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Emerging Frontiers in Chemical Sciences – 2022
EFCS 2022
Farook College (Autonomous)
National Conference

Day 1: 19 January 2023
Thursday

Registration & Inaugural Ceremony

8:45 am – 9:15 am	Registration and assemble at Yousef Al Saqer Auditorium
9:15 am- 10:00 am	Inaugural Ceremony Programme briefing: Prof. T. Pradeep, Chairman, Organizing Committee(IIT Madras) Inauguration: Prof. S. Chandrasekaran , SERB Distinguished Fellow, IISc, Bangalore
10:00 am- 10:20 am	Tea Break

Technical Session 1

Venue: Yousef Al Saqer Auditorium

	Chairman: Prof. Narayanan Kuthirummal, College of Charleston, USA
10.20 am – 11.10 am	Prof. S. Chandrasekaran , IISc, Bangalore
11.10 am – 12.00 pm	Prof T. Pradeep , IIT Madras
12.00 – 12.40 pm	Prof. Manzoor K. , Amrita University, Kochi
12.40 – 1.00 pm	Conference Photo Session
1.00 – 2.00 pm	Lunch Break

Technical Session 2

	Chairman: Prof. K. K. Unnikrishnan, Retired Professor, President, FALChem
2.00 – 2.40 pm	Prof. Prakash P. Neelakandan , DST-INST, Mohali
2.40 – 3.20 pm	Dr. Neena Susan John , CeNS, Bangalore
3.20 – 4.00 pm	Dr. Subinoy Rana , IISc, Bangalore
4.00 – 4.20 pm	Tea Break

Technical Session 3

Chairman: Dr. Ranimol Stephen, St. Joseph's College, Devagiri, Calicut	
4.20 – 5.00 pm	Dr. Susmita De , University of Calicut
5.00 – 5.40 pm	Prof. Evans Coutinho , St John Technical Campus, Palghar
5.40 – 6.10 pm	Oral Presentations
7.00 – 9.30 pm	Conference Dinner

Day 2 : 20 January, 2023

Friday

Venue: Yousef Al Saqer Auditorium

Technical Session 4

Chair: Dr. V. M. Abdul Mujeeb, Vice Chairman, EFCS	
9.00 – 9.50 am	Dr. Ashish Lele , Director, CSIR-NCL, Pune
9.50 – 10.30 am	Prof. Arun Mohan Isloor , National Institute of Technology Karnataka
10.30 – 10.50 am	Tea Break

Technical Session 4

Chair: Prof. K. Koyatty, Rtd. Professor, Farook College	
10.50 am – 11.30 pm	Prof. G. Anilkumar , MG University, Kerala
11.30 – 12.10 pm	Dr. Mousumi Das , IISER, Kolkata
12.10 – 2.00 pm	Lunch Break & Poster Presentation

Technical Session 5

Chair: Prof. K. M. Abdur Rasheed, Former Registrar, Kannur University	
2.00 – 2.40 pm	Dr. Jayaramulu Kolleboyina , IIT Jammu
2.40 – 3.20 pm	Dr. Ananya Baksi , Jadavpur University, Kolkata

Valedictory Session

3.20 – 3.50 pm	Valedictory Function and concluding remarks
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Atomically Precise Clusters for Applications

T. Pradeep

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Atomically precise clusters are a new class of materials with diverse properties. Many of their properties can be used for applications to address current needs. However, most of these materials have inherent limitations. Advancements made in the recent past make sure that these challenges can be addressed effectively. In this presentation, I will present the subject area of atomically precise clusters concisely followed by the current advancements. I will also present some of the new results in the area. One interest in presenting such results is to induce similar activities in colleges, even with limited infrastructure.

Chemistry of Nanoparticle Vaccines that Saved the World

Manzoor Koyakutty

Amrita Centre for Nanoscience and Molecular Medicine

Last three years, we witnessed a ‘magical realism’ of how chemistry, in the form of novel nanoparticles vaccines, saved the world population from the grip of COVID 19 pandemic. Like never before in recent human history, we realized the importance of science, especially chemistry, in saving human lives. With the approval of mRNA as vaccines, a new era in nucleic acid-medicine is evolving with extraordinary potential. In this talk, we will describe the science of nanoparticle based mRNA and peptide vaccines for SARS COV 2 and other upcoming vaccines for Cancer.

Multistimuli Programmable Organic Single Crystals for Flexible Electronics

Prakash P. Neelakandan

Institute of Nano Science and Technology, Sector 81, Mohali 140306, Punjab, India

There is an ever increasing need for the development of flexible electronic devices and components owing to the rapid growth of artificial intelligence and wearable devices. High-performance organic crystalline materials are considered strong candidates for next-generation flexible electronics such as displays, image sensors, and artificial skin.^{1,2} They are superior to the conventional materials in terms of flexibility, molecular diversity, low-cost, solution processability, and inherent compatibility with flexible substrates. Adaptable single crystals of small organic molecules have the potential for development as alternatives to conjugated-polymer-based crystalline semiconductors.³ This presentation will focus on our work on the mechanical and optical properties of luminescent materials prepared from Schiff bases.⁴⁻⁷ As the side chains are known to affect the photophysical and self-assembly properties of organic molecules, we have designed and synthesized a series of compounds based on salicylideneimine and naphthalideneimine moieties as the core and the side chains were varied systematically. While the flexible side chains had a minimal effect on the luminescence of the core moieties, the rigid side groups aided the formation of charge-transfer states that played a major role in defining the photophysical properties of these compounds. Further, it was observed that the luminescence and mechanical properties of these compounds could be modulated using external stimuli. The unique stimuli-induced self-assembly and mechanical properties of these compounds, and their applications in optoelectronics will be discussed.

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Role of high valent Ni in nickel oxide catalysts for efficient electrochemical urea oxidation

Neena S. John

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Electrochemical hydrogen generation from water splitting is hailed as the future of renewable energy technology. Urea oxidation reaction (UOR) holds great significance for replacing oxygen evolution counter part of water electrolysis with a less overall cell potential. Hence, UOR possesses three main advantages; less energy input for hydrogen generation, direct deployment as a fuel in direct urea fuel cells and environmental remediation by processing urea waste. Ni based electrocatalysts are popularly employed for UOR facilitated by the formation of NiO(OH) active site that plays a crucial role in achieving higher activity. However, sustained activity and long-term usage of the catalysts are retarded by CO_x poisoning, a by-product of UOR. We have explored tuning of these catalysts to aid the formation of active sites via promotion of Ni²⁺ into Ni³⁺ states and stabilizing these sites with higher tolerance for CO_x. Higher valent Ni ions can be promoted by introducing surface defects in nickel oxides by physical methods or employing Ni(III) oxide that inherently contain higher number of Ni³⁺ ions. The surface treated NiO exhibits better UOR activity than pristine NiO in alkaline medium and can be associated with the higher number of Ni³⁺ ions on the surface leading to enhanced formation of NiO(OH) active species. The dominant surface poisoning resultant of the enhanced activity is shown to be dealt by increasing KOH concentration. Ni₂O₃ shows six times higher UOR activity than NiO catalyst with retention of 70 % UOR performance even after 25 hours at an average current density of 25 mA/cm². The higher

activity, durability and sustained UOR activity of Ni₂O₃ can be correlated with the highly tolerant Ni³⁺ ions in Ni₂O₃ systems towards CO_x poisoning.

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Adaptive Enzyme-Equivalent Biomaterials with Superior Activities

Subinoy Rana

Indian Institute of Science, Bangalore

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Robust functional materials that can augment enzyme activity would provide effective tools for biotechnological applications. Herein, I will present a supramolecular approach to introduce a self-assembled vesicle that enhances the activity of natural enzymes. These out-of-equilibrium assemblies are designed in such a way that they form as long as a fuel (adenosine triphosphate, ATP) is present in the system. With ATP hydrolase-dependent dissipation of the assemblies, the activity of single enzyme and cascade pairs is precisely regulated in the time domain. Altogether, the tailorable nonequilibrium assemblies provide a biomimetic system that augments enzyme activity in a fuel-dependent manner. Likewise, we introduced new materials with excellent enzyme-like activities, often surpassing that of the natural enzymes. I will discuss about laccaselike activity of Cu_2O nanospheres, fabricated using a one-pot microwave-assisted method. These enzyme equivalents show superior enzymatic activity both in physiological and harsh conditions. The robustness of the enzyme equivalents extends practical applicability of enzymes in pollutant removal and biosensing. Furthermore, I will discuss a new class of dissipative enzyme equivalents, which exhibit oscillatory enzyme activity as a function of the fuel concentration. Overall, new materials with excellent biomimetic properties and practical applications will be demonstrated.

Understanding Proteins through Chemistry. What and How?

Susmita De

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We can put a set of alphabets together in innumerable permutations to make words each with its own meaning and with words we can make sentences, but only certain combinations in a particular order are meaningful for communications. Likewise, an endless number of poly-amino acid sequences can be formed with varying amino acid composition connected via peptide bonds. However only a certain, though roughly millions, number of possible amino acid sequences are represented in nature as proteins, each having a specific function. The function of protein is linked to the unique 3D structure attained by folding of the polypeptide chain, where the composition, sequence and position of specific amino acid are accountable. How the changes in the position, sequence and composition of the amino acid residues affects the activity of a protein at the molecular and atomic level towards controlling protein function and regulation of activity will be discussed based on recent works on ion channels,[1,2] immune proteins[3] and enzymes.[4]

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Using the right molecular modeling tool for the right application

Evans Coutinho

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For nearly two decades molecular modeling has made a deep impact on drug design, discovery and development. There are a variety of molecular modeling tools available for modeling specific end points. Broadly speaking, the information content available will decide the tool to be used. If knowledge about the receptor is available then tools like structure-based ligand design, docking, virtual screening may be adopted. However, in the event that nothing or very little is known about the target then QSAR, pharmacophore mapping, ligand similarity searches etc. may be used to model the end point. This lecture will cover the fundamental ideas about each one-of these tools along with some successful examples.

Trapeze Artistry in Smart Polymeric Hydrogels

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Thermoreversible hydrogels undergo temperature dependent volume phase transitions. These gels find applications in biomedical devices, smart windows, soft robotics and sensors. We have undertaken theoretical and experimental research on understanding the molecular basis of volume phase transitions, and we have shown that a fine balance of hydrophilic and hydrophobic interactions is necessary to induce sharp volume transitions near a critical temperature. We have demonstrated other unusual properties of such gels due to this fine balance of molecular interactions. In this talk I will summarize some of the interesting aspects of our work in this area.

Improving the Performance of the Membranes using Zwitterionic Polymer Nanoparticles as Novel Additives

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The rapid urbanization and industrialization has resulted in pollution and scarcity of the pure potable water. Among the different available technologies for the purification of the water, membrane technology is the most efficient and economical one. The performance of the membranes is dependent on the chemistry of the used materials/polymers. Researchers across the globe are actively involved in improving the performance and lifespan of the membranes. Current lecture highlights about novel synthesis zwitterionic polymer nanoparticles, which were prepared by Distillation Precipitation Polymerization (DPP) / Quarternization Precipitation Polymerization (QPP) methods. Structural elucidation of these novel derivatives were performed by different spectral as well as morphological studies. Further these zwitterionic polymer nanoparticles were used as additives for membrane fabrication. There is significant improvement in the performance properties of the membranes.

Synthesis of Medicinally Important N-heterocycles by Transition Metal Catalysis

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Heterocycles constitute one of the most important classes of compounds in organic chemistry. They are present in a large number of natural products, natural and synthetic drugs, agrochemicals and materials. In majority of drugs, the heterocyclic core acts as the active scaffold. Naturally, synthesis of these important compounds has attracted great attention, and several groups around the world are working to achieve medicinally relevant heterocycles using various synthetic protocols. In this scenario, we have developed a few methodologies based on transition metal catalysis involving Copper, Zinc, Iron, Manganese etc. in the synthesis of some nitrogen and oxygen heterocycles. In addition, we have also developed some green protocols for heterocycle synthesis without using any transition metal catalysis. These catalytic reactions will be discussed.

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Importance of Low-Lying Excited States of Carbon Based Molecules in Optoelectronic Properties

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In the field of optoelectronics and molecular electronics, carbon based organic conjugated molecules and their nanostructures are the centre of interest due to their immense applicability. Optoelectronic properties in light emitting devices and solar cell applications are governed by relative energy ordering of low-lying excited states of these molecules in singlet and triplet subspaces. This talk will highlight how low lying excited states can be calculated for these conjugated molecules within model Hamiltonian approach [1]. Small molecules can be solved exactly but comparatively larger systems are investigated with efficient Density Matrix Renormalization Group (DMRG) technique [2]. Theoretical and computational investigations on some of these molecules show they are promising candidates in the field of light emitting devices and designing singlet fission materials[3-6].

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Hybrid (2D) Porous Materials towards Sustainable Applications

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Metal organic frameworks (MOFs) are a unique class of materials comprising of metal centers linked by organic ligands, forming three-dimensional (3D) and/or two-dimensional (2D) porous networks. Striking characteristics, including high surface area, tunable pore structures, large pore volume, high redox activity, and tunable physicochemical properties, make MOFs candidate materials for sorption and electrochemical applications. However, MOFs are challenged by the issues associated with their limited chemical stability, poor electrical conductivity and inaccessible, intricate pores. Hybridization of MOFs with layered materials (graphene, Mxene, Clay) may be beneficial if the host structure provides appropriate interactions for stabilizing and improving the desired properties. Moreover, these hybrid (2D) Porous materials are known for their compositional versatility and formation of a range of structures with rich surface chemistries. In my presentation, comprehensive discussion on the remarkable recent efforts on hybrid porous for various applications are highlighted and potential future directions of rapidly evolving hybrid materials.^[1]

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Unravelling Molecular Materials using Mass Spectrometry

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Noble metal clusters are considered to be the bridge between atoms and nanoparticles where every atom counts. Ligand protected clusters show distinct absorption and emission feature in their condensed phase. Such atomically precise cluster molecules were identified as “Molecular Ion” in the gas phase using mass spectrometry (MS). Alongside solving their condensed phase structure through single crystal XRD, gas phase structure of such systems are equally important to create a rational link between their structure and properties. Advanced instrumentation plays a key factor to approach the growing quest for structure-property correlation and fundamental understanding of such complex systems. Application of different types of MS techniques for the synthesis, identification of new clusters, understanding cluster growth, multiple reaction monitoring and reaction mechanism establishment will be covered during the presentation. Integration of ion mobility separation (IMS) with MS adds a third dimension to a mass spectrum where ions are separated with respect to their size and shape, in addition to their m/z giving the flexibility to identify different isomer and conformers in the gas phase. Total structure analysis using density functional theory (DFT) and calculating collision cross section (CCS) of the ions enabled us to understand the experimental results by comparing them with the plausible isomeric forms.

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Green Synthesis of Chromonyl Chalcone and Pyrazoline as Potential Antimicrobial Agents – DFT, Molecular Docking and Antimicrobial Studies

**Mohammed Musthafa T.N.^{a*}, Snigdha K.^a, Abdullah M. Asiri^{b, c},
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The synthesis of biologically important chromonyl chalcone and pyrazoline derivative, via an impressive as well as an eco-friendly green approach, using LaCl₃/nano SiO₂ catalyst under solvent-free heating method has been discussed here. In this methodology, chromonyl chalcone prepared from 3-formylchromone and 5-acetylthiobarbituric acid by Claisen Schmidt condensation reaction was further used as an intermediate for the synthesis of a novel bioactive pyrazoline derivative. The novel compounds structures were established by FTIR, NMR and mass spectroscopic techniques. Antimicrobial activities were assessed for compounds against a set of bacterial and fungal strains using disk diffusion method, which revealed compounds as good antibacterial and antifungal agents. Geometry optimizations of newly synthesized compounds have been performed on DFT level of theory by the B3LYP acting along with Gaussain 16, revision B.01 to calculate the geometric and electronic structure parameters. The molecular docking study was carried out using the structure of DNA bacterial gyrase with newly synthesized chromone-based pharmacophore scaffolds.

Flexible Non-enzymatic Electrochemical Sensor Based on Nickel Hydroxide/ MWCNT Composite for the Real-time Detection of Glutamic Acid Using Invitro Stroke Model

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The development of miniaturized electronics for economical diagnostics which offer a timely output on demand is a major concern in the present biomedical research.¹ The lack of precisely determined chemical biomarkers has hindered such early diagnostics, especially in the case of brain disorders.² The ability of neurotransmitters to serve as critical biomarkers has sparked considerable interest in the scientific community.³ One of such most studied neurotransmitter which act as a biomarker in both physiological and social domains is Glutamic acid (Glu).⁴ Hence the sensitive and selective real-time monitoring of Glu has piqued the interest of the scientific community.⁵ The introduction of integrated sensors with a timely output can open the door to the mass production of miniaturized devices for the selective and sensitive detection of Glu.

Here, we report an easily synthesized nickel hydroxide/ multiwalled carbon nanotube (NH/MWCNT) modified non-enzymatic sensor for the detection of Glu. The NH/MWCNT composite-modified sensor showed excellent detection of Glu with a detection limit of 72 nM, even in the presence of many interfering groups. The practicality of the sensor in medical technology was established by its ability to detect the Glu released by both regular and oxygen-glucose deprivation-subjected SH-SY5Y neural cells, which act as an invitro model for stroke. Finally, as a proof of concept, an in-house

flexible sensor was fabricated to monitor Glu released by human neural cells. We anticipate that the present work will promote the development of cutting-edge third-generation non-enzymatic sensors for Glu monitoring.

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An Efficient Synthetic Protocol for Accessing *O*-Propargylated Oximes of β -Acetamido Ketones as Potential Candidates for Unusual Peptidomimetics

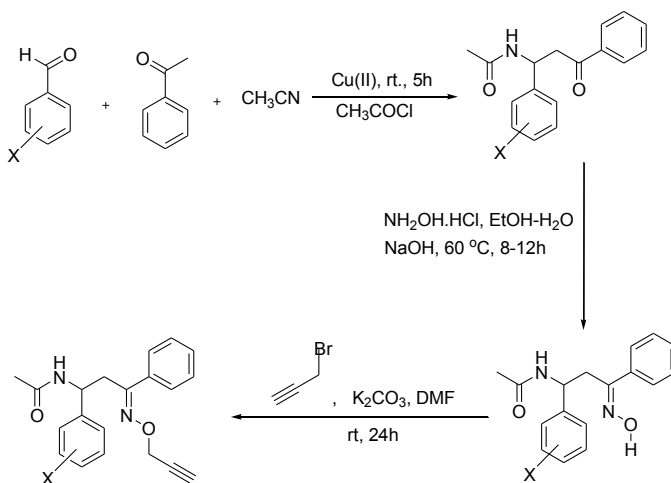
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Oximes holds great importance in organic chemistry on account of its easy synthesis from carbonyl compounds and their facile conversion to chemically relevant compounds like nitriles, amines, nitro compounds and heterocyclic compounds. The present work depicts the synthesis of *o*-propargylated oximes from β -acetamido ketones. The propargylated oximes of β -acetamido ketones will be potential candidate for accessing unusual peptidomimetic compounds via azide-alkyne click reaction. An efficient synthetic protocol is being reported for accessing a library of these potential candidates and the compounds were characterized using spectroscopic techniques such as FT-IR, ^1H NMR and ^{13}C NMR and also by elemental analysis. The present protocol is found to be simple and efficient as it afforded the products in very good yield and purity without intervention of column chromatography.

Graphical Abstract



Quantum Chemical Studies for Corrosion Inhibition of Mild Steel in Acid Media by the Schiff Base from Camphor and Tyrosine

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Schiff^o base ligand was synthesized and its inhibition action on mild steel was followed using weight loss method at 298 K – 328 K under 0.5 M HCl. The experimental results suggest that this inhibitor is efficient to control corrosion and its efficiency increases with increase in inhibitor concentration. The energy of activation and the thermodynamic parameters were calculated and evaluated from the results of temperature studies. From this study it is revealed that the inhibition efficiency depends on both the concentration of the inhibitor and the temperature of the system. Adsorption of this compound on mild steel surface obeys Langmuir isotherm model and the ΔG^0 value suggests mixed type nature of adsorption. The quantum chemical calculations were done by using Gaussian 16 software and geometry optimization were carried out by DFT- B3LYP/631G+G (d,p) basic set. Calculated parameters are agreed with experimental data.

Interfacial Tension-Induced Self-Assembly of MnO₂-Attached Pyrrole Oligomers and Subsequent Tailoring of Ultrathin Polypyrrole Sheets

Subin Kaladi Chondath¹, Subramanyan Namboodiri Varanakkottu², Mini Mol Menampambath*¹

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The liquid/liquid interface-assisted method represents an efficient and facile route for synthesizing two-dimensional (2-D) thin films of potential materials.¹ The underlying mechanism behind thin film formation at the liquid/liquid interface involves the preferential adsorption of nano-sized particles at the interface.² The spontaneous tendency of the interface to minimize high interfacial tension acts as a driving force for the adsorption and subsequent thin film formation at the interface.³ Here, a water/chloroform interface-assisted method is employed for the one-pot synthesis of highly crystalline polypyrrole/manganese dioxide (PPy/MnO₂) sheets. The synthesis strategy uses pyrrole as the monomer and potassium permanganate as the oxidant. The time-dependent decrease in the dynamic interfacial tension (from $32.35 \pm 0.23 \gamma$ mN/m to $17.63 \pm 0.62 \gamma$ mN/m) observed in pendant drop tensiometry proved the preferential adsorption of PPy/MnO₂ sheets at the water/chloroform interface.⁴ The ultra-thin sheet-like morphology and uniform distribution of ~ 6 nm MnO₂ nanoparticles were evidenced by transmission microscopy and atomic force microscopy images.⁴ UV-Visible spectroscopy and Raman spectroscopy were employed to assess the mechanism of polymerization and interfacial adsorption of nanoparticles during the synthesis of PPy/MnO₂ sheets.⁴ The predominance

of interfacial polymerization in retaining the electrochemical activity of the PPy/MnO₂ sheets is elucidated for the electrochemical detection of nicotine.⁴ Thus, the proposed synthesis strategy can be utilized to synthesize ultra-thin films of a wide range of multi-functional polymer nanocomposites.

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Carbazole Appended *trans*-Dicationic Pyridinium Porphyrin finds Supremacy in DNA Binding/Photocleavage over Non-Carbazolyl Analogue

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Cancer has been ranked as the second leading cause of mortality worldwide by World Health Organization (WHO).¹ Photodynamic therapy (PDT) using highly efficient photosensitizers (PSs) is an extremely promising tool for fighting against this unconquered malady. DNA targeted PSs that can generate reactive oxygen species are under active research. In this regard, cationic porphyrins/metalloporphyrins find an important space among the PSs.² By expecting an enhanced photosensitizing property, a carbazole appended cationic *trans*-pyridyl porphyrin (**2**) and its Cu(II) (**3**) and Zn(II) (**4**) complexes were designed and synthesized from porphyrin **1**, which is the non-cationic form.³ All the compounds were characterized by modern spectroscopic techniques. The DNA binding property of **2**, **3**, and **4** has been explored against calf thymus-DNA (CT-DNA) and it was quantized using intrinsic binding constant (K_b) that was calculated by UV-visible absorption spectroscopy, which follows the order **2** > **4** > **3**. Further, the fluorescence quenching efficiency and ethidium bromide quenching assay suggested an intercalative mode of interaction by the compounds towards the CT-DNA. This observation was then supported by the docking studies. Moreover, a notable DNA cleavage was observed by **2-4** by executing gel-electrophoresis experiment. The mechanistic studies revealed that the cause of DNA cleavage is the generation of singlet oxygen and this was confirmed by the

good singlet oxygen quantum yield observed for the compounds. Furthermore, we are expecting to draw these compounds for clinical applications.

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Microwave Assisted Green Synthesis of Fluorescent Carbon Dots from Sweet Flag (*Acorus Calamus*) for Fluorescent Sensing of 4-Nitrophenol

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In this piece of work, we devised a biogenic fluorescent probe from natural resource, sweet flag (*Acorus calamus*) through greener route by using microwave energy for the first time with best of our knowledge. The as obtained carbon dots with excellent fluorescence properties were designated as SFCDs. SFCDs were well characterized by different techniques including transmission electron microscope (TEM), X-ray diffraction (XRD), Fourier transform infrared FTIR, etc. The selective and specific interaction of the nano probe with 4-NP resulting the fluorescence quenching and it was made use to fabricate the probe as label free 4-NP sensor in water medium. 4-NP extensively used in various fields, the over usages of this compound mainly results in the ground water contamination. The lower level detection of 4-NP was highly demandable. The proposed probe selectively detect the 4-NP with LOD of 0.207 μM and linear range of 0-14.28 μM , the detection limit was found to be lower than allowed concentration of this pollutant in drinking water. The potentiality of the probe was implemented for the sensing application in real samples. The real sample analysis gives satisfactory level of statistical parameters including recovery percentage. After investigating the mechanism of quenching through different experiments, it was finally concluded that the observed turn-off in fluorescence is due to a combination of both static quenching and IFE.

Structural, Optical and Electrical Transport Properties of Zn Doped CuCrO₂ Crystallites

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CuCrO₂ is a p-type delafossite with potential applications such as solar cells, transistors, gas sensors, etc. Doping is one of the methods to alter the properties. Here we used Zn²⁺ as a dopant in Cr site of CuCrO₂ since it is a good candidate for creating point defect in the lattice and for improving band gap. Solid state reaction route was the method for the synthesis of the samples and XRD analysis were used for phase confirmation. FTIR, Raman and SEM investigations have revealed the structural and morphological modifications in the lattice. Carrier concentration and conductivity were measured by Hall measurements techniques and found as increased with increasing doping percentage of Zn²⁺. Optical studies were done by UV-Vis analysis and found the maximum band gap of 3.05 eV for 0.5 wt% doped CuCrO₂ hence the material has high optical transmission at visible wavelength and can be used as transparent conducting oxides (TCO) in products ranging from energy efficient low-e windows to photovoltaics.

Green Solvothermal-Assisted Synthesis of Mixed Nickel Oxide - Graphene Nanocomposite using Ball-Mill Produced Graphene for Supercapacitor Applications

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Development of high performance electrode materials for energy storage applications as in supercapacitor is a challenge in materials science research and technology. Due to the flexible valences, transition metal oxides can offer reversible faradic reactions leading to high specific capacitance and energy density. Oxides of nickel are one of the active transition metal oxide electrodes. The synergistic effect of nickel oxide with graphene can offer a better electrochemical performance in supercapacitors. Ball-mill assisted graphene preparation is a greener, scalable and economical approach for the bulk production of graphene and its composites. In this study, graphite is exfoliated using glycerol as a milling agent and the exfoliated graphite is dispersed in green solvent, isopropyl alcohol and the nickel oxides are then incorporated by precipitation followed by hydrothermal treatment. From the XRD patterns, formation of mixed oxides of nickel as well as metallic nickel is evident from the characteristic peaks present along with the major peaks corresponding to the cubic structure of NiO. Raman spectra reveal the well exfoliated and less-defective nature of graphene in the nanocomposite. The composite showed a high specific capacitance of 896 F/g at a scan rate of 5 mV and 837.5 F/g at a current density of 2 A/g in a three-electrode system using KOH electrolyte. The cyclic stability of composite is also investigated to prove its suitability as a supercapacitor electrode material.

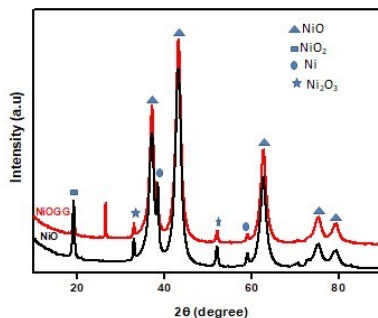


Figure 1. XRD pattern of nickel oxide graphene nanocomposite (NiOGG) and nickel oxide (NiO)

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Mononuclear Copper(II) Schiff base Complexes as Potential Phenoxazinone Synthase Models

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A series of structurally related mononuclear copper(II) complexes **1-4** of the type [Cu(L)(SCN)] **1-3**, and [Cu(L)(N₃)] **4**, containing tridentate N₂O Schiff base ligands have been synthesized and characterized using the modern analytical techniques. For instance, the transition around 640 nm corresponds to *d-d* transitions of **1-4** complexes and their EPR parameters $g_{\parallel} > 2.1 > g_{\perp} > 2.0$ reveal the square planar geometry that encompasses the copper(II) centre in the solution. The structural characterization of **3** by single-crystal X-ray diffraction study reveals a distorted square planar geometry encircling the copper(II) centre. Further, complexes **1-4** were subjected to phenoxazinone synthase mimicking activity in methanol, and it was found to promote the conversion of *o*-aminophenol (OAP) into 2-aminophenoxazin-3-one (APX) effectively under saturated dioxygen environment. Furthermore, this reaction follows the Michaelis-Menten model of enzyme kinetics and provides significant turnover numbers in the range of $2.4 \times 10^5 \text{ h}^{-1} - 6.2 \times 10^6 \text{ h}^{-1}$. More importantly, we have also identified the complex–substrate adduct [Cu(L)(OAP)] (**5**) using mass spectrometry and substantiated the radical-centred transient species forming through the the mono-adduct using computational analysis. Overall, the work presents that the complexes exhibit excellent activity in mimicking PHS and the detailed results will be presented during the presentation.

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Tailoring Au-Ag Alloy Embedded PEDOT Nanostructures for the Non-enzymatic Electrochemical Detection of Histamine

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The synergistic effect between conducting polymers (CPs) and metal nanoparticles appears with great perspective for new assemblies and applications. When alloys are formed in the nanoregime, the properties of monometallic nanoparticles are improved. Without utilising risky or expensive chemical agents, it is frequently challenging to produce Au-Ag alloy nanostructures under controlled conditions. Liquid/liquid interface-assisted polymerization offers a scalable methodology to fabricate hybrid materials, in contrast to the conventional and ubiquitous routes. We introduce this versatile approach toward the fabrication of well-tailored Au-Ag alloy nanostructures in a CP matrix, PEDOT (poly(3,4-ethylenedioxythiophene)). Due to its outstanding performance in a variety of applications, PEDOT has recently risen to the top of the list of CPs. In-situ polymerization at the hexane/water interface has generated Au-Ag alloy embedded PEDOT nanostructures without the need of any external reducing agents. Effective nanostructure tuning has been accomplished by altering the molar ratio of $\text{Au}^{3+}/\text{Ag}^+$ in the reaction mixture. The as-synthesized composite was further modified to detect histamine (HA), a biomolecule that naturally occurs in food and beverages and is known for its regulatory functions in the human body. The consumption of abnormal doses of HA can lead to allergic reactions and neuropsychiatric disorders. The sensor displayed high sensitivity towards HA with a limit of detection (LOD) of 1.5 nM. The proposed sensor's ability to detect HA generated by sub-cultured human neural cells SH-SY5Y and canned tuna fish demonstrated its practical

viability. Therefore, PEDOT/Au-Ag alloy nanohybrids can serve as an ideal non-enzymatic sensor HA detection.

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In Situ Polymerisation Induced Delamination of Ti₃C₂ MXene

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MXenes, the newly emerged 2D transition metal carbides or nitrides have attracted much attention of the research community due to their layered structure, polar surfaces and excellent chemical properties. The abundant polar groups endow them with good dispersibility in water even without any surfactant and enable them to interact with polar moieties by forming H- bonds and Van-der-waals force of attractions. These exceptional properties make MXene a promising candidate to be used as fillers in polymer nanocomposites. The layered structure of MXene promotes the intercalation of the monomer to the interlayer spacing which subsequently leads to polymerisation and hence causes the expansion and delamination of the MXene layers. Pyrrole is chosen as the monomer and is polymerized in the presence of Ti₃C₂ MXene by in situ polymerisation method. The physico-chemical investigations of the delaminated MXene-polymer sheets are then studied and compared with that of few layer MXene. The effectiveness of in situ polymerisation induced delamination of Ti₃C₂ MXene will be discussed in detail using various characterization techniques such as, electron microscopy, UV-visible and XRD in the presentation.

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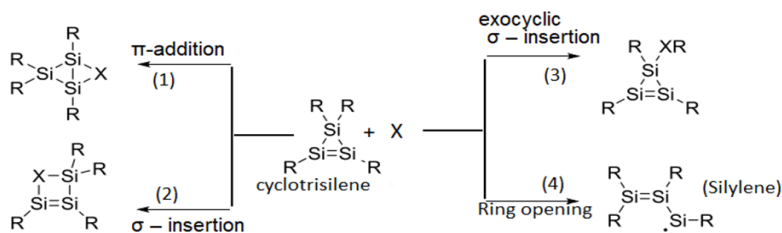
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Substituted Cyclotrisilene Generates Stable Silences - The Divalent Silicon Compound: The Latest in Silicon Chemistry

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The interaction of cyclotrisilenes with unsaturated molecules principally advance in two pathways: (1) The [2+2] π -addition of the unsaturated reactant across the silicon - silicon double bond of the cyclotrisilene, leading to the formation of a pentagonal product bearing no Si - Si double bond and (2) σ - insertion of the substrate into one of the endocyclic silicon – silicon single bonds, resulting in the ring expansion¹⁻⁴ with the formation of a pentagonal product with a Si - Si double bond. However, there are reported reactions in which, (3) the unsaturated reactant find place between a ring Si atom of the cyclotrisilene and its substituent (exocyclic - σ insertion)^{5,6}. Even though the carbon analogue of the cyclotrisilene readily undergo ring opening reactions, it is not common with the silicon dude. Despite that, in 2013, M. J. Cowley et.al reported such a reaction (4) in which aryl substituted cyclotrisilene undergoes an equilibrium ring opening reaction with N-heterocyclic carbene (NHC)^{7,8}. Therefore, one can expect four distinct interplays between an unsaturated reagent (X) and cyclotrisilenes on their encounter⁹.



In this presentation, we plan a computational analysis of the reactions of 1,2,3,3-tetramethyl cytotrisilene with $\text{CH}_3\text{-C}\equiv\text{CH}$ and $\text{C}_6\text{H}_5\text{-C}\equiv\text{CH}$. The energetics of all the four types of the expected reaction pathways: π -addition, σ – insertion, Exocyclic σ – insertion and ring opening were scrutinised with both substrates. All calculations were made using the B3LYP/6-31G level of density functional theory adopting Gaussian suite of programs. Minima were determined by IR frequency analysis and saddle points were located using single imaginary frequency.

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Biomimetic Polymer Membrane Based Potentiometric Sensor for Trace Level Detection of Atrazine in Ground Water

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Pesticides are biologically active compounds used by farmers to increase the yield of crops. The unethical usage of these pesticides adversely affects the non-targeted species in the environment. So it's highly recommended to develop sensors for detecting the trace amount of such pesticides. Here we developed a biomimetic potentiometric sensor for the trace level detection of Atrazine in ground water using Molecular imprinted polymer(MIP)¹ as ionophore . A thin composite film containing MIP was casted on the specified area of carbon cloth. The MIP was characterized using FTIR² and FESEM.³ The developed sensor shows good selectivity and can reliably be used for field monitoring.

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Green synthesis of Ag NPS from *Murraya Koenigii*, *Ocimum sanctum* and Spearmint leaves

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Green synthesis is an eco-friendly alternative method for the metal nanoparticles synthesis. Plants offer a better platform for the synthesis of nanoparticle since they are free from toxic chemicals and provide natural capping agents.¹ Silver nanoparticles are extensively known for their unique characteristics such as antimicrobial, anticancer, antiviral, sensors and catalyst.² Due to the biological applications, the green synthesized silver nanoparticles are also being used to find solution for environmental problems especially the dye degradation. We have synthesized silver nanoparticles from aq. silver nitrate through a simple route, using leaf broth of *Murraya Koenigii* (curry tree), *Ocimum sanctum* (Tulasi) and Spearmint (pudina) as reductant and stabilizer. The uv- visible spectra and microscopic images suggested that the formation of silver nanoparticles. The morphological studies was studied using FE –SEM and TEM .By using TEM, we can visualize the size, shape, and morphology of silver nanoparticles. From this, it is clear that most of the nanoparticles are spherical in shape and are well dispersed. Also we have conduct catalytic studies like dye degradation of methylene blue, methyl orange and 4- Nitro phenol with bio reduced silver nanoparticles. And also, we analyse colorimetric sensing of mercury with silver nanoparticles because mercury is a toxic pollutant.

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An Experimental and Theoretical Study on Heavy Metal Ion Adsorption by a Bischalcone-Based Mesoporous Polymer

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Wastewater from industries contains large amounts of heavy metal ions, which can cause a serious health hazard to humans and the environment¹. So, there is a great need to develop new methods, materials, and strategies for actively eradicating such contaminants. Adsorption is considered as one of the most efficient methods and porous polymers are one of the promising candidates in this group for the removal of heavy metal ions². By keeping this in mind we have synthesized a novel bischalcone-based thiophene-containing mesoporous polymer PTCA by FeCl₃-promoted oxidative coupling polymerization³. Even though the synthesized polymer exhibited low surface area, it displayed excellent adsorption of Zn²⁺ and Pb²⁺ ions due to their exceptional physiochemical properties such as porous nature, thermal and chemical stability, tunable functionality, presence of electron-rich heteroatoms, etc. The maximum adsorption capacity of the polymer PTCA for Zn²⁺ and Pb²⁺ was calculated as 729.4 mg/g and 569.1 mg/g respectively. The desorption study reveals that the synthesized polymer shows a maximum percentage recovery of 76.9% and 79.9% for Zn²⁺ and Pb²⁺ ions respectively. The theoretical study conducted using the Gaussian 09 program also supports the experimental findings.

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Swelling Characteristics of Biocomposites of Natural Rubber and Chitosan in Polar and Nonpolar Solvents

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The transport properties of different polar and non-polar aromatic solvents through chitosan (Ch) reinforced natural rubber (NR) were studied using sorption gravimetric analysis at room temperature. The effects of filler loading, curing system and penetrant size on the sorption properties were investigated. It is found that the diffusion and transport of solvents through the composites were decreasing with increase in filler loading which is due to the increased resistance to solvent penetration due to better interaction of chitosan on the rubber matrix. The overall mobility and flexibility of polymeric chains restricted with the addition of chitosan into the NR matrix, which reduces the ability of solvent penetration into the matrix. It was observed that as the size of the penetrant molecule increased, the solvent uptake decreased. The structural changes that take place to NR upon the incorporation of chitosan was analyzed by FTIR. By using SEM the morphological aspects of Chitosan NR composites were evaluated.

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Studies on Cellulose Fibres as Reinforcing Fillers in Rubber Based Biocomposites

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The need for biodegradable polymer composites is increasing in recent years because of the increased environmental concern and sustainability issues. Plant derived sustainable materials such as polysaccharides, cellulose, lignin, biochar, etc as reinforcing agents in polymer matrix are extensively investigated. Biocomposites with cellulosic natural fibers can be used as reinforcing fillers that can replace inorganic fillers, such as carbon black, silica, etc. in polymer matrix because of their good mechanical properties, easy availability, lower cost, renewable nature, production with less environmental pollution, non-toxic nature and low health hazards. In this work cellulose fibres is used as the reinforcing agent in acrylonitrile butadiene rubber/Natural rubber (NBR/NR) blend. The biopolymer composites were prepared in a two-roll mixing mill. The cure characteristics, mechanical properties and swelling properties were studied. The mechanical properties was found to be improved on the addition of the filler to the matrix. From the results it can be observed that cellulose fibres act as a promising reinforcement in the rubber matrix.

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Studies on Thermal and Bacterial Degradation of Biocomposites of High Density Polyethylene and Starch

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Starch from non edible tubers were used as reinforcing agent in high density polyethylene and composite materials were prepared. Starch from a non edible tuber was mixed in to HDPE using internal mixture. Maleic anhydride is used as the reinforcing agent. The effect of starch on the mechanical properties of HDPE was studied. The thermal and bacterial degradation of the composites was also studied. The structural changes that take place to HDPE upon the incorporation of tuber starch was analysed by FTIR. It has been found that the properties of HDPE have been improved in presence of non edible tuber starch.

The studies show that starch loading of tuber starch in HDPE and maleic anhydride, the tensile strength is very high as compared to the other HDPE-starch composition. The bio- degradability of HDPE polymer is varied by starch loading. Tensile strength and modulus is much lower when the samples are subjected to ageing fewer than 40 and 60 degree. By preparing the compositions of HDPE with starch from tuber, degradability of the polymer can be increased.

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Thin SiO₂ Shell Overcoating Enhances the Photostability of Silver phosphate Semiconductor for Photocatalytic Applications

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Semiconductor photocatalyst is a promising cost-effective alternative method for degrading hazardous organic contaminants from water. Ag₃PO₄ is a highly efficient visible-light photocatalyst for dye degradation and water splitting for the production of O₂. However, self-degradation is an unavoidable disadvantage of this semiconductor that limits the use of Ag₃PO₄ for real outside-the-lab applications. In this work, we demonstrated that the thin silica coating enhances the photo-stability by keeping the photocatalytic activity unaffected. Furthermore, the Ag₃PO₄, in combination with the SiO₂ shell, leads to enhanced photocatalytic activity in the degradation of Methylene blue (MB) and Rhodamine B (Rh B) even after five cycles.

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Synthesis and Characterization of Polyethylene Glycol Added Zinc Sulphide Nanoparticles

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PEG 400 (PEG) was used as a surfactant during the hydrothermal synthesis of zinc sulphide nanoparticles in order to study how the characteristics of ZnS nanoparticles change with varying PEG molecular weights. The presence of ZnS in the given sample was validated by X-Ray Diffraction, which provided insights to the crystal structure via Bragg's equation. The average grain size was also determined using the Scherrer formula, which ensured that the manufactured particle was nano-sized. The Scanning Electron Microscopy (SEM) provided details on the exterior morphology, and UV-Visible spectroscopy verified the optical characteristics. The blue shift in the band gap of ZnS nanoparticles was visible using UV-Visible absorption. ZnS nanoparticle sizes are also being determined using dynamic light scattering. The thermal stability of the sample is studied by thermogravimetric analysis (TGA) and the sample is thermally stable

Sustained Release Drug-Excipient Composites Via CO₂-induced Glassification

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Supercritical (sc) CO₂ ($T_c = 31.1^\circ\text{C}$, $P_c = 73.8\text{ bar}$) has been used as a safe and green solvent in the pharmaceutical industry. Non-toxicity, low processing temperature and ease of complete removal of CO₂ has made it an attractive alternative to conventional volatile organic solvents. ScCO₂ processing can bring about morphological and structural changes that affect release kinetics in drug-excipient composites. For instance, it was reported from our group that the CO₂-philic, sucrose octaacetate (SOA) forms a glass upon treatment with scCO₂.¹ Herein, we report the drug release behavior of the composites of Ibuprofen (IBU) in the SOA glass.

IBU and SOA (1:20) were stirred together in scCO₂ as a solvent, for an hour at 35° C and 80 bars. The resulting formulation had a smooth glassy surface with needle-like crystals localized inside as evidenced from XRD as well as optical imaging. Raman imaging revealed a homogeneous dispersion of drug in the matrix. Drug was released in a sustained manner from the excipient, owing to its entrapment inside the glassy matrix of SOA.

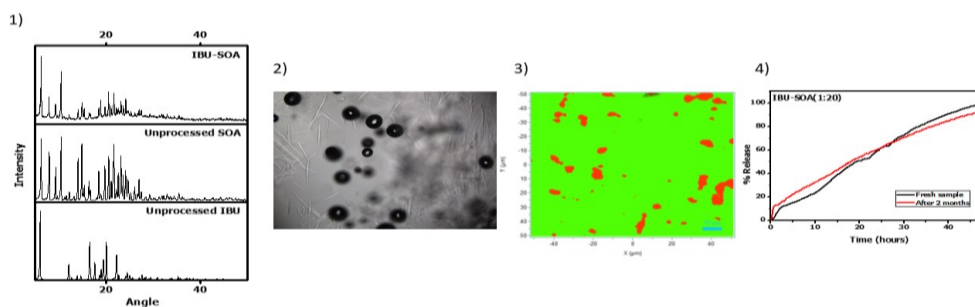


Figure 1 “XRD patterns of unprocessed IBU; unprocessed SOA; scCO₂ processed IBU-SOA (1-20).” **Figure 2** “System microscopic image of IBU-SOA processed in scCO₂ showing smooth glassy surface with needle-like crystals and pores localized inside.” **Figure 3** “Small area, high resolution (HR) Raman Image of Ibuprofen in SOA matrix.” **Figure 4** “Release patterns of fresh sample and sample after two months”.

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Nano Silver Synthesis and Antimicrobial Studies Using Nanocellulose from Pistachio Nut Shells as A Multifunctional Template

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The present study identified nano cellulose (NC) derived from pistachio nut shells with partial lignin and effective binding, complexing and reducing abilities, as an eco-friendly template for nano silver synthesis. The as-synthesized nanocellulose silver hybrid (NCAg) was characterized using Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-vis), high resolution transmission electron microscopy (HRTEM), and dynamic light scattering (DLS). Instantaneous color change at pH 10 suggested that reduction was facilitated by the formation of desulphated nanocellulose at this pH. The prepared NCAg was light orange with UV absorption at 406nm confirming the formation of nano silver. Crystallite size of nano silver calculated from XRD using the Scherrer equation was 11.62 nm and is comparable with the data obtained from DLS and TEM. FCC crystalline structure of nano silver was confirmed using XRD, HRTEM, and SAED data. The antibacterial activity of the NCAg hybrid against E. Coli, S. aureus, and B. subtilis bacteria was analyzed the zone of inhibition, optical density measurement, and the number of colonies forming units per ml studies. The NCAg hybrid with controlled morphology and size exhibited excellent antibacterial activity can offer valuable applications in the fields of active packaging films, wound treatment, separation membranes and as anti-biofouling films with good reinforcement ability.

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Development of Chitosan Modified ZSM-5 Framework

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The superior performance of zeolite catalysts is related to the presence of well-defined micropores. Normal zeolites are nano or micro porous materials which are size and shape selective catalysts. However, the presence of nano or micropores causes some limitations on their application^{1,2}. But the presence of a wide range of porosity (micro, meso and macro pores) has made hierarchical zeolites better catalysts than conventional zeolites^{3,4}. Hence, the use of the hierarchical porous ZSM-5 catalyst has become attractive for the acid catalyzed organic reactions.

In this work, Hierarchical ZSM-5 zeolite has been successfully synthesised using chitosan as a macro-template. The synthesized samples characterized using FTIR, FESEM, XRD, BET surface area analysis by N₂ adsorption-desorption, and NH₃ –TPD^{5,6}. The diffraction pattern obtained from XRD studies confirmed the typical Mobile five structure of ZSM-5. The acid sites on the surface investigated by temperature programmed desorption of ammonia (NH₃-TPD) and pyridine adsorption of sample followed by FTIR analysis⁷. The nitrogen sorption studies and FESEM analysis reveals that modified samples are mesoporous. The better pore properties and acidic properties of modified ZSM-5 make sure that it can be used as a suitable solid acid catalyst for organic reactions.

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Biomass Derived porous Carbon by Chemical Activation for Energy Storage

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Due to our current, inescapable need for energy, we need other alternative energy sources more frequently in our daily lives in order to combat the energy shortage. Energy storage and conversion received more attention in order to more effectively promote the energy sector due to the rapid energy consumption. Given the aforementioned fact, nanoporous carbon-based materials have gained more interest due to their larger surface area and potential use in the energy storage industry. This biomass-derived material is appealing because of its low cost, large surface area, and straightforward processing techniques. In this work, activated carbon was created using a kind of straightforward chemical activation process. The activating agent used in this activation is zinc chloride, and the activation method used is impregnation. By performing additional high-temperature carbonization under inert atmosphere, the activation was finished. The crystalline lattice structure and crystallinity are confirmed by the structural characterizations. Additionally, the variations in porosity and surface area with the activating agent content relative to precursor amount. Activated samples have better surface area in the range of 1700 m²/g. The prepared carbon is effectively used as the electrochemical energy storage with a specific capacitance of 91.58 F/g at 1V in symmetrical arrangement.

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Sorption Studies of Natural Rubber Composites Filled With Light Magnesium Carbonate Rich Industrial Waste

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Light magnesium carbonate (LMC) is utilized in various industries for flooring, dusting powder, toothpaste, cosmetics, fire proofing, fire extinguishing compositions, etc. The discarded LMC from various industrial units were subjected to landfill which is a principal cause for the hardness of water. This LMC waste is reutilized as a reinforcing filler in Natural rubber (NR) for the preparation of NR-LMC composites by two roll mill mixing method. The prepared composites were characterized by Fourier transform infrared spectroscopy (FTIR) and field emission scanning electron microscopy (FESEM) techniques. Swelling behaviour of these composites in various solvents like toluene, xylene and hexane were investigated in detail in terms of filler loading and penetrant size. The order of solvent uptake is in the order hexane < xylene < toluene. The solvent uptake is found to decrease with increase in filler loading and also with increase in molecular size of the solvent. Hexane showed least penetration behaviour due to its lower solubility parameter even though it has lesser molecular size. The transport mechanism is investigated and found to show deviation from normal Fickian trend.

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A Study on Thermal Decomposition Kinetics of HDPE/Chitosan/ Hydroxyapatite Composite Using Thermogravimetric Analysis

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Composites are the combination of two or more materials *viz a viz* matrix and filler, envisaged to generate a superior yet unique material^{1,2}. The modification of commercially available thermoplastic polyethylene implants by introducing the chitosan / hydroxyapatite as fillers lead to the formation of a ternary hybrid composite system. However, the extent of interaction between the hydrophobic matrix and hydrophilic fillers becomes a challenge for the mechanical and thermal stability. Thermal modeling studies using Flynn-Wall-Ozawa (FWO) and Kissinger-Akira-Sunose (KAS) models enable the determination of activation energy of the composites that contributes towards establishing the kinetics of the degradation mechanism. The activation energy values obtained by both the methods coincide indicating the suitability of the methods to study the degradation kinetics of the materials³. The thermal properties of the HDPE chitosan hydroxyapatite hybrid composite series with varying concentration of hydroxyapatite were investigated for heating rate of 5⁰C/min, 7⁰C/min, 10⁰C/min, 15⁰C/min .The activation energies were calculated and analyzed which describes the thermal stability as well as degradation profile of the composite. From FWO studies, highest actvation energy of 270.676 kJ/mol was determined for the chdpe sample. Similar results were also showed in KAS studies. The higher Ea values provide better thermal resistance to them. These composites can be further investigated for their usage in food packaging applications.

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Sweet Preparation of Graphene and its Decoration with Co₃O₄ for the Electrocatalytic Oxygen Reduction Reaction

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A green and cost-effective strategy for high quality graphene preparation is a major requisite since the present common method of graphene synthesis via graphite oxide suffers from the use of hazardous chemicals as well as defects in the graphene sheets. Here a promising alternative strategy for the large scale production of less-defective graphene is reported, where the ball milling of graphite with sucrose as a supporting milling agent is carried out. The non-conventional H-bonding interaction of carbohydrates with graphitic surfaces enhances the exfoliation of graphite layers during the mechanochemical treatment. Since energy conversion and energy storage systems gain high demands, the development of an efficient catalyst for oxygen reduction, which is the crucial cathodic reaction in fuel cells and metal-air batteries, is highly desired. The spinel Co₃O₄, a low-cost metal oxide is anchored on the ball-mill produced graphene sheets here via the precipitation method followed by calcination, which resulted in a hybrid material with superior electrocatalytic activity. The synergetic interaction between the metal catalyst and the graphene can facilitate the conductivity and oxygen reduction catalytic activity and reduces the agglomeration of metal nanoparticles as well as the restacking of graphene layers thus resulting in a stable catalyst configuration. The well-exfoliated graphene

layers and their less-defective nature is evident from various characterization results such as XRD, FTIR spectra, HRTEM, and Raman spectral analysis, which also revealed the uniform distribution of Co_3O_4 over the graphene sheets. The Co_3O_4 /graphene nanocomposite is found to be a promising catalyst for oxygen reduction reaction with an onset potential of -0.01 V.

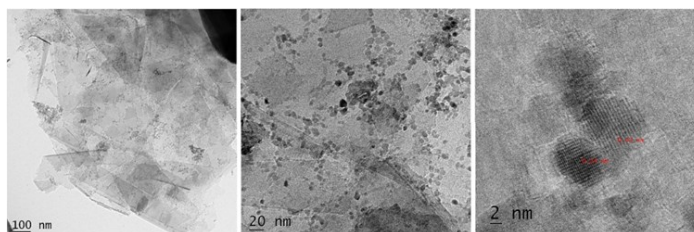


Figure 1. TEM and HRTEM images of the Co_3O_4 /graphene nanocomposite.

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An Eco-friendly Polyvinyl Alcohol/Soy Protein Isolate Hydrogel Films for Slow-Release Fertilizer Delivery

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Low nutrient efficiency and its environmental concerns, low water retention of the soil are significant challenges in the agricultural field¹. Hence slow release fertilizer hydrogels have become a potential solution². In this work, slow-release urea fertilizer(SRUF) based on polyvinyl alcohol(PVA) and soy protein isolate(SPI) blend films were successfully fabricated via the solvent casting method and were investigated for their structural properties by FTIR and XRD, thermal properties by TGA&DSC and morphological studies by SEM. The optimized blend solution was cross-linked with various weight percentages of citric acid(CA) ranging from 5-30%. The esterification reaction between citric acid and PVA in the semi-interpenetrating network was evidenced by FTIR spectra which showed the presence of the carbonyl absorption band of citrate ester at 1712 cm⁻¹. This crosslinking and robust hydrogen bond between PVA and CA enhanced the thermal stability and mechanical properties of PVA-SPI hydrogel films. In addition, the water absorbency decreased as the CA percentage increased. The urea release in water and soil was measured using spectrophotometry and exhibited a typical slow-release behaviour. Meanwhile, the water holding capacity and water retention behaviour of SRUF were studied and it was increased with an increase in gel content. The water retention of SRUF was more than 20% even after 30 days. The degradation behaviour of the coating material in soil was observed by SEM analysis. A degradation rate of 23% was attained when the SRUF was buried in the soil for 30 days. Thus these low-cost and eco-friendly hydrogel films with good water retention and slow-release property could be promising for application in agriculture.

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Ammonia Induced Reversible Structural Transformation of CsPbBr₃ Perovskite Nanocrystals

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In search for new materials for light energy harvesting and display devices have arrived at Lead halide perovskites as a result of their interesting properties like tunable band gap, soft crystal structure, easier carrier extraction, long exciton diffusion length, high emission yield, etc. However, the structural transformation/decomposition of lead halide perovskites in the presence of small molecules like water is the major concern. Herein, we present the structural transformation of immobilized CsPbBr₃ perovskite nanocrystals in the presence of vapour ammonia. The presence of vapour ammonia resulted in the quenching of visible absorption of CsPbBr₃ perovskite nanocrystals. Also, it resulted in the appearance of a new peak around 370 nm corresponding to CsPb₂Br₅. Interestingly, the structural transformation is reversible with time. The evaporation of ammonia from the substrate resulted in the reappearance of visible absorption and the emission from the CsPbBr₃ perovskite nanocrystals. The structural transformations are reversible up to five cycles. Thus, herein, we propose, the perovskite immobilized paper/glass substrates for the cost-effective sensing of ammonia vapours. Also, this will give insights towards the structural transformation of CsPbBr₃ perovskite nanocrystals in the presence of small molecules.

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Morphology-Controlled Synthesis of V_2O_5 Nanorods for Enhanced and Efficient Photocatalytic Degradation of Methylene Blue

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Controlling pollution brought on by the presence of dyes and pigments in wastewater released to rivers, lakes, and the ocean has emerged as one of the most challenging environmental issues. Utilizing $[VO(O_2)_2(OH_2)]$ as the starting material, V_2O_5 nanorods were successfully made using a template-free hydrothermal method without the need for organic surfactants or inorganic ions. By using X-ray powder diffraction (XRD), scanning electron microscopy (SEM), and Brunauer Emmet Teller (BET), Fourier-transform infrared spectroscopy, the produced samples were analyzed. The outcomes showed that this hydrothermal approach may easily convert per oxovanadium (V) complexes to V_2O_5 nanorods. The photocatalytic efficiency of the synthesized V_2O_5 nanorods was evaluated using methylene blue (MB) photodegradation. Due to better visible-light adsorption and a decreased rate of photoinduced electron-hole pair recombination in one-dimensional nanostructures, V_2O_5 nanorods showed higher photocatalytic activity in the degradation of methylene blue when compared to commercial vanadium pentoxide. Methylene blue (MB) worked best under basic conditions¹, better under neutral pH conditions, and poorly under acidic conditions. By using the PL emission of newly formed photoluminescent species 2-TAOH to scavenge the increasingly formed OH radicals, it was possible to understand why methylene blue's (MB) photodegradation was rising. It has been shown that active O_2 radical plays a significant role in the breakdown of methylene blue (MB). The methylene blue (MB) in an aqueous solution was consistently, repeatedly, and successfully degraded by the V_2O_5 nanorods.

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Thermal Decomposition Kinetics of Melt-Mixed EVA/Chitosan Composites Using Thermogravimetry

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Composites of ethylene-co-vinyl acetate (EVA) with chitosan (CS) and chitosan-g-PANi (CS-PANi) have been developed via a melt-mixing process by varying the composition of fillers. Investigations on the degradation mechanism of thermoplastics lead to insights of their performance at high temperatures. The decomposition kinetics of the composites was determined by plotting thermograms at different heating rates. The model-free Flynn-Wall-Ozawa and Kissinger method has been used to estimate the energy of activation (E_a) of the developed ¹⁻³. The activation energies of EVA/CS composites lie between 162 and 209 kJ/mol and EVA/chitosan-g-PANi composites within the range of 145-256 kJ/mol. The activation energy values varied toward higher conversion levels, which suggested multistep kinetics for the degradation of the material. The calculated E_a has been found to be in good agreement with the literature reports⁴.

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Evaluation of Lubricant Properties of Mustard Oil/CaO Nanoparticle Biolubricant Systems for Industrial Application

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There has been growing concern for the use of mineral oils as lubricants because of the world-wide interest in environmental issues. Many vegetable oils are preferred over mineral oils as lubricating base oils due to their high biodegradability, renewability and low toxicity.¹ Modifying vegetable oils to produce an alternative product to petroleum-based materials is one of the most important emerging industrial research areas today because of the adverse effects of petroleum products on the environment and the shortage of petroleum resources. Sustainable additives have attracted special attention recently because of their enhanced multifunctional performances and biodegradability compared with commercial additives.² In this work, natural oil- nano incorporated systems have been developed and examined for their physico-chemical, thermal, rheological and tribological properties. Mustard oil has been identified as the base oil after an optimization protocol. CaO nano particles have been synthesized and used as the additive in different compositions. TGA, DSC and UV examination of the systems have been carried out. Flash point, cold flow properties, temperature resistance and oxidation stability have been analyzed. An ideal lubricant with better properties, compared to the commercial SAE 30 oil has been developed with comparatively better biodegradability, for industrial lubrication.

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Application of Fruit Peel Extract as Plasticizer in Starch Films

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Food packaging aims at ensuring food safety from physical, chemical and biological factors and thus to extend their shelf life. The impressive physical properties and mechanical resilience of plastic packaging films made people to use it with passion from decades. As more and more people are now aware of the adversities brought by plastic packaging, the scientific community were prompted to find a biodegradable alternative even though it is impossible to discard the use of plastic completely. When it came to the food industry, the most radical solution proposed to boycott plastic packaging was to introduce ‘Edible films’, which can not only increase the shelf life, but also can improve the quality of the human and environment health in total.

Polysaccharides are easily available in bulk quantities than most biopolymers. Out of these polysaccharides, the extraction and purification of starch is the least cumbersome, hence it is popular as the polymer matrix in edible films. Even being a tuber native to South America, tapioca is cultivated as a staple food in Kerala. Being gluten-free, it has become quite popular as an alternative to cereals like wheat. Tapioca starch is obtained from the cassava tubers, which has about 15% starch content. Pure tapioca films have weak mechanical strength, feeble resistance to moisture and low processability.

The pectin rich fruit peel extracts were used to tackle the brittleness of starch films, thereby making them flexible and easy to handle for future packaging application.

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Phenothiazine Appended Cyanostilbene Systems: Twisted Intramolecular Charge Transfer and Mechanoluminescence Properties

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Conjugated Donor- π -Acceptor molecules have considerable interests due to the vast applications such as security links, opto-electronic devices, organic light emitting diodes (OLED), solar cells, sensors etc.¹⁻² Among various class of luminogens studied cyanostilbene based molecules received special interest owing to their excellent solid state emission properties along with stimuli responsive emission under the stimuli such as temperature, pressure, pH, solvent etc. Generally, the cyanostilbene based dyes are non-fluorescing or weakly fluorescing in the solution state, however these molecules highly emissive in the solid state. Herein, we designed and synthesized a D- π -A system which emissive in both solid and solution state with stimuli responsive emission properties. The present phenothiazine appended cyanostilbene based design relies on intramolecular twisted charge transfer and aggregation induced enhanced emission. In this study we demonstrate the solvatochromic emission along with multistimuli responsive reversible fluorescence switching in the solid state.

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Influence of Traffic on Contamination of Roadside Soil

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Heavy metal accumulation in roadside soils from traffic emission is one of the significant urban environmental issues, which is critical for environmental management. In this study, we collected soil samples from zones of three different traffic density at three different distances from road of Calicut city and investigated the impact of traffic density on physical and chemical soil properties (pH, EC, P, K, N, etc) along with available lead content in the soil and its influence on soil pH and total organic matter. The studies have been confirmed that, load of heavy metal contents in topsoils and their variability depend upon the traffic density and the distance from road. Higher Lead concentrations were found in sites with a high traffic volume on main roads. Results suggest a strong positive correlation between pH and soil organic matter with Lead content in soil.

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Theoretical Investigation into the Effect of Water on the N₂O Decomposition Reaction over Cu-ZSM-5 Catalyst

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Cu-exchanged zeolites are promising catalyst for the direct decomposition of N₂O. In the presence of water vapor, the decomposition reaction is inhibited and their application is greatly restricted. In the present study, we examined the mechanism of direct decomposition of N₂O over dicopper active sites that are located on the opposite sides of 10-membered ring in Cu-ZSM-5. It was shown that the formation of [Cu–O–Cu]²⁺ and [Cu–O₂–Cu]²⁺ moieties occurred during the decomposition of first and second N₂O over dicopper active centers. The N₂O decomposition over [Cu–O₂–Cu]²⁺ is kinetically unfavourable due to its high activation barrier. We also investigated the mechanism of decomposition of N₂O in the presence of water vapor. The activation barrier in the water incorporating mechanism of decomposition is higher than in the absence of water. The theoretical results shown that the formation of [Cu–(OH)–Cu(OH)]²⁺ have a crucial role in the inhibitory process of N₂O decomposition. Therefore, This study helps to understand the mechanism of N₂O decomposition and gives an idea about the effect of water on the fields of heterogeneous catalysis.

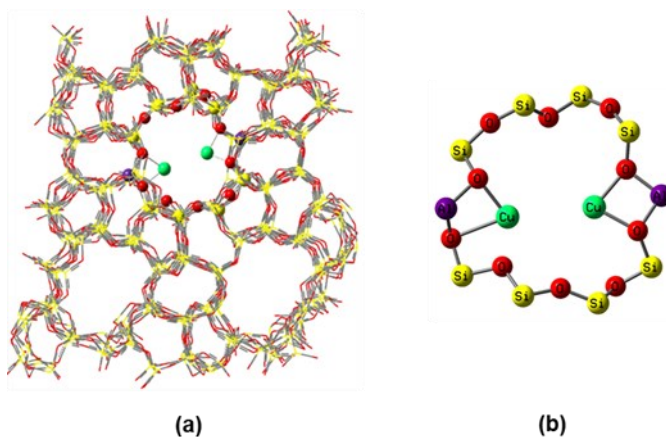


Fig. 1 (a) Representations of ZSM-5 model used in the study. Balls and stick represent the QM treated region, and the rest indicates the MM treated region. (b) 10- membered ring used for QM calculation.

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

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Atomically precise nanoclusters have recently emerged as ideal building blocks for constructing self-assembled multifunctional superstructures. The existing structures are based on various non-covalent interactions of the ligands on the nanocluster surface, resulting in inter-nanocluster interactions. Despite recent demonstrations on light-induced reversible self-assembly, long-range reversible self-assembly based on dynamic covalent chemistry on the nanocluster surface has yet to be investigated. Here, we show that Au₂₅ nanoclusters containing thiolated umbelliferone (7-hydroxycoumarin) ligands allow [2+2] photocycloaddition reaction-induced self-assembly into colloidal-level toroids. The toroids upon further irradiation undergo inter-toroidal reaction resulting in macroscopic supertoroidal honey-comb frameworks. Systematic investigation using electron microscopy, atomic force microscopy, and electron tomography suggests that the nanoclusters initially form spherical aggregates. The spherical structures further undergo fusion resulting in toroid formation. Finally, the toroids fuse into macroscopic honeycomb frameworks. As a proof-of-concept, we demonstrate a cross-photocycloaddition reaction between coumarin-tethered nanoclusters and an anticancer drug (5-fluorouracil) as a model photo-controlled drug release system. The model system allows systematic loading and unloading of the drug during the assembly and disassembly under two

different wavelengths. Our results suggest that the dynamic covalent chemistry on the nanocluster surface offers a facile route for hierarchical multifunctional frameworks and photocontrolled drug release.⁵

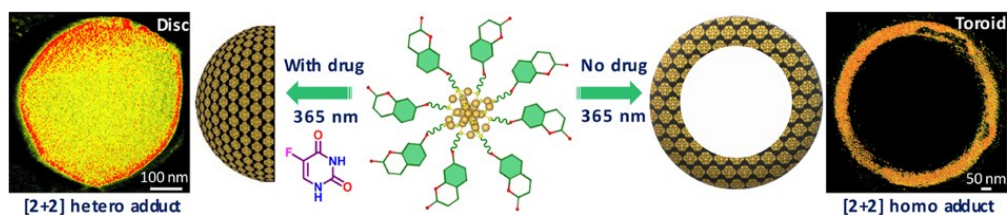


Figure 1. Schematic representation of the [2+2] photocycloaddition-assisted self-assembly and drug loading in thiolated coumarin-stapled Au₂₅ nanoclusters

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Role of Charge Transfer State Together with ESIPT in Tuning the Emission of Salicylidene-2-anthrylamine in Solution

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Salicylideneaniline is a well-known Schiff base for showing Excited State Intramolecular Proton Transfer (ESIPT), a process in which photoexcited molecules relax their energy through tautomerization by transfer of protons. Anthracene substitution to salicylidene plays a vital role in tuning the radiative decay process and ESIPT thus tunes the molecule to be a potential candidate in devices which are having applications in emission based turn on/off sensors. Herein, we report a Charge Transfer (CT) state of an anthracenebased Schiff base, Salicylidene-2-anthrylamine (2ASD), in addition to the commonly showing ESIPT through which a keto isomer is formed from the enol isomer by proton transfer. Theoretical studies also revealed a stable excited CT state formed by the rotation around the imine linkage of the trans-enolic form of 2ASD. We firmly believe that this study will help to understand the excited state process of other such salicylidene systems.

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Effect of NO \cdots H Interactions in Nitric Oxide Adsorption on Various Metal-loaded ZSM-5

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Adsorption characteristics of NO on various metal-loaded zeolites have an unprecedented role in explaining the mechanism of NO decomposition reactions.¹⁻⁶ In this work, we investigate the role of hydrogen bond present between adsorbed NO and Brønsted acid sites (NO \cdots H) in the adsorption characteristics of NO on various metal-loaded ZSM-5 (M = Fe⁺, Co⁺, Ni⁺, Cu⁺, Zn⁺, Pd⁺, Ag⁺ and Au⁺) by using DFT calculations. The M-ZSM-5 model considered for this study is depicted in Figure 1. The NO \cdots H hydrogen bonding interaction enhances the stabilization of NO-adsorbed complexes of most metals. A substantial hydrogen bonding stabilization is found for Zn, Fe, and Co metals in NO adsorption, and a reasonable stabilization for Ni, Cu, and Ag metals, whereas hydrogen bonds in NO complexes of Pd and Au show an anomalous effect in stabilization. However, a moderate N–O bond weakening due to NO \cdots H interaction is detected through Mayer bond order and QTAIM analyses in all NO adsorbed M-ZSM-5 complexes. Moreover, a noticeable redistribution of Mulliken spin densities and NBO charges on M-atom and atoms of NO are observed due to NO \cdots H interaction in all complexes. Interestingly, the correlation between hydrogen bond (NO \cdots H) distance and potential value at O-atom of NO (V_O) obtained by MESP analysis suggests V_O as a descriptor for measuring the hydrogen bond strength. Therefore, this theoretical exploration provides useful insights into the designing of an M-ZSM-5 catalyst for effective NO adsorption and further their applications.

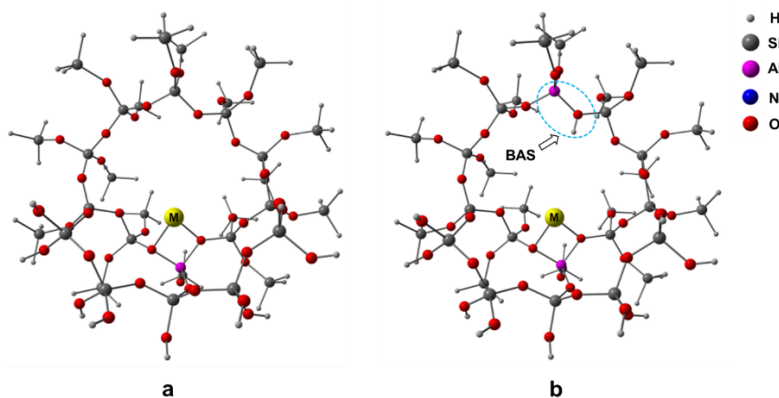


Figure 1. The model of M-ZSM-5 primarily used in this study. (a) System without Brønsted acid site (BAS). (b) System with BAS (marked with blue dotted lines). In the structures, M denotes (Yellow spheres) the monovalent transition metal ions (M = Fe, Co, Ni, Cu, Zn, Pd, Ag, and Au).

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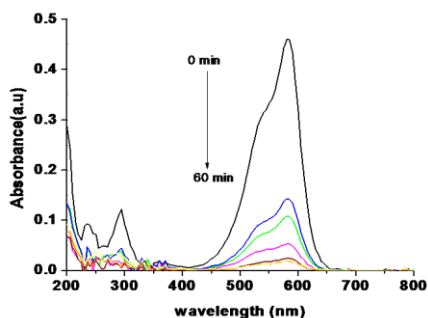
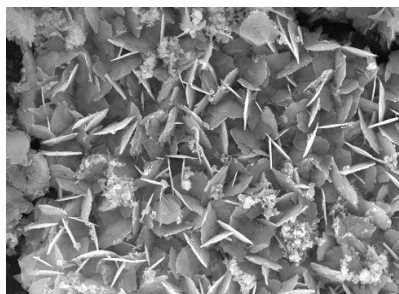
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Microwave mediated synthesis of BiOBr/CdS heterostructure photocatalyst for efficient degradation of Crystal Violet under Visible light

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Semiconductor photocatalysis is an emerging solution to address the world's energy crisis and environmental pollution. One of the compounds in this regard that has been heavily studied is Bi-based semiconductors due to their narrow energy gaps, disperse valance band, and nontoxicity. However, the rapid recombination of internal electron and hole pairs has a significant impact on the efficacy of these individual semiconductors. It has been reported that creating heterojunctions is a promising strategy for increasing the photocatalytic efficiency of these photocatalysts.¹⁻³ In the present work, a one-step microwave irradiation method was used to create a BiOBr/CdS heterostructure. The as-prepared samples were characterised by X-ray diffraction (XRD), scanning electron microscopy (FE-SEM), diffuse reflection spectroscopy (DRS), Raman spectroscopy, and photoluminescence (PL). BiOBr/CdS exhibited 96% photocatalytic activity and high stability for crystal violet (CV) degradation when exposed to visible light. The scanning electron microscopic image and the optical absorption sperctum BiOBr/CdS heterostructure are shown below.



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