryptolepine, isocryptolepine, and neocryptolepine exhibit diverse pharmacological activities, including antimalarial, antifungal, antibacterial, antiprotozoal, antitumoral, anti-inflammatory, antihyperglycemic, hypotensive, antithrombotic, and vasodilatory effects[1]. While numerous synthetic strategies for constructing indoloquinolines have been reported[2,3], this study highlighting the efficient and eco-friendly method utilizing *p*- toluenesulfonic acid (*p*-TSA). The Pictet-Spengler cascade approach involves the condensation of 2-(1*H*-indol-2-yl) aniline with aldehydes, cyclisation, followed by aromatization in moderate yields.

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PP 14

A Formal Vinylic Substitution Reaction for the Synthesis of α, β-Unsaturated Enol Esters and Their Anticancer Potential

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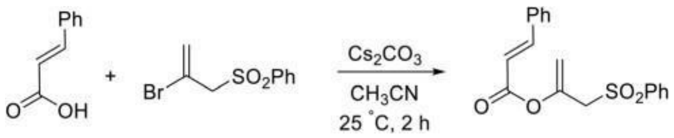
Keywords: α, β-Unsaturated enol esters, Formal vinylic substitution, 2-Bromoallyl sulfones, Antiproliferative activity

A novel and efficient Cs_2CO_3-mediated synthesis of α, β-unsaturated enol esters via formal vinylic substitution[1] of 2-bromoallyl sulfones with cinnamic acids is presented. The approach demonstrates a metal-free sp^2 carbon–oxygen coupling and yields enol esters bearing arylsulfonyl groups.



Scheme 1: Cs_2CO_3-mediated reaction of cinnamic acid and 2-bromoallyl sulfone

Synthesis of aryl sulfonyl tethered enol esters, shows diverse functional group tolerance and delivers moderate to good yields over a range of substrates. Preliminary biological evaluations reveal that selected synthesized compounds exhibit significant antiproliferative activity against human lung adenocarcinoma cells, while six derivatives showing greater potential than the standard anticancer drug carboplatin. Mechanistic investigations suggest the reaction proceeds via dehydrobromination to form an allenyl sulfone[2] intermediate, followed by a hetero-Michael addition to yield the desired product. Under the same conditions, thiophenol and 2-bromoallyl sulfones reacted to produce α-thiophenyl-α'-tosyl acetone through aerial oxidation. The present work can further be extended to the development of suitable pharmacophore - enol ester hybrids with promising anticancer activity.[3]

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PP 15

Tuning of Photoluminescence and Conducting Properties in Oligo (Phenyleneethynylene) Based Cocrystals

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Keywords: Charge transfer cocrystals, Phenyleneethynylene, Tetrachloroterepthalonitrile, Tetracyanobenzene, Charge carrier mobility.

Cocrystalline systems with customized charge transport properties are essential for various electronic applications, such as field-effect transistors, photovoltaic cells, photoconductivity, ferroelectricity, and magnetoelectricity.[1-5] This study highlights the potential of cocrystal engineering to manipulate molecular arrangements and weak intermolecular interactions—such as hydrogen bonding, π-π stacking, and halogen bonding—to attain tailored optoelectronic properties.

Cocrystals of oligophenyleneethynylene (OPE) with two electron acceptors, 2,3,5,6-tetrachloroterephthalonitrile (TCPN) and 1,2,4,5- tetracyanobenzene (TCNB), were synthesized to investigate its photophysical and charge transfer behavior. In the solid state, OPE exhibited a redshifted emission at 524 nm compared to its dilute toluene solution, highlighting the influence of molecular packing. Interestingly, OPE-TCPN displayed a slight blueshift in emission, while OPE-TCNB showed a pronounced redshift. Photoluminescence lifetime studies confirmed fluorescence emission in the nanosecond range. Single-crystal X-ray diffraction analysis revealed that π-π stacking and intermolecular interactions significantly impact optical properties. Mixed-stacking systems integrating OPE with both TCPN and TCNB demonstrated improved tunability in bandgap, charge carrier mobility, and energy levels. These results highlight the versatility of cocrystal engineering in developing advanced materials with customizable optoelectronic features, paving the way for innovative applications in electronic and photonic devices.

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PP16

Niosome-Loaded Agarose and Chitosan Composite Film with the Incorporation of ZnO@HNTs Nanocomposites for the Dual Moad of Drug Delivery System for Anti-Cancer Treatment.

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Keywords: Drug delivery, Antibacterial properties, Thin film

Developing improved drugs delivery methods is crucial for increasing treatment effectiveness while limiting adverse impacts. In this study, we propose the synthesis and characterization of an agarose (AG) chitosan (CS) composite film including halloysite nanotubes (HNTs) surface modified with zinc oxide (ZnO) nanoparticles, designed to serve as a biodegradable carrier for niosome (Nio)-encapsulated medicines. The composite thin film was prepared by casting, ensuring uniform dispersion of HNTs@ZnO and Nio within the polymer matrix. Morphological analysis using scanning electron microscopy (SEM), Transmission electron microscopy (TEM) revealed a porous structure conducive to drug loading and release. The physical and chemical properties were assessed through Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD), demonstrating improved mechanical stability and biocompatibility. Drug loading studies indicated a significant encapsulation efficiency of the niosomes within the film, while in vitro release kinetics showed a controlled and sustained release profile. Antimicrobial activity tests confirmed the ZnO component's potential to enhance the composite's antibacterial properties. These findings suggest that the agarose chitosan HNTs@ZnO composite film loaded with niosomes is a promising platform for effective drug delivery applications.

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PP 17

Amberlyst-15 Mediated Unprecedented Oxidation: Tunability of Diarylmethanols to Ketones or Ethers

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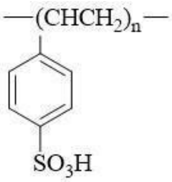
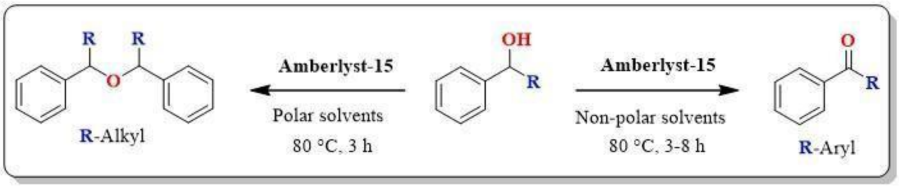
Keywords: Amberlyst-15, Diarylmethanols, ether formation.



Amberlyst-15

Oxidation of alcohols to the carbonyl compounds and protection of alcohols to ethers are important and routine transformations useful for the variety of organic synthesis.[1] An extensive variety of reagents have been developed for the transformation of secondary alcohols to ketones and etherification well documented in literature.[2-5] All the previously reported methods suffer some of the disadvantages. To overcome the limitations associated with the earlier mentioned methods, a new class of catalysts, solid supported heterogenous catalysts, have emerged. Among the solid acid catalyst, Amberlyst-15, an heterogenous catalyst, with sulfonic acid groups serves as excellent source of strong Bronsted acidity.[6] We have discovered a novel, unprecedented, environmentally benign method for the selective oxidation of diaryl alcohols to ketones and etherification of alcohols mediated by Amberlyst-15 by varying the polarity of solvents and obtained moderate yields.



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PP 18

Layer-By-Layer Constructed mPEG-b-PCL-b-PEC Micelle- Embedded Membranes Functionalized with Folic Acid for Targeted Cancer Therapy

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Keywords: Targeted drug delivery, Layer-by-Layer assembly, Camptothecin, Triblock copolymer, Cancer therapy.

Development of precision drug delivery systems is essential in advancing cancer therapeutics. In this work, we present a novel membrane platform constructed via the Layer-by-Layer (LbL) assembly technique that embeds micelles of mPEG-b-PCL-b-PEC triblock copolymers functionalized with folic acid for targeted drug delivery. Synthesized through 2 step ring-opening polymerization (ROP) catalyzed by stannous octate (Sn(oct)2) and TBD 1,5,7-triazabicyclo [4.4.0] dec-5-ene respectively and designed to encapsulate chemotherapeutic agent camptothecin within the core of its micelles[1]. The LbL assembly approach allowed for accurate deposition of drug-loaded micelles into stable and uniform membranes, with high drug-loading capacity and structural integrity. The detailed characterization using NMR, FT-IR, GPC, TEM, and DLS provided evidence for successful copolymer production and micelle generation. The functionalized membranes showed receptor-mediated targeting of cancer cells overexpressing folate in addition to regulated drug release, which improved therapeutic efficacy and lowered systemic toxicity[2].

This novel approach, therefore, shows potential by integrating layer-by-layer assembly with micelle-embedded membranes in advanced cancer treatment, where drug delivery will be highly targeted and release regulated[3].

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PP 19

Efficiency Enhancement of Porous Coordination Polymers based Supercapacitor by Implementation of Organic Redox Mediator

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Keywords: Co-Ordination Polymers, Redox Mediator, Supercapacitor, Energy Storage

Quest to improve the efficiency of supercapacitors seems to be a perpetual one. The task requires innovation in development of sophisticated electrode and electrolyte materials. Porous coordination polymers (PCPs), also known as metal organic frameworks (MOFs), while serving as an emergent material, have their shortcomings which include low intrinsic conductivity, electrolyte incompatibility and reduced electrochemical stability.[1] These limitations can be obstructive in practical applications, but can be overcome by assorted techniques. These techniques include addition of composite materials to PCPs, optimization of electrolyte, and surface modifications by annealing process.[2] In this presentation, we will elaborate the utilization of our organic redox mediator in improvement of the electrochemical performance of the prepared PCPs and an augmentation in overall efficiency of the supercapacitor.

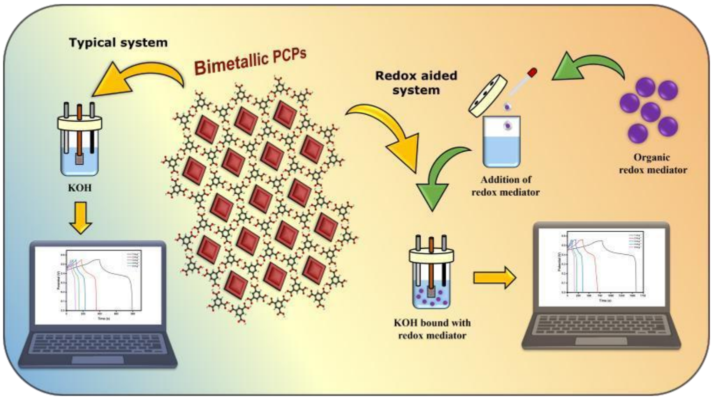

Figure 1. Graphical abstract of the redox aided system for supercapacitor

Herein, a mesoporous bimetallic PCPs were synthesized, having high surface area and are utilised as active electrode material. The prepared material was studied in a half-cell system, where excellent electrochemical properties were observed. A novel redox mediator in organic potassium salt, bound with KOH were implemented to improve the electrochemical performance of the prepared material. This system showed a maximum specific capacitance of 931.47 F g^{-1} at the current density of 1 A g^{-1}. The material retained 88.23% of its original capacitance after 5000 charge- discharge cycles, which was not affected in the presence of redox mediator, indicating that the material was not degraded by augmentation of its performance. This study indicates an improvement in overall efficiency of the material by implementation of the proposed redox mediator in the electrolyte. (See Figure 1)

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PP 20

A Novel Temperature Sensor Driven by Cooperative Actuation of Multistep Electrochemical Molecular Machines in Polypyrrole/ Chitosan Hybrid Films

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Keywords: Conducting Polymer, Polypyrrole, Cooperative Actuation, Temperature Sensor

Polypyrrole/hydrogel hybrid film, fabricated through *in situ* chemical polymerization of pyrrole, is proposed as a flexible model for the intracellular matrix of ectothermic muscle cells that respond to ambient thermal energy[1]. This hybrid film can undergo a series of reversible, consecutive conformational changes under electrochemical control and function as a multi-step macromolecular motor. When subjected to a constant electrochemical stimulus (cyclic voltammetry), increased available thermal energy drives deeper conformational movements of the polymer chains due to the cooperative actuation of the film's chemical components, which facilitates the exchange of larger amounts of counterions and solvent to maintain charge balance and osmotic equilibrium. The extent of the reaction, as defined by the coulovoltammetric charge, varies as a semi-logarithmic function of the inverse temperature and functioning as a self-sensor for reaction thermal conditions (reaction self-awareness). Under galvanostatic conditions, the hybrid film sense or respond to the thermal energetic perturbation of the surrounding environment by adjusting the electric energy they consume and allowing them to self-adapt to the newly imposed energetic conditions[2]. These findings offer the development of biomimetic sensing motors (intelligent devices) based on a polypyrrole/chitosan hybrid film, mimicking biological functions, where both driving and sensing signals can be monitored at any instant of the reaction using the same two connection wires.

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PP21

pH-Dependent Optical Tunability of C-2-Phenylethenil Calix [4] Resorcinarene

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Keywords: Calix [4] resorcinarene, Density Functional Theory (DFT), UV-Visible Spectroscopy

Calix [4] resorcinarene, a macrocyclic compound consisting of a cyclic array of four resorcinol units, has attracted significant attention in fields ranging from materials science to environmental engineering and pharmaceutical sciences. This versatile molecular platform is particularly well-suited for encapsulating metal nanoparticles and has been extensively studied in host- guest chemistry. The present study investigates the influence of pH variations on the structural and optical properties of C-2- phenylethenilcalix[4]resorcinarene (CPECR), combining theoretical and experimental approaches to provide deeper insights into its behaviour. Density Functional Theory (DFT) calculations were performed to analyse how structural modifications induced by pH changes affect the electronic configuration of CPECR. These calculations revealed pH-induced structural deformations induce a significant redshift in the absorption spectrum of CPECR. The theoretical findings were corroborated experimentally using UV- Visible spectroscopy, which demonstrated a pronounced shift in the absorption peak from 280 nm to 310 nm when the pH was altered to the basic region. This study highlights the potential of systematically tailoring the absorption of this compound makes it a promising candidate for applications in advanced materials, including sensors, optical switches, and other photonic devices.

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PP 22

Triazole Containing Dipicolylamine as A Sensor for Zn^{2+} in Water Milieu

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Keywords: Di-(2-picolyl) amine, Receptor molecule, Quenching

Metal ions are widely present in biological systems and participate in many critical biochemical processes.[1] Among various biologically relevant metal ions, zinc ion is the second richest metal ion in the lifesystem. Therefore, the rapid and efficient early detection of Zn^{2+} has important research significance in the fields of medicine, chemistry, biology, agronomy, and environmental sciences. The receptor molecule containing di-(2- picolyl) amine (DPA) plays an important role in the field of sensing for the detection of ions and molecules due to the presence of four pyridyl-nitrogen groups. The receptor molecule,**1**(Figure**1**) was prepared by the click reaction between 1,8-naphthalimide and DPA molecule through a triazole linker. Among 11 biologically relevant metal ions studied, the receptor molecule shows excellent selectivity towards Zn^{2+}. It detects Zn^{2+} through fluorescence turn-on mechanism with a fluorescence enhancement fold of~

4.5. The competitive titration also confirms the selectivity of sensor towards the Zn^{2+} while marginal interferences caused by Cu^{2+} and Ni^{2+}. Based on Job's plot analysis, the stoichiometry of the complex is 1:1 and the limit of detection is1.5 ⍰ 10^{-5} M. The secondary sensing abilities of **1** has been studied towards anions and nitro compounds. Among 11 anions, the in-situ prepared zinc complex of **1** (**1.Zn**) shows selectivity towards $CO3^{2-}$. Also, among 16 nitro compounds, **1.Zn** exhibits selectivity towards picric acid and 4- nitroaniline. Both the sensing of anions and nitroaromatics were identified through fluorescence quenching mechanism. Further, we explored the practical use of sensor **1** to detect the zinc ion in the tissue of living organism.[2] It has been found that **1** acts as a very powerful sensor probe to detect Zn^{2+} in larval zebrafish.

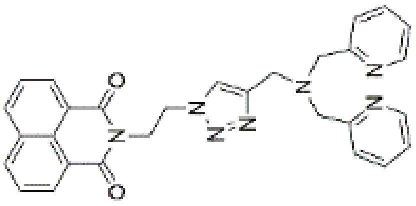

Figure 1: Receptor molecule, **1**

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PP 23

Synthesis, Characterization and Antibacterial Investigations of N^4-Phenyl Subsituted Semicarbazone Based Ligand and its Trinuclear Zinc (II) Complex

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Keywords: Semicarbazones, Zinc (II) complex, DFT, Antibacterial

Semicarbazones are gaining attention for their unique metal coordination, notable toxicological potential, and strong chelating abilities.[1] A novel ligand, 2,4-dihydroxy benzaldehyde-4-phenyl-3-semicarbazone (H4L) and its trinuclear zinc (II) complex (**1**) were synthesized and physicochemically characterized. The structure of the ligand was confirmed by single crystal X- ray crystallography (SCXRD). DFT study is performed to analyse the electronic structure, stability, reactivity, and molecular properties for insights into chemical interactions and potential applications. To achieve better insight into electronic structure, several quantum chemical calculations including Mulliken charge distribution and molecular electrostatic potential (MEP) study were carried out. The antibacterial activity of the ligand and the zinc complex against Gram-positive (*S. aureus*) and Gram-negative (*E. coli*) strains was evaluated using the agar well diffusion method. The zones of inhibition indicate that the ligand is more effective against *S. aureus* compared to *E. coli*, while the complex is more active against *E. coli.* Also, the activity against *S. aureus* of both the compounds are found comparable with the standard.

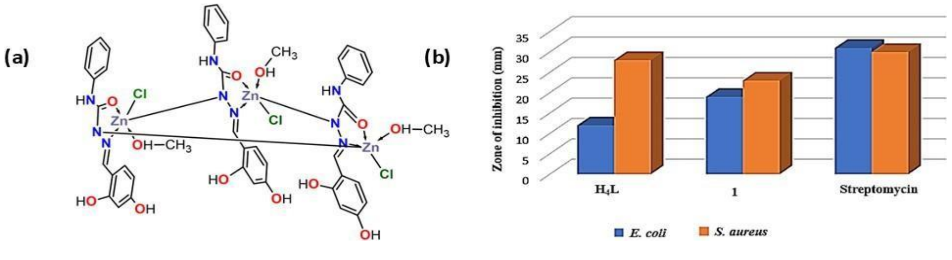

Figure:(a) Tentative structure of **1**, Fig. (b) Zones of inhibition of H4L, **1**, and Streptomycin at 1000 µg against *E. coli* and *S. aureus*.

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PP 24

A Hierarchical Porous Sheets of Bimetallic Terephthalate Frameworks for Sensitive Detection of Theophylline Drug

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Keywords: Electrochemical sensor, metal organic frameworks, theophylline, drug detection.

Methylxanthines are a group of drugs drawn from innumerable plants and animals. Among this, theophylline (TPH) is an alkaloid drug which was mainly used in the treatment and prevention of a number of respiratory diseases such as asthma and chronic bronchospasm in adults. Unfortunately, it has become a focal point in research due to its narrow therapeutic window and potential side effects making it as a toxic drug when used above its therapeutic range of 10 to 20 mg/mL[1]. To avoid the complications, TPH levels must be carefully recommended. So, electrochemical method plays a significant role in detection of TPH compare to other conventional methods[2]. For this, porous materials received much attention, one such material is metal-organic frameworks (MOFs) also called as porous coordination polymers (PCPs), which are crystalline solids with infinite lattices synthesized from secondary building units (SBUs)[3]. These novel hybrids are formed through the strong coordination bond between metal ions or clusters and organic linkers with permanent porosity leading to increased sensitivity towards detection of TPH.

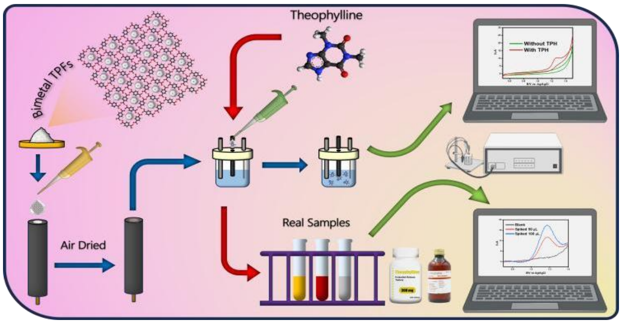

Figure 1: Graphical abstract of the electrochemical detection of TPH.

In this work, a novel bimetal terephthalate framework was synthesized by a facile hydrothermal method and characterized by various microscopic/spectroscopic techniques. Subsequently, the prepared material was casted on the glassy carbon electrode for the amperometric sensing of theophylline (TPH), a drug for various respiratory diseases. The electrochemical experiments were performed with Britton–Robinson (B-R) buffer solution for irreversible electro-oxidation of TPH. The modified sensor shows greater stability, selectivity, reproducibility with low limit of detection (LOD) and limit of quantification (LOQ) of 0.05 µmol L^{-1} and 0.18 µmol L^{-1}, respectively within the linear range of 1.0 x 10^{-6} to 1.50 10^{-4} mol L^{-1} and sensor mechanism was found to be diffusion-controlled phenomena. The proposed sensor offers a promising approach to monitor TPH levels in real-time (synthetic urine samples and TPH tablet and syrups solutions), allowing healthcare providers to adjust dosages and prevent toxicity. (see Figure 1)

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PP 25

Fluorescence Turn-on Sensor for Zn^{2+}, and Al^{3+} by Imine Based Conjugates

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Keywords: Schiff's base, Fluorescent sensors, Colorimetric sensors, *Turn-on* Fluorescence

The detection and quantification of metal ions are paramount owing to their crucial role in various biological processes.[1] Both excessive and inadequate consumption of metal ion can result in severe health issues in humans.[2] For instance, Zn^{2+} plays vital role in the structural, functional, catalytic, and signal transmission of biological systems. Similarly, iron, the most important trace element, involved in number of electron transfer as well as oxidoreductase process. The toxic metal ions such as Al^{3+}at higher concentration causes adverse effects to the human body.[3] Hence, the detection of biologically relevant ions and toxic ions are important areas of research. Schiff bases have proven to be best candidates for the selective detection of metal ions due to their strong coordination ability and structural variations. Hence, we have synthesized and characterized Schiff's base conjugates containing salicylaldehyde and 2-hydroxy-1-naphthaldehyde groups. The salicylimine **(SB1)** displays selectivity towards Zn^{2+} and Al^{3+} with a fluorescence enhancement fold of ~10 and ~20 respectively based on fluorescence spectroscopy. The limit of detection of **SB1** was 1.8×10^{-6} and 1.6×10^{-6} M towards Zn^{2+} and Al^{3+} respectively. The naphthylimine **(SB2)** displays selectivity towards Al^{3+} based on fluorescence spectroscopy [Figure 1]. The **SB2** effectively binds with Al^{3+} to form a 1:2 complex and exhibits LOD value of 3.2×10^{-6} M. The imine conjugate was capable of detecting Fe^{2+} and Fe^{3+} by colorimetric techniques, offering a sensitive and selective response with potential for real sample analysis.

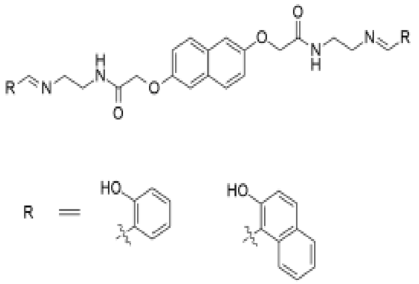

Figure 1: The structure of receptor molecule**, SB1** and **SB2**.

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PP 26

One-Pot Synthesis of a Fluorescent Cyan-2-Aryl Benzimidazole for Applications in Environmental Sensing, Luminescent Ink, and Coating Technologies

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Keywords: BBI, Picric acid, Fluorescent ink, Luminescent gel, Static quenching, IFE.

A highly efficient luminescence sensor has been developed using a one-pot green synthesis method to detect picric acid (PA).[1] The sensor was characterized through various spectroscopic techniques, along with absorption and fluorescence emission analysis, to evaluate its sensitivity and selectivity. It shows a limit of detection (LOD) of about 1.22×10^{-7} M and a quenching constant of 1.67×10^{5} M^{-1}, based on fluorescence data. The sensing mechanism was thoroughly investigated through both experimental and theoretical approaches.[2] To test the sensor's practical application, water and soil samples were analyzed. The detection process was further simplified using solid-phase paper strips and glass coating methods. Additionally, luminous ink and gel were created for fluorescent writing, surface coating, and molding applications.

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PP 27

Exploring The Potential of Strontium Substituted High-Entropy Oxides for Supercapacitors and Photocatalysts

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Keywords: High entropy oxides, Multicomponent systems, Functional properties, Specific capacitance, Photocatalytic dye degradation.

High entropy oxides (HEOs) represent a new category of advanced ceramic materials, distinguished by their remarkable functional properties. Since the first synthesis by Rost et al. in 2015, (HEOs), particularly (CuZnNiCoMg)O, have received significant attention and have been extensively studied. In this work, we substituted magnesium (Mg), the only non-transition element in the (CuZnNiCoMg)O composition, with another divalent atom from the same group, strontium (Sr). The structural and functional properties of the resulting HEOs are thoroughly examined for their potential applications in supercapacitors and photocatalysts. The novel (CuZnNiCoSr)O nanocrystalline HEO was synthesized through the coprecipitation method. The structural properties of as-synthesized nanostructured materials were analyzed using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and energy dispersive X-ray spectroscopy (EDX). X-ray photoelectron spectroscopy (XPS) was used to examine their elemental composition. The electrochemical properties of (CuZnNiCoSr)O were analyzed using a three-electrode system. The photocatalytic activities of the synthesized nanostructures were assessed by the photocatalytic degradation of methylene blue (MB). HEO compositions with strontium substitution demonstrated its *potential* to enhance performance in various applications.

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PP 28

Mechanistic Insights into Electrocatalytic Reduction of 4-Nitrophenol on Co_3O_4/Graphene Nanocomposite Synthesized Via a Green Method

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Keywords: Co_3O_4/graphene, electrocatalyst, 4-nitrophenol

Graphene holds promise as an electrocatalyst because of its key features, such as high surface area and excellent electrical conductivity[1]. Co_3O_4, a cobalt spinel oxide, exhibits strong redox electron transfer capabilities that aid in the transformation of organic molecules. However, its effectiveness is hindered by particle agglomeration, which limits the availability of active sites. Co_3O_4/graphene nanocomposite is synthesized here using the solvothermal method, while graphene is obtained through ethyl cellulose- assisted liquid-phase exfoliation of graphite. The structure and morphology of the prepared nanocomposite is investigated using characterization techniques like XRD, HRTEM images, and FT-IR spectroscopy etc, which indicated the strong interaction between graphene and cubic Co_3O_4. 4- Nitrophenol (4-NP), commonly used in the production of dyes, pharmaceuticals, and other industrial products, is a hazardous pollutant that easily leaches into soil and water[2]. Its persistent presence in the environment can cause long-term damage to the ecosystems and public health. In this study, the synthesized Co_3O_4/graphene nanocomposite is employed for the electrochemical reduction of 4-NP a synthetic intermediate, as demonstrated by the clear redox peaks in cyclic voltammetry, which indicate the reaction mechanism involving both adsorption and diffusion control. The redox peak currents show a linear increase with the square root of the scan rate ranging from 20 to 200 mV/s, suggesting a diffusion-controlled process and at a higher scan rate it follows a combination of adsorption and diffusion- controlled reaction. Similarly, the irreversible reduction peak of 4-NP to 4- aminophenol exhibited the same adsorption as well as diffusion-controlled behavior.

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PP 29

Metal Interconnected Transition Metal Dichalcogenides Meets Conducting Polymer Arrays to Give an Efficient and Stable Cathode Material for Asymmetric Hybrid Supercapacitors

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Keywords: Transition Metal Dichalcogenides, Conducting polymer, Doping.

Energy is one of the most important needs of the human race; Nowadays, the demand in energy storage devices, as well as the need for a green environment, has become a major global force in past years. In recent decades, hybrid supercapacitors (SC) pay an attention of quick charge and discharge device, which shows advantages such as fast rechargeable feature and extreme energy output.[1] Generally, Various materials such as metal oxides, conducting polymers (CPs), metal chalcogenides, etc exhibits pseudocapacitance. Contemporarily, researchers have increasingly focused on transition metal dichalcogenides (TMDs) and CPs due to their excellent performance in supercapacitors and other energy storge applications.[2] This approach offers the potential for scalable and eco-friendly material synthesis, supporting the development of sustainable energy technologies.

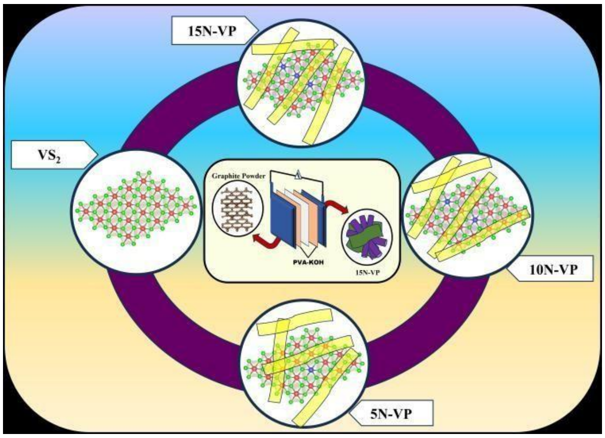

Figure 1: Graphical Representation for this work.

We present an innovative hybrid electrode material, Metal doped TMDs/conducting polymer(N-VP), synthesized through a sustainable hydrothermal strategy. By systematically adjusting the M1 and M2 precursor concentrations (5:95, 10:90, 15:85, 20:80) with the constant polymer (see Figure 1), we produced three distinct N-VP variants, namely 5N-VP, 10N-VP and 15N-VP each having unique morphological features. Among these, the optimized 15N-VP variant exhibited excellent crystallinity and a branched rodlike structure, delivering a high specific capacitance of 1047.9 F/g at 1 A/g. Furthermore, it maintained 90.52% of its initial capacitance even after 5,000 charge-discharge cycles, underlining its long- term electrochemical stability. To evaluate the capabilities of 15N-VP, we fabricated a hybrid material asymmetric supercapacitor (HMASC) device. The device unveiled admirable energy-storage performance, with a specific capacitance of 30.5 F/g at 1 A/g, power density of 870.87 W kg^{-1} and an energy density of 34.31 Wh kg^{-1}. Additionally, it maintained 92.17% of its capacitance even after 10,000 cycles, highlighting its durability and longevity. These results indicate the N-VP hybrid material as a highly promising candidate for future supercapacitor technologies.

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PP 30

Impact of Particulate Fillers on the Electrorheological Behaviour of Polymers

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Keywords: Electro-rheological behavior, Particulate fillers, Carbon black, Polymer composites, Dielectric polarization.

The incorporation of particulate fillers into polymer matrices significantly enhances their electro-rheological (ER) properties by introducing dielectric polarization and altering microstructural dynamics.[1] Recent advancements highlight that fillers such as carbon black, silica, and titanium dioxide can modulate the ER behaviour by affecting parameters like conductivity, particle size, and surface chemistry.[2] The addition of carbon black has been shown to improve the ER effect due to its high dielectric constant and superior dispersion characteristics within the polymer matrix.[3] Furthermore, studies demonstrate that the alignment and orientation of filler particles under an electric field contribute to the development of anisotropic structures, thereby enhancing the overall mechanical and rheological performance of the composites.[4] These findings suggest a promising avenue for tailoring the ER properties of polymers for applications in smart actuators, sensors, and advanced electronics.[5] The synergy between filler type and polymer matrix is a critical factor in determining the ER response, as evidenced by variations in dielectric relaxation and yield stress across different systems.[2] In particular, the use of nano-fillers such as carbon nanotubes and graphene has opened new possibilities for achieving superior ER effects due to their exceptional conductivity and surface area. Annealing and post-treatment processes further refine the filler-polymer interactions, enhancing microstructural stability and ER efficiency. [5] Future research must focus on optimizing filler loading, particle size distribution, and interfacial interactions to maximize performance while minimizing energy consumption. [1]These insights pave the way for the development of next-generation ER materials with improved functionality and adaptability to diverse technological applications. [3]

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PP 31

Energy Enhancement of a Nickel–Cobalt-Mixed Metallic Metal–Organic Framework Electrode and a Potassium Iodide Redox Mediator Bound with an Aqueous Electrolyte for High Performance Redox-Aided Asymmetric Supercapacitors

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Keywords: Metal organic frameworks (MOFs), Asymmetric supercapacitors, KI

In recent years, increasing energy demands in industry and human science call for efficient, clean energy conversion and storage devices. Therefore, improved energy storage technologies are urgently required. Batteries and supercapacitors have emerged as promising possibilities, and they have seen a lot of use in electronic vehicles and electronic gadgets. Compared with batteries, supercapacitors exhibit a fast charge and discharge capability, high power density, and high cycle stability.[1] Generally, Various materials such as metal oxides, metal organic frameworks (MOFs), covalent organic frameworks (COFs), conducting polymers (CPs), metal chalcogenides, etc., exhibits pseudocapacitance. Contemporarily, researchers have increasingly focused on Metal–organic framework (MOF) materials with redox active metal ions have improved the pore structure and have been continually exploited for energy storage because of their unique Pseudocapacitive nature. [2] By using KI redox mediator electrolyte, pseudocapacitance can increase the power density, and cycle stability is observed in the electrode material for supercapacitors.

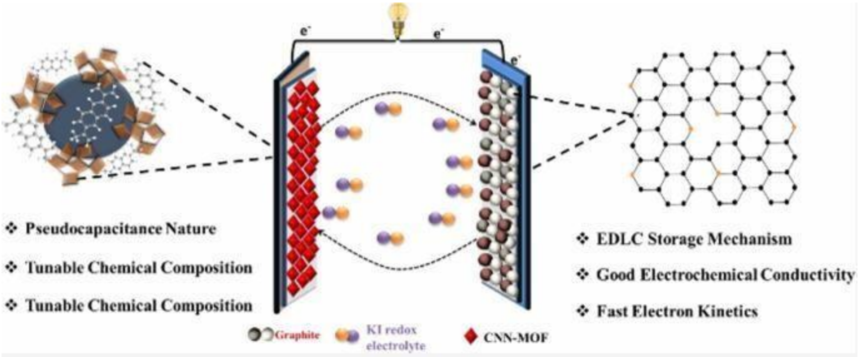

Figure 1. Graphical abstract of the fabricated RAASC device.

Enhancing the energy density of supercapacitors requires the development of novel electrode and electrolyte materials that can endure high voltages and exhibit fast electrochemical kinetics. Pseudocapacitance, high energy density, and specific capacitance can be achieved through electrodes and redox mediator electrolytes used in redox-aided asymmetric supercapacitors (RAASC), which are vital for their practical application. In this study, a rod and microsphere structure of Ni/Co-mixed metal-organic framework (MOF) was synthesized using a hydrothermal method for the positive electrode material. The rod and microsphere structure provides numerous active sites and smooth ionic channels, making Ni/Co-MOF a suitable material with three different organic linkers. The CNN-MOF material, which has a rod-like structure, demonstrated good capacitance. To further improve its capacitance, a KI redox mediator combined with a KOH electrolyte was introduced, achieving a specific capacitance of up to 612 F g^{-1} in a three-electrode system. Additionally, in the assembled RAASC, a graphite anode with CNN-MOF as the cathode and a KI redox mediator bound with a KOH gel polymer electrolyte exhibited electrical double- layer capacitor behavior. The RAASC device achieved an energy density of 84.2 W h kg^{-1} and a power density of 532 W kg^{-1}. It also displayed excellent cyclic stability, retaining 97.4% of its initial capacitance after 11,200 charge/discharge cycles. This work highlights the efficient fabrication of high-performance MOF electrodes and introduces the KI redox electrolyte-constructed RAASC device as a promising approach for advanced energy storage systems.

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PP 32

Flexible and Efficient Solid-State Interdigitated Microsupercapacitor based on Activated Carbon Microfibers

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Keywords: Microsupercapacitors, Layered Activated Carbon, Solid-state flexible device

Microsupercapacitors have a competitive advantage in tiny energy storage devices for wearable and portable electronics. Devices are increasingly in need of materials with high activity and cheap cost, as well as straightforward manufacturing processes. Here, we report the activated carbon microfiber electrode using an electrochemical activation method. This allows for an increase in the specific surface area and growth of the surface oxygen functional groups in the microelectrode. The as-developed carbon microelectrode achieved a greater areal capacitance of ~30.5 mF cm^{-2} (stability up to 50,000 cycles and 142.8 % capacitance retention). A full cell symmetric solid electrolyte microsupercapacitor with an energy density of 0.015 μW h cm^{-2} at 0.3 mA cm^{-2} and power density of 11.24 μW cm^{-2} with high cycling stability up to 20,000 cycles (125 % capacitance retention) is also demonstrated.

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PP 33

Novel High-Performance Supercapacitors Based on NGQDs and Conducting Polymers

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Keywords: Nitrogen doped graphene quantum dots, Supercapacitors, Galvanostatic charge/discharge, Cyclic voltammetry

Novel nitrogen-doped graphene quantum dots (NGQDs) were synthesized using conducting polymer as a precursor via a one-step hydrothermal method. Subsequently, NGQDs/PPy composites with varying NGQD concentrations were prepared through an *in situ* chemical oxidative polymerization process. The incorporation of crystalline NGQDs into the polypyrrole matrix significantly enhanced the electrochemical performance by improving charge-transfer efficiency and ion migration kinetics. The successful formation of NGQDs and their composites was validated through optical and morphological analyses. Transmission electron microscopy (TEM) confirmed the size, shape, and monodispersed nature of the NGQDs, while X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy provided detailed structural insights. Among the composites, NGQDs/PPy-10 exhibited the highest specific capacitance of 664 F/g at a current density of 0.8 A/g, outperforming pure PPy. An all-solid-state symmetric supercapacitor, assembled using NGQDs/PPy-10 as the electrode material and PVA/NaCl gel as the electrolyte, achieved a specific capacitance of 432 F/g at 1 A/g. The device also demonstrated a high energy density of 86.4 Wh/kg, a power density of 593.5 W/kg, and excellent cycling stability, retaining 94% of its initial performance after 3000 cycles at 5 A/g. These results highlight the pivotal role of NGQDs in enhancing the performance of hybrid supercapacitor devices.

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PP 34

Computational Insights into the Differential Efficacy of Nucleotide Analogues: A Study on Remdesivir and Sofosbuvir Across Viral Infections

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Keywords: Broad-spectrum Antiviral, Remdesivir, Sofosbuvir

Viruses exploit host cell machinery for replication, posing significant global health challenges. Although vaccines mitigate viral infections, limitations such as allergic reactions, partial efficacy against variants, and resistance underscore the need for alternative therapies. Re-purposing antiviral drugs, the evaluation of approved drugs for known viruses against new viruses, is cost-effective and time-saving [1]. Viral replication and transcription rely on polymerase enzymes, including RNA- dependent RNA polymerase (RdRp), DNA-dependent DNA polymerase, and DNA- dependent RNA polymerase, making them prime targets for antiviral drug development [2]. Broad-spectrum antivirals may act against all viruses, RNA viruses, or specific viral families [1]. This computational study focuses on two nucleotide analogues: Remdesivir, an adenine analogue and the first FDA-approved antiviral for COVID-19, which inhibits viral RNA replication via chain termination. [3] and Sofosbuvir, a uridine analogue and the first FDA-approved inhibitor of the HCV NS5B polymerase.[4], Despite their efficacy, Remdesivir exhibits reduced potency against HCV, while Sofosbuvir has limited efficacy against Ebola. This study aims to investigate the molecular basis for these limitations and optimize nucleotide analogues for diverse viral infections.

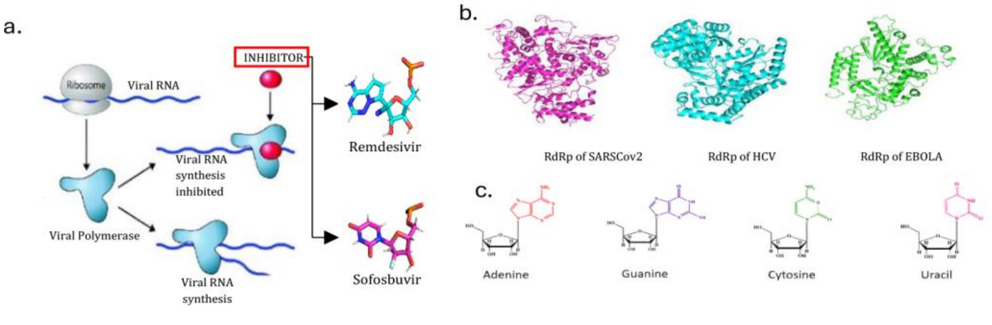

Figure 1: a. RdRp Polymerase b. Selected Viral Proteins c. Natural

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PP 35

Analysis of Surface Binding Sites in PET Hydrolases for Selective PET Binding–A Theoretical Study

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Keywords: PET hydrolases, Binding sites, Specificity

Plastic biodegradation represents a promising strategy for upcycling plastic and managing plastic waste[1]. PET hydrolases, a group of enzymes within the α/β hydrolase family are known for their ability to hydrolyze PET, which is a major polymer valued for its strength, chemical resistance, and recyclability across a wide range of applications[2].To industrially scale this process, structure-based rational engineering is essential. Enzyme- substrate complex formation, a critical step in catalysis determines the specificity and selectivity of the reaction[3]. There are reports on mutations on PETases that enhance enzymatic activity[4]. But enzyme-substrate complex formation step has not been extensively studied. In this work, we attempt to explore the specificity of enzyme-substrate complexes in some wild-type and mutated PET hydrolases with the help of molecular dynamics simulations. In this study, we focus on five specific PET hydrolases— *Is*PETase, LCC, *Tf*Cut2, *Ca*PETase, and Lipase (Figure 1a). Our results revealed additional surface binding sites, leading to the understanding that these sites could interfere with selective binding to the active site, potentially reducing catalytic efficiency. (Figure 1b) These findings suggest that eliminating non- specific binding sites through targeted mutations can improve the catalytic efficiency of PET hydrolases, facilitating more effective plastic waste biodegradation on an industrial scale.

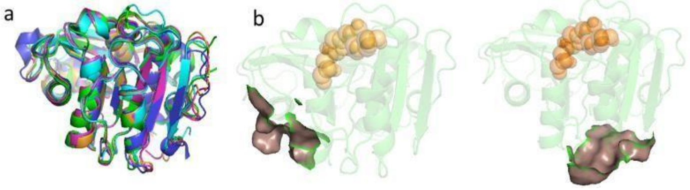

Figure 1: a. Superimposed structure of 5 selected PET hydrolases b. Surface representation of two major additional surface binding sites on *Is*PETase (catalytic residues represented as orange spheres)

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PP 36

Theoretical Investigation of Zeolite Confinement Effects on N_2O Decomposition Reaction

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Keywords: Zeolites, N_2O decomposition, Confinement

Copper exchanged zeolites are highly efficient catalysts for the direct decomposition N_2O. The topology of the zeolite and pore confinement play crucial roles in catalytic reactions.[1,2] The present study investigates the mechanism of N_2O decomposition in various types of zeolites - AEI, CHA, MFI, FAU, and MAZ - using quantum mechanics/molecular mechanics (QM/MM) calculations. Our results demonstrate that large pore zeolites FAU and MAZ exhibit higher activity for the activation of N_2O compared to medium and small pore zeolites. Quantum theory of atoms in molecules (QTAIM) analysis is performed to explain the difference in the O_2 desorption energies. This study provides a molecular level understanding of N_2O activation over topologically different zeolites.

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PP 37

Poly (Methyl Methacrylate)/Copper Oxide Nanocomposites for Flexible Optoelectronic Devices

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Keywords: Conductivity, CuO, Nanocomposites, Physical properties, Poly (methyl methacrylate)

Polymethyl methacrylate (PMMA) with varied compositions of copper oxide (CuO) nanoparticles was synthesized using in-situ free radical polymerization. UV–visible, FT-IR, FE-SEM, DSC, and TGA were employed to examine their structure, morphology, and thermal properties. The broadening and intensification of UV absorption, as well as the shift in IR peaks of PMMA with the addition of CuO, confirm their interactions. The reduction in optical band gap values with the reinforcement of nanofillers confirms the existence of intermediate energy bands in nanocomposites. The FE-SEM image revealed that the dispersion of CuO altered the nonporous, rough surface of PMMA into a homogeneous shape. The reinforcement of CuO enhanced the thermal stability and glass transition temperature of PMMA. The mechanical strength, modulus, impact strength, and rigidity of PMMA were significantly improved through in-situ polymerization. The electrical property analysis revealed that the AC conductivity increased with frequency, temperature, and filler content. The reduction in activation energy of AC conductivity with temperature points toward their semiconducting nature. PMMA/CuO nanocomposites with higher tensile strength, lower bandgap energy, higher conductivity, and thermal properties can be used to make flexible optoelectronic devices.

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PP 38

Vibrationally Resolved Absorption Spectra and Third-Order Nonlinear Optical Properties in Adamantane Derivatives – A DFT Study

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Keywords: TD-DFT, Adamantane, Non-Linear Property, Vibronic Spectra.

The quantum chemical calculation analyzes the third-order Non-Linear Optical (NLO) characteristics of adamantane (Ad) derivatives. The study involves the vibronic spectral and third-order NLO analysis of the adamantane derivatives. The trend shows that the energy gap (ΔE) is a crucial factor in determining the third-order NLO characteristics and the substituted adamantane possesses the highest second-order hyperpolarizability and exhibited the maximum intensity at a longer wavelength than ideal adamantane which is influenced by the enhanced intramolecular charge transfer (ICT) and lower vibrational frequency and thus results that the substituted adamantane can be a potential candidate for high-performance third-order NLO materials. These insights help to deepen the understanding of the potential of substituted adamantane for integration into next-generation optical devices.

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