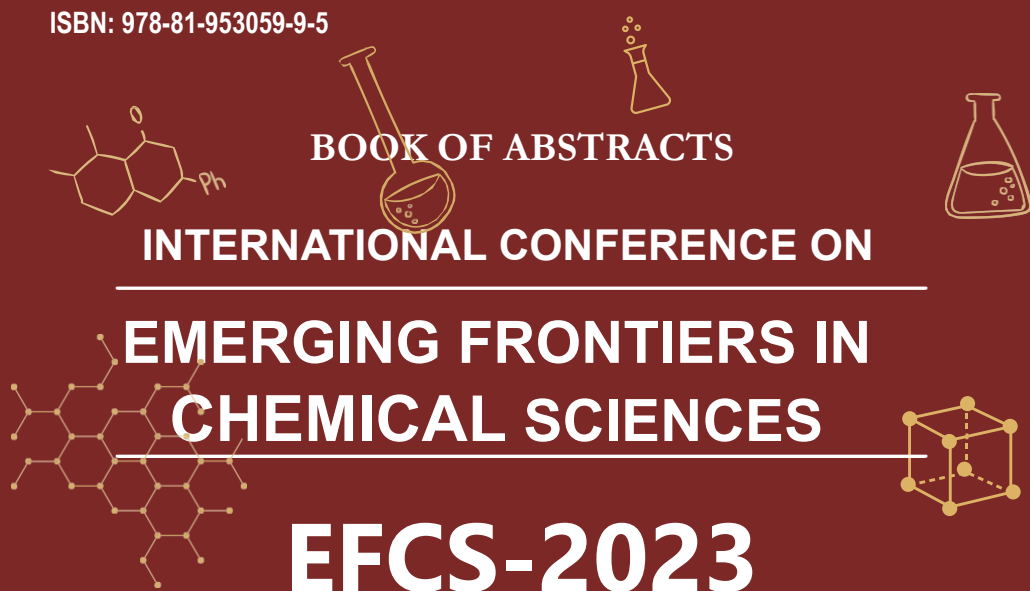


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**BOOK OF ABSTRACTS**  
**INTERNATIONAL CONFERENCE ON**  
**EMERGING FRONTIERS IN**  
**CHEMICAL SCIENCES**  
**EFCS-2023**

19 – 21 DECEMBER 2023



POSTGRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY

**FAROOK COLLEGE (AUTONOMOUS)**

P.O. Farook College, Kozhikode, Kerala, India- 673 632

Aided by Govt. of Kerala and Affiliated to the University of Calicut

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## Preface

The Postgraduate & Research Department of Chemistry, Farook College (Autonomous) is very pleased to release the Book of Abstract of the International Conference on "Emerging Frontiers in Chemical Sciences, EFCS-2023" conducted during December 19-21, 2023. This volume is an account of most of the contributions presented at the conference.

EFCS 2023 is the seventh conference of the EFCS series and the fourth international event hosted by Farook College with a view to provide a platform for young researchers and science aspirants to communicate with international and national experts. This event is very rich with the participation of eminent scientists of international and national reputation. The most respected Prof. N. Kalaiselvi, Director General of Council of Scientific and Industrial Research, New Delhi is the inaugural speaker of EFCS 2023. Another attraction of the conference is the honouring ceremony of Prof. K. Koyatty, Retired Professor, Farook College by EFCS Lifetime Achievement Award for his outstanding service to academics and society. The EFCS committee also recognise the efforts of young researchers by honouring with EFCS Young Scientist Award and Dr. Nygil Thomas, Assistant Professor, Nirmalagiri College, Kuthuparamba is selected for this recognition.

We would like to thank all the academicians, delegates and participants for their contributions to the Conference. We are much grateful to the sponsors of the programme including SERB, CSIR, KSCSTE ACS, M/s Ambernath Organics Pvt Ltd., Mumbai and the College Managing Committee.

In this volume, abstracts of invited lectures are given at the beginning, followed by abstracts of papers presented at the conference. The editorial board has tried its level best to make this collection a comprehensive one. This book of abstracts presents a snapshot of the state of development other subject at the time and would be invaluable for that reason.

We thank all those who have contributed to the successful organisation of the conference.

December 10,2023

Organising Committee

EFCS 2023



*Programme Schedule*

**EMERGING FRONTIERS IN CHEMICAL SCIENCES  
EFCS-2023  
INTERNATIONAL CONFERENCE  
19-21 DECEMBER 2023  
FAROOK COLLEGE (AUTONOMOUS)**

**Day 1: 19<sup>th</sup> December 2023 Tuesday**

*Venue: Yousef Al Saqer Auditorium*

***Registration & Inaugural Ceremony***

08:30 am – 09:00 am Registration and assemble at Yousef Al Saqer Auditorium

**09:00 am – 10:00 am Inaugural Ceremony**

**Programme Briefing: Prof. T. Pradeep**  
*Chairman, Organizing Committee (IIT Madras)*

**Inauguration: Dr. N. Kalaiselvi**  
*Director General, CSIR and Secretary, DSIR*

**Technical Session 1**

*Venue: Yousef Al Saqer Auditorium*

**Chair: Mr. P. A. Mohammed Ziyad**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

10:00 am – 10:50 am Atomically precise matter

**Prof. T. Pradeep**  
*Indian Institute of Technology Madras*

10:50 am – 11:30 Am Nature Inspired Circular Recycling for Soft Materials  
(NaCRe)

**Prof. Francesco Stellacci**  
*Institute of Materials Interfaculty Bioengineering, Ecole  
Polytechnique Fédérale de Lausanne (EPFL), Switzerland*

11:30 am – 11:45 am **Tea Break**

11:45 am – 12:00 pm **Conference Photo Session**

## Technical Session 2

*Venue: Yousef Al Saqer Auditorium*

**Chair: Dr. P. Rafeeque**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

12:00 pm – 12:40 pm      Metal Phosphate Rings, Chains, Cages, and Layered  
Materials: Energy Applications

**Prof. R. Murugavel**

*Indian Institute of Technology Bombay*

12:40 pm – 01:20 pm      Inorganic materials for energy storage

**Prof. G. Ranga Rao**

*Indian Institute of Technology Madras*

01:20 pm – 02:20 pm      **Lunch Break**

**Panel Discussion**

*Venue: Yousef Al Saqer Auditorium*

**Chair: Prof. V. M. Abdul Mujeeb**

*Vice Chairman, EFCS, Rtd. Head, Department of Chemistry University of Calicut*

02:20 pm – 03:00 pm      *Alumni Engagement for Strengthening Higher Education*

**Prof. Dr. Muhammed Basheer Ummathur**

*Principal, KAHM Unity Women's College, Manjeri*

**Mr. Abdul Latheef, E.K**

*Quality Assurance Manager, Al Wahaat Drinking Water  
Industry, Qatar*

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*Asst. Professor, Research institute for Electronic Science,  
Hokkaido University, Japan*

**Mr. Thabassum A. Nattikallungal**

*Research Scholar, University of Southern California, Los  
Angeles, USA*

## Technical Session 3

*Venue: Yousef Al Saqer Auditorium*

**Chair: Prof. Rajeev S. Menon**

*Head, Department of Chemistry, University of Calicut*

- 03:00 pm – 03:40 pm     2D materials-based smart membranes and their applications  
**Prof. Rahul Raveendran Nair**  
*University of Manchester*
- 03:40 pm – 04:20 pm     Ultimate clean energy Generation and storage device based on functional nanomaterials  
**Prof. Vinu Ajayan**  
*University of Newcastle, Australia*
- 04:20 pm – 05:00 pm     Carbon and Water Recycling for Sustainable Energy: A Journey from Fundamental Chemistry to Green Technologies  
**Prof. Sebastian Peter**  
*Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore*
- 05:00 pm – 05:15 pm     **Tea Break**

#### **Technical Session 4**

**Venue: Yousef Al Saqer Auditorium**

**Chair: Mr. Midhun Shah**

*Head, Department of Physics, Farook College, Calicut*

- 05:15 pm – 06:30 pm     Oral Presentations  
*Anjali C, University of Calicut*  
*Anjana K R, St. Joseph's college (autonomous), Devagiri, Calicut*  
*Athulya K R, Cochin University of Science and Technology*  
*Dipin Thacharakkal, Indian Institute of technology, Bombay*  
*Jazeel Raoof, University of Hyderabad*  
*P. Dhanyasree, Cochin University of Science and Technology*

- 07:00 pm – 09:30 pm     Conference Dinner (Hotel Copper Folia)

**Day 2: 20<sup>th</sup> December 2023 Wednesday**

#### **Technical Session 5**

**Venue: Yousef Al Saqer Auditorium**

**Chair: Dr. Reji Thomas**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

- 09:00 am – 09:40 am      Stabilising Gold in non-Cubic Crystal Structures  
**Prof. G. U. Kulkarni**  
*Jawaharlal Nehru Centre for Advanced Scientific Research,  
Bangalore*
- 09:40 am – 10:20 am      (Car)borane Cluster Molecules in Self-Assembly on Flat  
and Colloidal Metal Surfaces  
**Prof. Tomas Base**  
*The Czech Academy of Sciences, Czech Republic*
- 10:20 am – 11:00 am      Light-Induced Self-Assembly in Precision Noble Metal  
Nanoclusters: New Directions and Applications  
**Dr. Shibu Sidharth**  
*University of Calicut*
- 11:00 am – 11:15 am      Tea Break

### **Technical Session 6**

***Venue: Yousef Al Saqer Auditorium***

**Chair: Ms. Sumayya K**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

- 11:15 am – 11:55 am      Structural Design in Atomically Precise Silver and Copper  
Nanoclusters  
**Prof. Sukhendu Mandal**  
*IISER Thiruvananthapuram*
- 11:55 am – 12:35 pm      Synthesis of biogenic nanoparticles incorporated  
bionanocomposites and its applications  
**Dr. Bini George**  
*Central University of Kerala, Kasaragod*
- 12:35 pm – 01:30 pm      **Poster Presentation**  
01:30 pm – 02:30 pm      **Lunch Break**

### **Technical Session 7**

***Venue: Yousef Al Saqer Auditorium***

**Chair: Dr. Sajith P.K**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

- 02:30 pm – 03:10 pm      Transition Metal Catalysis for Heterocycle synthesis  
**Prof. G. Anilkumar**  
*MG University*



- 03:10 pm – 03:50 pm    Seeing Nanoscale Assemblies in 3D  
**Prof. N. Nonappa**  
*Tampere University, Finland*
- 03:50 pm – 04:30 pm    Exploring the Multiple Conformational States of RNA  
Genome through Network Analysis  
**Dr. Debashree Chakraborty**  
*NITK Surathkal*
- 04:30 pm – 04:45 pm    Tea Break
- 05:00 pm – 06:00 pm    Cultural Programme

### **Technical Session 8**

***Venue: Yousef Al Saqer Auditorium***

**Chair: Mr. Arshad T**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

- 05:30 pm – 06:30 pm    Cultural Program
- 07:00 pm – 09:00 pm    Dinner (Yousef Al Saqer Auditorium)

### **Day 3: 21<sup>st</sup> December 2023 Thursday**

### **Technical Session 8**

***Venue: Yousef Al Saqer Auditorium***

**Chair: Dr. Sr. Asha Thomas**

*Head, Department of Chemistry, Providence Women's College, Calicut*

- 09:30 am – 10:05 am    Ligand engineering in atomically precise metal  
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**Dr. Indranath Chakraborty**  
*IIT Kharagpur*
- 10:05 am – 10:40 am    Interfacial tension induced morphology tuning of polymer  
nanomaterial composites at the liquid-liquid interface  
**Dr. Mini Mol Menampambath**  
*NIT Calicut*
- 10:40 am – 10:55 am    **Tea Break**

## **Technical Session 9**

***Venue: Yousef Al Saqer Auditorium***

**Chair: Dr. Muhammed Yoosuf**

*Assistant Professor, Department of Chemistry, Farook College, Calicut*

10:55 am – 11:30 am      Heterogeneous Catalysis: Challenges and Opportunities in Methanol Synthesis, Oxygen Evolution Reaction and Oxygen Reduction Reaction

**Dr. Nygil Thomas**

*Nirmalagiri College Kuthuparamba*

11:30 am – 12:00 pm      Advanced technologies of secondary refining and 3D printing technology in high quality casting manufacturing

**Dr. Nithin Raj**

*Manager R&D, Peekay Steel Castings (P) LTD*

### ***Valedictory Session***

***Venue: Yousef Al Saqer Auditorium***

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12.30 pm – 01.30 pm      Lunch

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Shanavas Yoosuf and Shalina Begum T

# *Invited Lectures*



**IL-1****Atomically precise matter****T. Pradeep***Indian Institute of Technology Madras, Chennai, 600 036, India**E-Mail: pradeep@iitm.ac.in**https://pradeepresearch.org*

Research in the recent past has resulted in a large number of nanoparticles whose properties depend on the number and spatial arrangement of their constituent atoms. This distinct atom-dependence of properties is particularly noticeable in ligand protected atomically precise clusters of noble metals, which I will refer to as nanomolecules in this lecture. They behave indeed like molecules as revealed most elegantly by mass spectrometry. They show unusual properties such as luminescence in the visible and near-infrared regions. Their molecule-like behavior is most elegantly shown by atom and structure conserving chemical reactions between them. Several clusters, which are archetypal nanoparticles,  $\text{Ag}_{25}(\text{SR})_{18}$  and  $\text{Au}_{25}(\text{SR})_{18}$  ( $-\text{SR}$  = alkyl/aryl thiolate) have been used for such reactions. Despite their geometric robustness and electronic stability, reactions between them in solution at room temperature produce alloys  $\text{Ag}_m\text{Au}_n(\text{SR})_{18}$  ( $m+n = 25$ ), keeping their  $\text{M}_{25}(\text{SR})_{18}$  composition, structure and topology intact. We captured one of the earliest events of the process, namely the formation of the dianionic adduct,  $[\text{Ag}_{25}\text{Au}_{25}(\text{SR})_{36}]^{2-}$ , by electrospray ionization mass spectrometry.

Exploring this science further, we have studied rapid solution state exchange dynamics in nanoscale pieces of matter, taking isotopically pure atomically precise clusters as examples. As two isotopically pure silver clusters made of  $^{107}\text{Ag}$  and  $^{109}\text{Ag}$  are mixed, an isotopically mixed cluster of the same entity is formed, similar to the formation of HDO, from  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ . This spontaneous process is driven by the entropy of mixing and involves events at multiple timescales.

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**IL-2****Nature inspired circular recycling for soft materials (NaCRe)****Francesco Stellacci***Institute of Materials, Bioengineering Institute, and Global Health Institute  
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In 2070 the world will be inhabited by 11 billion people. One of the main problems, humanity will have to face is the sustainability of its materials production and consumption. By then, close to 1 billion tons of plastic will be produced yearly. Even if all polymers were to be bio-sourced and bio-degradable, there would still be a huge sustainability challenge both in terms of sourcing (to avoid problems such as deforestation or competition with food production) and of disposing (as those quantities would end up polluting earth at the very least by shifting ecosystems balances in significant ways). Clearly, humanity has to move towards the principles of circular economy where materials, once produced, remain in usage for the longest possible amount of time, taxing earth the minimum possible.

Interestingly when pausing to observe Nature's main polymers (e.g. proteins) it is possible to admire the circularity in their use. A vast over exemplification of protein metabolism shows that when a living specie eats, it will digest protein down into its monomers (the 20 proteogenic amino-acids), then the ribosomal synthetic cell machinery in the cell will reassemble them into completely different proteins in no way related to the original ones. One could state that Nature is teaching us the ultimate circular economy example for materials use, where recycling leads to the formation of materials that have limited commonality with the original ones, with the key building blocks (amino acids or nucleic acid bases) that are constantly in use.

In this talk, I will show the progresses my group is making towards showing that natural sequence-defined polymers can indeed be recycled into other polymers that have little in common with the original ones in the laboratory. Results involving various types of proteins and of nucleic acids will be presented. Efforts to translate this concept in the world of synthetic polymers will also be introduced.

**IL-3****(Car)borane cluster molecules in self-assembly on flat and colloidal metal surfaces****Dr. Tomas Base***Institute of Inorganic Chemistry  
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Carborane clusters have become an important class of molecules for self-assemblies. Their rigid molecular structures and rich isomeric forms enable to investigate particular physical properties of their 2-D assemblies while keeping the surface pattern either identical or close to identical. The respective self-organized monolayers exhibit fewer types and lower total number of surface defects, partly as a consequence of their low conformational freedom. In our laboratories we have been using these molecules as basic constituents for better understanding of some of the most fundamental self-assembly principles and intermolecular interactions that lead to a certain supramolecular structure and function. We shed more light on several key aspects such as the interaction of these molecules with flat gold and silver surfaces, we analyzed and showed the effect of their dipole moment orientation and magnitude on the surface properties changes and, not the least, we opened these monolayers to further chemistries by introducing additional functional groups that are in their SAMs exposed from the surface. This interdisciplinary contribution summarizes several of the above- mentioned aspects but also shows how these species can be advantageously used to generate new types of stable interfaces for further research and applications in bio-medicinal sciences.



**IL-4****Ultimate clean energy generation and storage device based on functional nanomaterials****Ajayan Vinu**

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In this talk, I will present a novel, stable and ultraclean hybrid energy storage and conversion device that continuously supplies energy using naturally abundant resources such as Sun, water and CO<sub>2</sub>. This device is mainly composed of nanoporous semiconductors including carbon nitrides, phosphides, sulphides and carbon-based materials that will be incorporated into stable, cost-effective photocatalytic semiconductor devices, for the conversion of CO<sub>2</sub> or seawater into clean fuels using sunlight. This novel technology will not only reduce CO<sub>2</sub> levels but will also provide a source of clean energy. I will also present the development, capabilities, and current and future applications of multifunctional nanoporous materials. Especially, much focus will be given to the fabrication of new family of semiconducting nanostructures composed of carbon and nitrogen (carbon nitrides) with different pore diameters, nitrogen contents, and structures which is the major component of the ultimate clean energy and storage device.<sup>1-9</sup> Especially, I will focus on the preparation of novel mesoporous C<sub>3</sub>N<sub>5</sub>, C<sub>3</sub>N<sub>6</sub>, C<sub>3</sub>N<sub>7</sub> and C<sub>3</sub>N<sub>8</sub> materials and their structural elucidation using different spectroscopic techniques. I will also demonstrate how the chemical composition, structure, porosity and the functionalization of these unique materials can be tuned, as well as the fabrication of CN with single molecular precursors with C, N, S elements and with mono and bimetallic sulphides. In the second part of the talk, I will present on the energy storage and photocatalytic performance of these unique nanoporous carbon nitrides and their hybrids on water splitting and CO<sub>2</sub> capture and conversion. Much focus will be given on the bulk production of the functionalized carbon nanostructures and their commercialization including the demonstration of the pilot plant for CO<sub>2</sub> capture. Finally, I will demonstrate the integration of this CO<sub>2</sub> capture and conversion technology with fuel cells, batteries and supercapacitors to develop an ultimate energy storage and conversion device for the continuous supply of energy for mobile and automobile applications. It is expected that the energy produced from this energy conversion and storage device will also be used to reduce the CO<sub>2</sub> molecules in a continuous process.

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**IL-5****2D materials-based smart membranes and their applications****Prof. Rahul Raveendran Nair***National Graphene Institute and Department of Chemical Engineering**University of Manchester, Manchester, UK**E-Mail: [rahul@manchester.ac.uk](mailto:rahul@manchester.ac.uk)*

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

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**IL-6****Seeing nanoscale assemblies in 3D****Nonappa***Faculty of Engineering and Natural Sciences  
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Transmission electron microscopy (TEM) imaging has revolutionized modern materials science, nanotechnology, and structural biology. Its ability to provide information about materials' structure, composition, and properties at atomic-level resolution has enabled groundbreaking discoveries and the development of innovative materials with precision and accuracy. Electron tomography, single particle reconstruction, and microcrystal electron diffraction techniques have paved the way for the three-dimensional (3D) reconstruction of biological samples, synthetic materials, and hybrid nanostructures at near atomic-level resolution.<sup>1,2</sup> TEM tomography using a series of two-dimensional (2D) projections has been used extensively in biological science. In recent years, it has become an important method in synthetic nanomaterials and soft matter research. I will discuss how TEM tomography offers unprecedented morphological details of 3D objects, internal structures, packing patterns, growth mechanisms, and self-assembly pathways of self-assembled colloidal systems.<sup>3-8</sup> I will also present how it provides valuable data for computational simulations for predictive design and reverse engineering of nanomaterials with desired structures and properties.



**Figure 1.** An overview TEM tomography assisted 3D reconstructed colloidal superstructures.

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**IL-7****Stabilising gold in non-cubic crystal structures****G. U. Kulkarni***JNCASR, Bengaluru*

Cubic lattice structure preferred by noble metals (e.g., Au, Ag, Pd and Pt) is thermodynamically highly stable. These metals cannot be induced into lower symmetry crystal structures even under high pressures and temperatures. Observing a structural transformation in these metals is therefore fundamentally exciting and can possibly be useful in tuning their otherwise noble behavior. Recent explorations in this direction have focused on nanocrystals, as the energy needed for lattice distortion is relatively low when the size is only a few nanometers. Inducing lattice strain at larger length scales to cause structural transformation in the crystallite is indeed a herculean task. The same has been achieved in the laboratory by stabilizing decahedral nanocrystal seeds in tetragonal and orthorhombic lattices via a simple synthetic method. The grown crystals exhibit corrugated rice-like morphologies with interesting properties.

The presentation will describe the synthesis of Au decahedra nuclei and the growth aspects. The results obtained using in-house facilities, on the morphology of the microcrystals, the unusual lattice forms and their phase transitions, chemical reactivity etc., will be presented. Further, the insights obtained using nanofocus synchrotron X-ray beamline on individual crystallites on the distribution of the various phases, will be described.

**IL-8****Inorganic materials for energy storage****G. Ranga Rao***Department of Chemistry**Indian Institute of Technology Madras, Chennai 600036, India**Email: [grrao@iitm.ac.in](mailto:grrao@iitm.ac.in)*

It is believed that supercapacitors and supercapattery electrochemical devices could replace 50% of lithium-ion batteries in future. Efficient and stable materials for energy storage and retrieval on demand are crucial for developing such devices. Nanoscale inorganic materials with various functionalities can be exploited as potential materials for energy storage. In this context, metal oxide-carbon based materials, ternary metal oxides, MOF-derived oxides, conducting polymer hybrid materials, polyoxometalates, metal oxynitrides, LDH materials etc have been investigated extensively. Various synthetic methods have also been devised to obtain nanoscale energy materials with different morphologies to enhance the energy storage and cycling stability. One of the major goals of our lab is to design efficient nanostructured materials for energy storage which led to the investigation of various simple and mixed metal oxides, graphene based-oxide composites, inorganic materials such as transition and lanthanide-based metal-organic frameworks (MOFs), MOF-derived materials, coordination polymers and transition metal chalcogenides (sulfides, selenides, tellurides). These materials possess required porosity and redox properties for energy storage applications. An overview of the synthesis strategies and the influence of nanostructure properties on charge storage will be discussed with examples.

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**IL-9****Metal phosphate rings, chains, cages, and layered materials: energy applications****Ramaswamy Murugavel***Indian Institute of Technology Bombay, Powai, Mumbai 400076*

Reaction of  $\text{H}_3\text{PO}_4$  mono aryl esters with a divalent metal such as  $\text{Zn}^{2+}$  in a donor solvent (L) leads to the isolation of tetranuclear metal phosphates  $[(\text{RO})\text{PO}_3\text{Zn}(\text{L})]_4$  whose inorganic core resembles the zeolitic D4R SBU.<sup>1,2</sup> In recent times, we have also unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions.<sup>3</sup> On the other hand the reaction of phosphoric acid mono and dialkyl esters yield either 1-D polymers or 2-D materials which thermally anneal to produce ceramic materials at temperature lower than 300 °C.<sup>4</sup> Rationalization of these building principles will be presented in this lecture, apart from highlighting the use of this class of compounds as molecular magnets,<sup>5</sup> phosphorus based perovskites and other energy materials.<sup>6</sup>

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**IL-10****Carbon and water recycling for sustainable energy: a journey from fundamental chemistry to green technologies****Sebastian C. Peter***New Chemistry Unit and School of Advanced Materials**Jawaharlal Nehru Centre for Advanced Scientific research, Bengaluru, Karnataka, India-560064**sebastiancp@jncasr.ac.in, sebastiancp@gmail.com*

Two most imminent scientific and technological problems that mankind is facing now are energy and climate. The energy production and utilization in modern society is mostly based on the combustion of carbonaceous fuels like coal, petroleum and natural gas the combustion of which produces CO<sub>2</sub>, which alters earth's carbon cycle. 30 billion of tons of CO<sub>2</sub> per year get emitted globally as waste from the carbonaceous fuel burning and industrial sector, which if converted to valuable chemicals have the potential to change the economy of the world. We, in our lab, are trying to address both issues and are keen upon translating our innovative technologies from the lab to the industrial and commercial scale. In this talk, I will discuss about our recent discoveries of materials based on intermetallics, chalcogenides, oxides, organic-inorganic hybrids, etc as efficient catalysts for the conversion of CO<sub>2</sub> to chemicals/fuels.[1-15] We are capturing CO<sub>2</sub> from industrial flue stream and converting it to value added chemicals/fuels such as methanol, CO, methane, dimethyl ether, C<sub>2</sub>-C<sub>5</sub> & C<sub>5</sub>-C<sub>11</sub> gasoline hydrocarbons. I will also cover our activities to produce green hydrogen via electrochemical pathway.[16] The utilization of hydrogen and other fuels like methanol/ethanol through fuel cells also will be discussed.[17] Catalyst design is at the heart of all these technologies, and we have developed customized catalyst systems for targeted product conversions as per the need of different industries. Development of these catalyst via various methods, the driving force behind the enhancement in activity and the mechanistic pathways will be explained with the support of various in-situ (DRIFTS, IR, XAFS), ex-situ (XPS, XRD, IR, XAFS) and theoretical (DFT calculation) studies. The talk also will cover the industrial viability of these catalysts.

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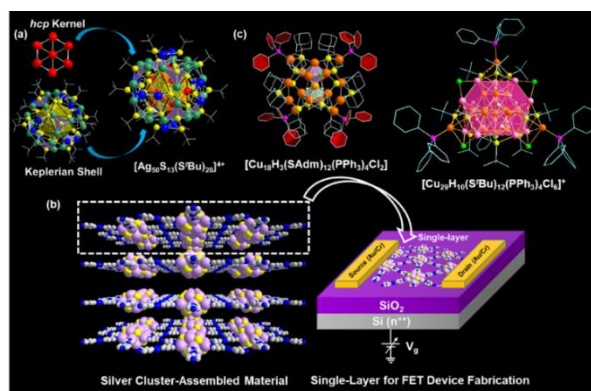
## IL-11

## Structural design in atomically precise silver and copper nanoclusters

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Atomically precise metal nanoclusters (NCs), a new class of materials are composed of tens to hundreds of metal atoms in the core and possess unique structures, high stability, and attractive properties. Built on the significant success of Au NCs, Ag and Cu NCs have recently received increasing attention. Synthesis and structural elucidation of these NCs are challenging because the zero-valent oxidation states of Ag and Cu are very reactive and prone to oxidization.<sup>1</sup> We have designed a new strategy to synthesize Ag and Cu NCs and then correlated their structure-property relationship. Here, we will discuss the following: (a) A new Ag-S NC  $[\text{Ag}_{50}\text{S}_{13}(\text{S}^t\text{Bu})_{20}][\text{CF}_3\text{COO}]_4$  with its unique hcp  $\text{Ag}_{14}$  kernel and  $\text{Ag}_{36}$  Keplerian shell-based structural architecture and its photoresponsivity;<sup>2</sup> (b)  $\text{Ag}_{12}$ -based two-dimensional cluster-assembled materials and their optoelectronic properties;<sup>3</sup> (c) Presence of unique structural geometry in  $\text{Cu}_{18}$  and  $\text{Cu}_{29}$ -based NCs (Figure 1).<sup>4</sup> **Figure 1.** Structural illustration of the newly synthesized atom-precise Ag and Cu NCs.



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**IL-12****Transition metal catalysis for heterocycle synthesis****Dr. G. Anilkumar***School of Chemical Sciences, Mahatma Gandhi University,**Priyadarsini Hills P O., Kottayam, Kerala, India-686560**E-Mail: anilgi1@yahoo.com, anil@mgu.ac.in*

Heterocycles constitute the most important class of compounds in organic chemistry. These have accumulated much significance mainly in chemical, biological and industrial domains. Nitrogen-based heterocyclic motifs have always been a fascinating arena pointing towards their irreplaceable presence in pharmaceuticals, natural products, and fundamental materials. We have developed various methods of synthesis of heterocycles such as indole, benzofuran, imidazopyridine, aminothiazole, aminobenzothiazole, pyrrole etc. using transition metal catalysis involving Copper, Zinc, Iron, Manganese, Nickel and Cobalt.

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**IL-13****Exploring the multiple conformational states of RNA genome through network analysis****Debashree Chakraborty***Biophysical and computational lab**National Institute of Technology Karnataka, Mangalore 575025, India*

The structural variation of RNA is often very transient and can be easily missed in experiments. Molecular dynamics simulation studies along with network analysis can be an effective tool to identify prominent conformations of such dynamic biomolecular systems. Here we describe a method to effectively sample different RNA conformations at six different temperatures (288 K, 303 K, 318 K, 333 K, 348 K and 363 K) by using relative orientations of the stems of the RNA molecule as the basis for the construction of a conformational network. This is a new methodology. This method gives us information about the prominent states of the RNA as well as the probability of the existence of different conformations and their interconnections during the process of evolution. The commonly used structural parameters such as RMSD, RGyr values often fail to give this information as many of the important details of the RNA might be neglected when we deal with the statistically averaged out data. We have taken SARS-CoV-2 RNA Genome as the system for this study.

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**IL-14****Ligand engineering in atomically precise metal nanoclusters****Indranath Chakraborty**

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Atomically precise metal nanoclusters consist of a well-defined metal core and a ligand shell. Generally, the diversity in ligand types is rare for most NCs except for a few gold NCs (e.g., Au<sub>25</sub>) reported so far. This is primarily because the ligand contributes significantly to determining the atomicity of the resulting NCs. Metal–ligand interactions during the NC formation are particular to individual metals and kinetic parameters used in the synthesis. For example, Ag<sub>25</sub> NC was reported to be synthesized only with 2,4-dimethylbenzenethiol (DMBT), while Au<sub>25</sub> NCs are reported with a wide variety of ligands, although both the NCs have identical crystal structures. Both secondary and primary ligands and their functionalities play a significant role in their optical properties, especially in photoluminescence. However, the mechanism of photoluminescence in NCs is still not clear. This talk will explain how ligand engineering can affect their resultant optical and structural properties, which can help understand the photoluminescence mechanism.

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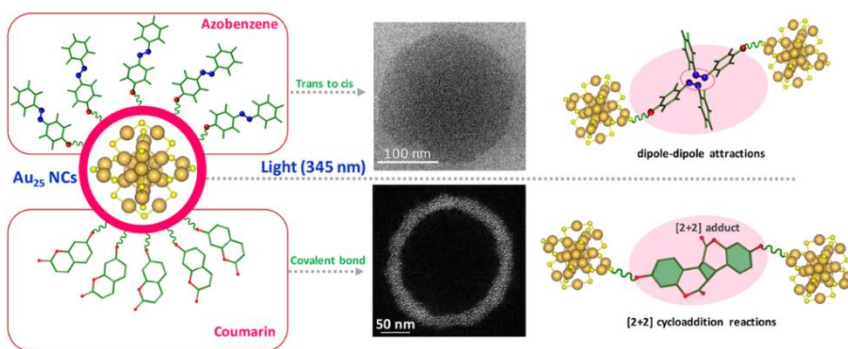
## IL-15

## Light-induced self-assembly in precision noble metal nanoclusters: new directions and applications

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Atomically precise noble metal nanoclusters (NCs) have recently emerged as ideal building blocks for constructing self-assembled multifunctional superstructures. In this talk, the light-induced assembly of Au<sub>25</sub> NCs fabricated with two different chromophores (azobenzene and coumarin thiols) will be discussed in detail. In the presence of 345 nm light, azobenzene-tethered NCs showed a disc-like assembly, whereas the coumarin-tagged NCs formed a toroidal assembly due to the difference in the photochemistry behind each chromophore (**Scheme 1**). Though the trans-to-cis photoswitching followed by the dipolar attractions played a major role in the first case, an efficient photocycloaddition-assisted dynamic covalent chemistry resulted in the selective formation of toroids. The same chemistry has been further extended to study the interplay of chromophore spacer lengths in the assembly and drug loading/unloading.



**Scheme 1.** Shows two different photochemistry-induced assemblies in Au<sub>25</sub> NCs.

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**IL-16****Synthesis of biogenic nanoparticles incorporated bionanocomposites and its applications****Dr. Bini George***Department of Chemistry, Central University of Kerala*

Green nanotechnology has, in recent years, been accorded increasing importance for two reasons, namely, its contribution towards the elimination of harmful reagents and its ability to facilitate the synthesis of valuable products in a cost-effective manner. The green synthesis of nanoparticles involves more compatible, eco-friendly, low cost and less time-consuming processes compared to other synthetic methods such as chemical and physical methods of synthesis, which has been widely used to achieve the same ends. This green synthesis method explores the advantages of inexpensive and non-toxic precursors. An economical, facile and eco-friendly method is described for a greener synthesis of metal and metal oxide nanoparticles using the natural hydrocolloids gum Arabic and gum Kondagogu. Abundantly available binding sites, adequate functional groups and desirable physical properties of these hydrocolloids make it a good template for nanoparticle synthesis. The synthesis and characterization of metal and metal oxide nanoparticles using natural hydrocolloid materials. The cytotoxic effects of synthesized nanoparticles in HepG2 and HEK 293 cell lines to screen least toxic nanoparticles for further applications. The fabrication of a carbon paste based modified electrode for the electrochemical detection of  $Pb^{2+}$  ions with the synthesized  $TiO_2$  NPs. The real time application of the fabricated electrode was explored by applying them for the detection of trace amount of lead content in plastic toys.

An affordable, simple and ecologically sound technique for synthesizing metal and metal oxide nanoparticles utilizing the leaf extracts as a reducing and stabilizing agent for sensor and packaging applications. The fabrication of CH-AgNPs modified glassy carbon electrode used for the electrochemical detection of  $H_2O_2$ . The preparation and characterization of CH/GE/AgNPs bionanocomposite films using a simple solution casting method. Physicochemical and mechanical properties, biodegradability and toxicity of films were evaluated. The real-time application of the films was tested by evaluating the shelf-life existence of carrot pieces covered with the composite films.

$CeO_2$  NPs were synthesised in a single-pot green method using *C. tamala* aqueous leaf extract. The biocompatible NPs were incorporated into the chitosan matrix, forming  $CeO_2$ /chitosan nanocomposites ( $CeO_2$ /CS) by the solution casting method. The well characterised  $CeO_2$ /CS nanocomposite was utilised for the fabrication of biosensors. The economically viable, easily prepared  $CeO_2$ /CS-MGCE can be applied for the development of sensor devices for neurotransmitters.

**IL-17****Interfacial tension induced morphology tuning of polymer nanomaterial composites at the liquid-liquid interface****Subin K. C. and Mini Mol Menamparambath***Department of Chemistry, National Institute of Technology Calicut**Email: minimol@nitc.ac.in*

The distinct interface between two immiscible solvents ensures a limited diffusion and mass transfer of molecules through two-dimensionally (2-D) confined few nanometers thick interfacial areas. Such liquid/liquid (L/L) interface assisted synthesis methods are easy, scalable, and eco-friendly. The polymerization at the L/L interface primarily involves the self-organization of monomer and initiator molecules at a localized region, i.e., an interface where interfacial tension is high. The initial stage of the proposed work focuses on the mechanistic investigation of the vital role of various oxidants in the self-assembly of reactive intermediates at the liquid/liquid interface in the formation of conductive polymers. In this presentation, an efficient and versatile approach toward the in-situ tailoring of polypyrrole/manganese dioxide (PPy/MnO<sub>2</sub>) nanostructures. The method verifies that ~6 nm MnO<sub>2</sub> NPs were successfully encapsulated in ultrathin PPy sheets without particle agglomeration. Therefore, the presentation will encompass a discussion on the distinctive synthesis strategy, interfacial polymerization, as well as its capability to tune physicochemical properties, and its potential applications.

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**IL-18****Heterogeneous catalysis: challenges and opportunities in methanol synthesis, oxygen evolution reaction and oxygen reduction reaction****Dr. Nygil Thomas***Department of Chemistry, Nirmalagiri College**Kuthuparamba, Kerala, India, 670701**E-Mail: [nygill@gmail.com](mailto:nygill@gmail.com)*

Heterogeneous catalysis deals with the acceleration of chemical reactions by solid catalysts. Heterogeneous catalysts are essential for a wide variety of industrial processes, including the production of fuels, chemicals, and pharmaceuticals. One challenge is the development of new catalysts with improved activity and selectivity. This is particularly important for reactions that are currently inefficient or difficult to carry out. Another challenge is the design of catalysts that are stable under harsh reaction conditions. This is important for extending the lifetime of catalysts and reducing costs. Oxygen evolution reaction (OER) and oxygen reduction reaction (ORR), are the key electrocatalysis technologies for the development of renewable energy conversion and storage systems like water splitting, metal-air batteries, and fuel cells. For the large-scale application of these technologies highly efficient, low cost and stable electrocatalyst are very important. Recently, non-noble metal-based OER electrocatalyst has drawn fabulous research interest. A comprehensive investigation is made on various types of nanostructured materials including Co, Ni, and Mn-based transition metal oxide and multi-metal oxides such as spinels, and perovskites as catalysts for OER and ORR. The crucial factors that are used to tune the activity are discussed including nanostructure development, phase, morphology, crystal facet, defect, mixed-metal, heteroatom doping, topological defects, and formation of metal-N-C.

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**IL-19****Advanced technologies of secondary refining and 3D printing technology in high quality casting manufacturing****Dr. Nithin Raj P***Head of Research and Development,  
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Casting is one of the oldest manufacturing processes in the world. The manufacturing process of a casting has several stages from designing to machining. The initial stages of the casting manufacturing are a complex combination of several processes. The casting process is basically making a product by pouring molten metal to a designed cavity to make a required shaped component. The presentation is on two of the modern technologies employed in the field for the production of high quality and precision castings 3D printing of the mold and the secondary refining technologies of molten metal. The introduction of 3D printing into mold making of casting has brought revolution to the field. The cavities and the component required are 3D printed using a combination of injectors depositing sand resin and hardener for creating micro sized layers for the precise creation of intended shape. The next step of manufacturing is melting the metal and preparing the required combination of chemical composition to create the alloy with all the required qualities for the component. For certain high end applications like nuclear, sub sea petroleum pipelines, sub zero temperature gas pipelined between countries, desalination plants etc.. The metal needs to be of highest purity and in some applications demands ultra low carbon content. A series of chemical reactions in technologies like Argon Oxygen Decarburization (AOD) and Vacuum oxygen Decarburization (VOD). Use of the range of chemical reactions and orders to obtain a highly accurate chemical composition is a very complex process which determines the final quality of the component.



# *Oral Presentations*



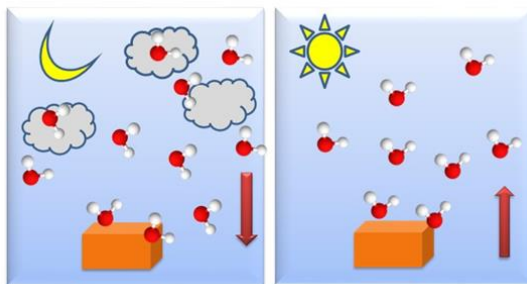


## OP-1

**CaCl<sub>2</sub> incorporated graphene oxide/PVA gel for atmospheric water harvesting****Anjali C, Renuka Neeroli Kizhakayil\****Advanced Materials Research Centre, Department of Chemistry**University of Calicut, Kerala-673 635, India.**Email: [renuka@uoc.ac.in](mailto:renuka@uoc.ac.in)*

Fresh water scarcity is a grave issue that the humanity faces, especially in the context of expanding population and worsening water pollution. Huge amount of water content in the atmosphere as moisture is an underutilised resource, that has the potential to address the above-mentioned issue. Atmospheric water harvesting (AWH) moisture sorption using suitable sorbents is being explored by the researchers, recently. This approach, when combined with the release of collected water from the sorbent using sunlight, constitutes an energy-efficient and sustainable solution to water scarcity.

Herein, we introduce a blend of hygroscopic salt and graphene oxide/polyvinyl



alcohol (GO/PVA) gel matrix as an efficient AWH material. The components mentioned perform the roles of sorbent, water releasing source, and storage medium, respectively in the order. An optimized composition of the gel shows a water capture capacity of 0.284 g/g and 0.83 g/g at relative humidity levels of 30% and 75%, respectively, following a typical 2-hour capture and 1-hour release cycle. To ensure sustainable water harvesting performance, ten such capture-release cycles are performed. The GO-based gel stands out not only for its effective water harvesting ability, but also for its advantageous characteristics such as low cost, easy scaling up and portability, making it a promising candidate for commercialization.

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**OP-2****Design and development of a potentiometric sensor for the selective determination of As (III) in ground water samples****Anjana K R, Saumya Varghese\****Department of chemistry**St. Joseph's college (autonomous), Devagiri, Calicut -673008, Kerala*

Arsenic is a metalloid found in air, water, and soil. Arsenic compounds show different oxidation states: -3, 0, +3, and +5. Out of these, As(III) has more potent toxic properties.<sup>1</sup> Different analytical methods, such as inductively coupled plasma,<sup>2</sup> atomic absorption spectroscopy,<sup>3</sup> stripping voltammetry,<sup>4</sup> neutron activation analysis,<sup>5</sup> and polarographic techniques,<sup>6</sup> have been used for arsenic determination in different samples. But the above methods are inconvenient for routine analysis. Potentiometric sensors have attracted great interest because they are simple and economically viable when compared to other electrochemical sensors. Here, a novel potentiometric sensor for the trace level detection of arsenic (III) in ground water using an ion imprinted polymer (IIP) was developed. The developed sensor exhibits a near-Nernstian response in a concentration range of  $1 \times 10^{-9}$  M to  $1 \times 10^{-2}$  M with a slope of -17.1 mV and a limit of detection of  $1 \times 10^{-10}$  M. The characterization of the IIP was done using FESEM and EDX. The developed sensor is highly sensitive and selective for the As(III) ion.

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**OP-3****Spectroscopic investigation of the stability of carbon dots derived from polyethylene glycol****Athulya K R,<sup>a</sup> Anitha C Kumar<sup>b\*</sup>**<sup>a</sup> *Department of Applied Chemistry,**Cochin University of Science and Technology, Kochi, Kerala,*<sup>b</sup> *School of Chemical Sciences, Mahatma Gandhi University, Kerala*athulya5598@cusat.ac.in, \* [anithackumar@mgu.ac.in](mailto:anithackumar@mgu.ac.in)

Carbon dots (CDs) are an exciting class of nanoparticles with a size of less than 10 nm and they have been receiving huge attention from the day it got discovered.<sup>1,2</sup> CDs are a family of quantum dots that came to the limelight again recently as the discovery of such nanoparticles was awarded the 2023 Nobel Prize in Chemistry. CDs can be synthesised from various carbon sources by various methods. Polyethylene glycol (PEG), a linear, non-conjugated biopolymer is an ideal choice for the fabrication of CDs as the source itself is biodegradable, the CDs are also expected to be biocompatible.<sup>3</sup> Here in this work, we synthesised CDs from PEGs of different molecular like 200, 300 and 400 g/mol using a facile and green method, i.e., microwave irradiation method as per the reported procedure. The stability study of prepared CDs was carried out by comparing the UV-Visible absorbance, fluorescence nature, Zeta potential values, and size of CDs synthesised from various PEGs on different days following the synthesis like 1, 15, 30, etc. days. Optical characteristics of manufactured CDs were assessed using UV-Visible spectral analysis as well as fluorescence spectra. DLS analysis has been used to perform size analysis. This study proves that CDs made of polyethylene glycols, regardless of their molecular weights, can last for a long period with the same qualities they displayed on the first day after synthesis. Applications like bioimaging might benefit from CDs that can endure stability over an extended duration without losing their fluorescence property. Keywords: PEG, carbon dots, fluorescence, bioimaging

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**OP-4****Plasmonic synergism in tailored metal-carbon interfaces for real-time single molecular level sniffing of PFOS and PFOA****Dipin Thacharakkal, Chandramouli Subramaniam***Department of Chemistry, Indian Institute of technology, Bombay  
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Generating plasmonic hot-spots through engineering of nanoscale interfaces offers exciting opportunities towards point-of-care analytical detection. The mutual trade-off between ultra-high sensitivity, specificity and reliability are major drawbacks for practical applicability with real-time samples. Fundamentally these originate from low photonic mode density, high ohmic losses, temporally fluctuating and chemically indistinguishable nature of electromagnetic hot spots. This work describes synergism of metallic plasmons from tailored interfaces of Ag-Au nanoalloys with conical nanocavities of nanocarbon florets (NCF), leading to strong metal-dielectric interfacial coupling. Such, Ag-Au-NCF nanohybrid delivers an unprecedented 1517-fold enhancement in surface-plasmon coupled directed emission (SPCE) of Rhodamine B (RhB) leading to robust (relative standard deviation, RSD < 10%) single-molecular-level detection of spectroscopically silent perfluoroalkyl substances (PFAS). The limit-of-detection demonstrated (PFOS = 0.005 ppt) is one-thousand times better than WHO recommendation and surpasses all existing reports. The specific cation-anion interactions between RhB and PFAS are substantiated through density functional calculations that concur with experimental findings. Finally, the emission from this SPCE platform can be visually tracked through a smartphone camera over wide range of PFOS concentrations (0.005 - 5000000 ppt) in water samples (lake, river, tap, drinking and ocean) and blood-plasma, offering transformative opportunities in analytical sciences.

**OP-5****Fabrication of an eco-friendly silver nanocomposite sensor film for removal and selective colorimetric detection of mercury in aquatic environments****P. Dhanyasree,<sup>1</sup> P. M. Sabura Begum,<sup>1</sup> Karuvath Yoosaf<sup>1,2\*</sup>**<sup>1</sup>*Department of Applied Chemistry,**Cochin University of Science and Technology (CUSAT), Kerala, Pin 682022, India,*<sup>2</sup>*Inter-University Centre for Nanomaterials and Devices,**Cochin University of Science and Technology (CUSAT), Kerala Pin 682022, India,**\* E-mail: [yoosafk@cusat.ac.in](mailto:yoosafk@cusat.ac.in)*

In the current research world, there has been a lot of interest in the fabrication of eco-friendly sensors that can detect and remove mercury ( $\text{Hg}^{2+}$ ) in its nanomolar concentration from aquatic systems. The highest concentration of  $\text{Hg}^{2+}$  that can be present in drinking water worldwide is approximately 2 nM. It can be challenging to detect  $\text{Hg}^{2+}$  concentrations at nanomolar levels, although there are several sophisticated techniques available. Interestingly, colorimetric analysis is rapid, inexpensive, and produces results with respectable accuracy. It uses a simple spectrophotometer to detect color changes in real-time analysis.<sup>1</sup> The sensor film shows are highly effective by the presence of silver nanoparticles that are incorporated into it. Nanoscale particles exhibit enhanced Surface Plasmon Resonance (SPR) and a greater surface-to-volume ratio in comparison to their bulk precursors.<sup>2</sup> An ideal concentration of AgNP is added to the biopolymer polymer blend to increase its stability. In the sensing mechanism, AgNP undergoes a redox-favored reaction and forms an Ag-Hg alloy.<sup>3</sup> The sensor films are inexpensive, biodegradable, and remarkably effective at detecting nanomolar concentrations. Additionally, we looked at the real sample analysis and selectivity using nearby water sources. The absorbance peak remains at 413 nm when added to the polymer nanocomposite film, confirming the absence of matrix and interparticle effects. Depending on the concentration of  $\text{Hg}^{2+}$  ions, this causes an immediate discoloration or color shift. Plotting the absorbance change vs concentration of  $\text{Hg}^{2+}$  ions produced a linear relationship that demonstrated the data's applicability to quantitative estimations. The absorption peak of the nanocomposite film does not significantly alter when different metal solutions, except  $\text{Hg}^{2+}$ . As a result, the sensor film exhibits strong  $\text{Hg}^{2+}$  ion selectivity. A Mercury analyzer was used to examine the film's capacity to remove  $\text{Hg}^{2+}$  ions.



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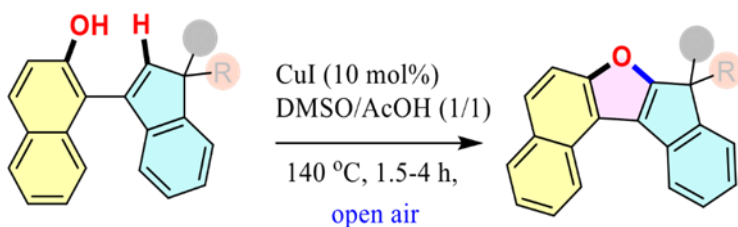
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## OP-6

**Cu-catalyzed oxidative C(sp<sup>2</sup>)-H cycloetherification of o-alkenyl arenols for the preparation of fused-furans**

**Srinivasarao Yaragorla\*, Tabassum Khan and Jazeel Raof**  
*University of Hyderabad*

An efficient and practical approach for the synthesis of functionally embellished indenonaphthofurans is developed using a copper-catalyzed, aerobic oxidation of 1-(1H-inden-3yl)naphthalen-2-ols. This intramolecular cycloetherification proceeds via C(sp<sup>2</sup>)-H oxygenation (C-H bond breaking and C-O bond forming) and enables the synthesis of poly fuse furans in high yields with large substrate diversity and is complementary to the previous methods for the synthesis of fused furans.

**Reference**

1. S. Yaragorla\*, T. Khan, J. Raof; Cu-Catalyzed Oxidative C(sp<sup>2</sup>)-H Cycloetherification of o-Alkenyl Arenols for the Preparation of Fused-Furans *J. Org. Chem.*, xxxx (Manuscript accepted)

# *Poster Presentations*



**PP-1****Photophysical properties and DNA binding studies of Dysproium(III) schiff base complex****Anjana T.M., Naseera C.M., Liyakath F.M., Sheeja S.R.\***

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**Abstract:** Recently, the rare earth complexes with hydrazone schiff base ligands have been a subject of growing interest owing to their promising applications in the field of optics and pharmacology. A Dysprosium(III) complex based on salicylaldehyde benzoylhydrazone ligand have been synthesized and characterized by partial elemental analysis, UV-Vis and IR spectroscopy. The photoluminescence properties of Dy(III) complex in the solid state and the solution state were also investigated. The lifetime studies of the Dy(III) complex and hydrazone reveal that they exhibit fluorescence. The fluorescence intensity of the Dy(III) complex have been tremendously increased when compared to the hydrazone.. The CT-DNA binding activity of the hydrazone and Dy(III) complex was studied by absorption spectra measurements and found that the Dy(III) complex has more binding activity than hydrazone.

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## PP-2

**Synthesis and characterization of Fmoc modified phenylalanine hydrogel at various pH****Arathy Chandran<sup>a</sup>, Anitha C Kumar<sup>b\*</sup>**<sup>a</sup> *Department of Applied Chemistry, Cochin University of Science and Technology, Kochi, Kerala, India*<sup>b</sup> *School of Chemical Sciences, M G University, Kottayam, Kerala, India  
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**Abstract:** A hydrogel is a three-dimensional network of polymers that can swell in water and hold a large amount of water while maintaining the structure due to the chemical or physical cross-linking of individual polymer chains. In biological applications, in general, the polymer backbone and its degradation products have to be biodegradable and biocompatible. There is the use of biomolecules for the preparation of hydrogels. Amino acids, proteins, and peptides are used for the preparation of hydrogels. Hydrogels prepared from amino acids received attention because peptides and proteins need further tedious synthesis. Amino acids are molecules used by all living things to make proteins. It is simply an organic molecule with amine and carboxylic groups. In the last few years, the self-assembly of single amino acids has been extensively studied owing to their properties: the ability to respond to external stimuli, cost-effectiveness with ease of synthesis, tunable structural properties, the capability to form different morphological nanostructures, and excellent biocompatibility, which make them applicable in various fields including drug delivery. Tissue engineering, wound healing, etc. Not only are single amino acids self-assessed, but amino acids modified with various groups are also extensively researched. In this category, the Fmoc group is more significant as an amine-protecting group with intrinsic aromaticity and hydrophobicity. Phenylalanine is an essential amino acid in humans. Phenylalanine is a component of several important proteins and enzymes. Herein, in this work, we discuss the details of the hydrogel formation by Fmoc-L-Phenylalanine in an aqueous buffer of different pHs involved in its formation. The present study focuses on the utilization of fluorescence spectroscopy to understand the self-assembly and gelation of the formed hydrogels. It is possible since the fluorescence studies give useful and important details regarding the changes in the microenvironment of the fluorophore molecule during the self-assembly and gelation processes. In the present study, the use of any extrinsic fluorescent probe is not required since phenylalanine has intrinsic fluorescence. The morphology, and properties of

hydrogels formed at different pHs, are compared and analyzed with the use of various spectroscopic and microscopic techniques.

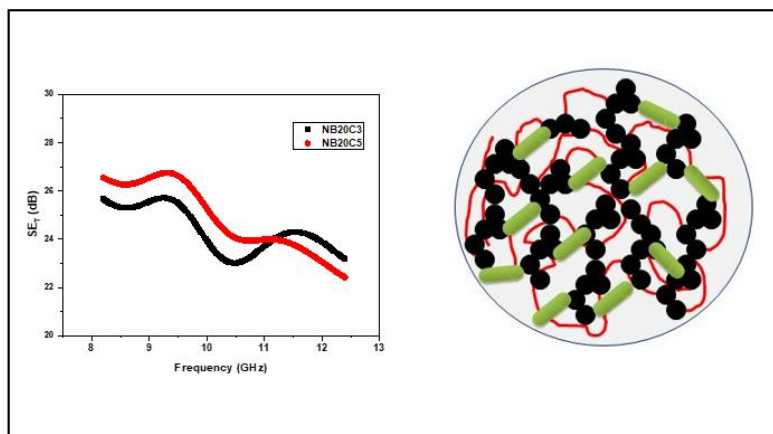
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**PP-3****EMI shielding properties of hybrid filler incorporated NR composites****Abhisha V.S, Ranimol Stephen***Department of Chemistry, St. Joseph's College (Autonomous), Devagiri**Calicut, Kerala- 673 008, India.**[ranistephen@gmail.com](mailto:ranistephen@gmail.com)*

**Abstract:** Natural rubber (NR) modified by the addition of conductive fillers such as, carbon nanotubes (CNT), conductive carbon black (CCB) and ionic liquid (IL) modified fillers are applicable for commercial electromagnetic interference (EMI) shielding. (1,2) EMI shielding property refer to the effectiveness of a material or structure in attenuating or blocking electromagnetic radiation and preventing its interference with electronic devices or systems. Conducting polymer composites offers advantages such as flexibility and stretchability while providing excellent EMI radiation shielding. These properties of NR composites are evaluated in terms of the homogeneous dispersion of fillers, as well as the physicochemical interfacial interactions established between the filler and the polymer matrix. Moreover, the ionic liquids modified fillers enhance the shielding properties of the composites.(3) Conductive fillers incorporated NR shows higher DC conductivity, which in turn has high EMI shielding effectiveness. EMI shielding performance of hybrid filler composites are measured in the X band frequency as it is important in the modern wireless communication devices. Ionic liquid plays an important role in dispersing and stabilizing CNTs within the composite, promoting better interfacial adhesion, and enhancing the conductivity of composites. The commercial requirement for EMI shielding device is satisfied by all hybrid filler systems and the highest EMI SE of 33.8 dB in the frequency range of 9-10 Hz is observed for the combination of CNT and rGO in NR containing 20 phr conductive carbon black.





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## PP-4

**Cu-doped Bi<sub>2</sub>MoO<sub>6</sub>/graphene nanocomposites under visible light irradiation: a DFT study****Aiswarya Chandran, Dr. Mausumi Chattopadhyaya**

**Abstract:** In this study, optical and electrical properties of Bi<sub>2</sub>MoO<sub>6</sub>, 1 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub> and 2 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>, Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene, 1:1 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene and 1:2 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>(010)/ Graphene were calculated using DFT calculations. Their photocatalytic properties were investigated through several electronic and optical property analysis. The optimization, optical band gap, projected density of states and charge transfer were investigated using DFT calculations. The study reveals that the doping of Bi<sub>2</sub>MoO<sub>6</sub> with Cu widens the band gap for bulk Bi<sub>2</sub>MoO<sub>6</sub>. The interface study reveals that the doping by Cu atom can influence the interaction and stability of heterostructures. From the adhesion energy analysis, the doped heterostructures were found to be more stable than undoped heterostructures. Also, the electronic and structural analysis shows the photocatalytic activity for 1:2 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene. For the heterostructure of Bi<sub>2</sub>MoO<sub>6</sub>(010)/graphene heterojunction the band gap is getting narrowed as the Cu concentration increases. Thus, 1:2 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene shows lower optical band gap which shows higher absorption of visible light. The projected density of states also reveals the influence of Cu doping on heterostructures rises the valence band and thus narrows the band gap. The charge density difference and work function analysis revealed that fast charge transfer occurs from graphene to Bi<sub>2</sub>MoO<sub>6</sub> surface in the case of 1:2 wt% of Cu: Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene. Thus, our theoretical study reveals that the doping of Cu on Bi<sub>2</sub>MoO<sub>6</sub>(010)/Graphene enhances the photocatalytic activity by improving the visible light absorption capacity.

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**PP-5****Extraction of amorphous nano silica from pennisetum polystachion  
(mission grass)****Ajmal Thayyullathil***Department of Chemistry, Government College Madappally, Vadakara-2*

**Abstract:** Mission Grass (MG) is an aggressive weed widely grown in the agricultural field and has no significant use. But it is a potential source of silica. Amorphous nano silica has wide application in the field of material science (Lu et al., 2010) and it can be prepared from MG through sol gel method. Powdered MG is calcinated at 600°C for 20hrs in a muffle furnace. It is then digested with 2M HCl to remove metal ions if present. It is filtered and the residue is heated with 3M NaOH for 3 hrs (Thuadaj and Nuntiya, 2008). The solution is filtered, and the filtrate is assumed to be sodium silicate. Dilute HCl is added drop by drop till the silica soil is obtained, which on heating silica powder is obtained and the percentage of yield is 1.68%. The sample is characterized by XRD, FTIR and SEM-EDX. XRD studies shows that the sample have typical amorphous nature, since the diffractogram is very broad. There is a characteristic broad hump from 15°-30° which shows that silica is in amorphous form (Lu and Hsieh, 2012). No other peaks are found, which shows its purity. The crystallinity index calculated is 43%. FTIR spectra is very broad and rounded peaks are observed, which conform the amorphous nature of silica. The prominent peak at 1056 cm<sup>-1</sup> is due to Si-O-Si asymmetric stretching vibration, the less intense band at 803 cm<sup>-1</sup> is due to symmetric stretching of Si-O-Si bond and the peaks at 465 cm<sup>-1</sup> is attributed to rocking vibration of Si-O-Si bond. There is a broad band at around 3000 cm<sup>-1</sup> is more diffused and irregular (Athinarayanan et al., 2015). This is because the sample is in agglomerated form and the O-H group is extensively H-bonded due to the presence of silanol group and adsorbed water molecule. SEM -EDX, shows that amorphous nano silica appears to be more agglomerated and there is no uniformity in the size of the particle. EDX data shows that the percentage of silica in the sample is 95.6%. Thus, it is concluded that MG is not merely a fodder but is good source of silica and highly pure amorphous nano silica can be synthesized from it.

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**PP-6****Characterization and performance evaluation of NR modified used cooking oil as bio-lubricant for industrial applications****Amina Hamnas, G Unnikrishnan\****Department of Chemistry,**National Institute of Technology Calicut, Kerala, 673601, India**unnig@nitc.ac.in*

**Abstract:** The growing concerns regarding environmental sustainability and the depletion of fossil resources have spurred research into alternative lubricants for industrial applications. This study presents a comprehensive analysis of bio-lubricants synthesized from used cooking oil (UCO) blended with mustard oil (MO) as the base oil, incorporating natural rubber (NR) as an additive. This research aims to assess the feasibility of UCO/MO-based bio-lubricants enhanced with NR for industrial use by evaluating their physicochemical properties, tribological performance, and thermal stability. The first phase of the research involved collecting and purifying UCO, followed by its acidity, viscosity, density, and chemical composition characterization. The collected UCO samples were then blended with MO (50/50) and then with NR to create biolubricant formulations. In the second phase, the physicochemical properties of the UCO/MO based bio-lubricants were thoroughly analyzed, including TGA, DSC, flash point, cold flow properties, and viscosity have been analyzed. Tribological assessments were conducted to evaluate their friction and wear properties using a four-ball tester under different operating conditions, simulating industrial applications. The obtained results were compared with conventional mineral-based lubricants to assess the performance of the bio-lubricants. Compared to the commercial SAE 20W40 oil, an ideal lubricant with better properties has been developed with comparatively better biodegradability for industrial lubrication.

The findings of this study demonstrate that UCO-based bio-lubricants with NR additives exhibit favourable physicochemical properties and promising tribological and thermal performance, making them a viable alternative to conventional lubricants.

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## PP-7

**g-C<sub>3</sub>N<sub>4</sub> based composites for partial oxidation of benzyl alcohol****Amrutha T.P. and Renuka Neeroli Kizhakayil\***

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**Abstract:** Partial oxidation of olefins to aldehydes holds importance in both organic synthesis and industrial chemistry. Here we discuss the catalytic activity of Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) based photocatalysts for partial oxidation of organics. Graphitic carbon nitride is considered as next-generation visible light-induced semiconductor photocatalyst which finds application in oxidation reactions. However, practical application of g-C<sub>3</sub>N<sub>4</sub> is limited due to poor visible-light absorption, fast recombination of excitons and low specific surface area. Band gap narrowing is an established strategy to overcome these drawbacks and optimize the electronic structure.

We have developed g-C<sub>3</sub>N<sub>4</sub> based binary and ternary composites of metal oxides, g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub> and g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub>/ZrO<sub>2</sub> systems for catalysing benzyl alcohol oxidation, an industrially significant reaction in view of its partial oxidation product, benzaldehyde. The catalysts are characterized using X-Ray Diffraction (XRD) analysis, Fourier Transform Infrared (FT-IR) spectroscopy, UV–VIS Diffuse Reflectance Spectroscopy (UV-Vis DRS), Scanning Electron Microscopy (SEM) analysis and Brunauer-Emmett-Teller (BET) surface area analysis. Studies show that the as-prepared g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub> and g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub>/ZrO<sub>2</sub> are considerably efficient in benzyl alcohol oxidation. The ternary system, g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub>/ZrO<sub>2</sub> shows maximum conversion, which increases with temperature, while the selectivity towards benzaldehyde is maximum for the binary system g-C<sub>3</sub>N<sub>4</sub>/V<sub>2</sub>O<sub>5</sub>.

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## PP-8

**A new Zirconium substituted phosphotungstate-PDPA composite: synthesis, characterization and electrochemical properties****Anjana P T<sup>a</sup>, Athif Ali<sup>b</sup>, Preetha B<sup>c</sup>**<sup>a</sup> Department of Chemistry, KMM Govt. Women's College, Kannur, India<sup>b,c</sup> Govt. College Madappally, Vadakara, Kozhikode, India

**Abstract:** The introduction of nanoscale reactive inorganic species in conducting polymers produces metal/organic hybrid composite structures with unique properties. The new composite, ZrPW-PDPA was synthesized by oxidative polymerisation of diphenylamine followed by reaction with the polyoxometalate, Zirconium substituted phosphotungstate. The use of various spectroscopic and non-spectroscopic techniques provided interesting information on the physicochemical characteristics of the material.

Distribution studies were carried out for various metal ions in demineralised water by batch process which showed high selectivity towards certain toxic metal ions. Dye degradation efficiency of the composite was also carried out. These results are very significant in environmental chemistry and can be utilized for applications involving separation and removal of toxic metal ions and conversion of dyes into harmless products.

The electrical conductivity of protonated composite was measured at room temperature on compressed pellet using the Keithley four-probe technique. The conductivity depends on the extent of oxidation of diphenylamine and protonation of the composite. The conducting organic polymer part and protonic conduction of the polyoxometalate contributed to the conductivity of the nanocomposite.

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## PP-9

**A facile *in situ* synthesis strategy to silver nanoparticle functionalized nitrogen doped graphene quantum dots and the remarkable antifungal activity thereof****R. Aswathi<sup>1,2</sup> and K. Y. Sandhya<sup>2</sup>**<sup>1</sup> PG and Research Department of Chemistry,  
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**Abstract:** In this work, we report a simple, green approach for the *in situ* formation of silver nanoparticles (AgNPs) on nitrogen doped graphene quantum dots (NGQDs) and used it for antifungal applications. NGQDs with an efficient nitrogen (N) doping and an aromatic structure with crystalline nature were initially prepared [1] by a simple hydrothermal route where polyaniline (PANI) was used as the precursor. Herein, we obtained AgNPs functionalized NGQDs (Ag-NGQDs) via a facile strategy in which NGQDs serve as both reducing agent and stabilizer/capping agent, silver nitrate solution being used as the precursor for AgNPs, and no additional reducing agent and stabilizer is necessary. The UV-Vis spectrum of Ag-NGQDs exhibit the characteristic surface plasmon absorption peak of AgNPs around 400nm. Also, HR-TEM images confirm the formation of Ag-NGQD composite, where N-GQDs were covered with Ag NPs of an average diameter of 10 nm. Silver has the inherent advantage of broad antimicrobial activities against bacteria and fungus. Also, Graphene based nanocomposites' antimicrobial activity exhibits great potential in clinical application [2]. Graphene quantum dots (GQDs) are emerging zero dimensional materials promising various novel applications due to their extraordinary physicochemical properties. Herein, we investigated the antifungal activity of Ag-NGQDs and NGQDs against the fungi *Aspergillus Niger* by the well diffusion method. Both NGQDs and Ag-NGQDs exhibited antifungal activity, Ag-NGQDs being better performers though. The enhanced antifungal activity of Ag-NGQDs has been attributed to the synergistic effect of antifungal activity of both NGQDs and Ag NPs that fosters the fungal inhibition.

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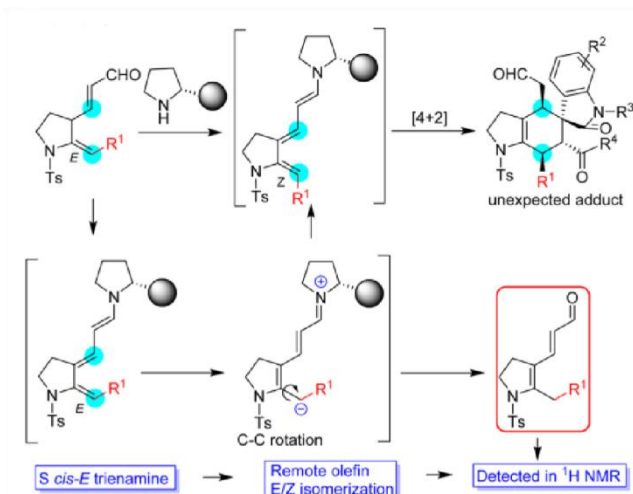
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## PP-10

**Trienamine-catalyzed remote olefin E/Z isomerization/[4+2]-cycloaddition for the asymmetric synthesis of siprohexahydroindole oxindoles****Madavi Shiva Prasad\*, Murugesan Sivparakash, Bharani sankar***Asymmetric synthesis and catalysis laboratory, Department of Chemistry**School of Basic and Applied Science, Central University of Tamil Nadu**Tiruvarur, India, 610101**E-mail: [shivaprasad@cutn.ac.in](mailto:shivaprasad@cutn.ac.in)*

**Abstract :** The advent of trienamine catalysis has offered an efficient and gentle method for constructing intricate carbocyclic frameworks via a single-step remote [4+2]-cycloaddition reaction [1]. Recent studies exploring the reaction of cross-triamines and tetraenamines with oxindole olefins have unveiled a stepwise mechanism, supported by the isolation of an oxindole organocatalyst intermediate [2,3]. Motivated by the biological significance and unique reactivity of oxindole olefins, we embarked on an investigation of their viability in the context of our designed dienal through trienamine catalysis [4].

In this study, we present the inaugural report on a trienamine-catalyzed remote olefin E/Z isomerization/[4+2]-cycloaddition reaction for the synthesis of a unprecedented stereoisomer of siprohexahydroindole oxindole. The reaction involves the pyrrolidine exocyclic dienal reacting with various oxindole olefins, showcasing remote olefin E/Z isomerization/[4+2]-cycloaddition to yield a diverse library of optically pure siprohexahydroindole oxindoles (33 examples). Remarkably, the reaction exhibits excellent yield and Scheme 1 Trienamine catalyzed [4+2] cycloaddition stereoselectivity, reaching up to 95% reaction yield, 99% ee, and a diastereomeric ratio exceeding 99:1. Through comprehensive NMR investigations, we propose the most favorable pathway for the reaction, shedding light on the intricate details of the remote olefin isomerization and [4+2]-cycloaddition processes. This study not only introduces a novel trienamine-catalyzed methodology for the asymmetric synthesis of siprohexahydroindole oxindoles but also expands the scope of oxindole olefins in trienamine catalysis [5].



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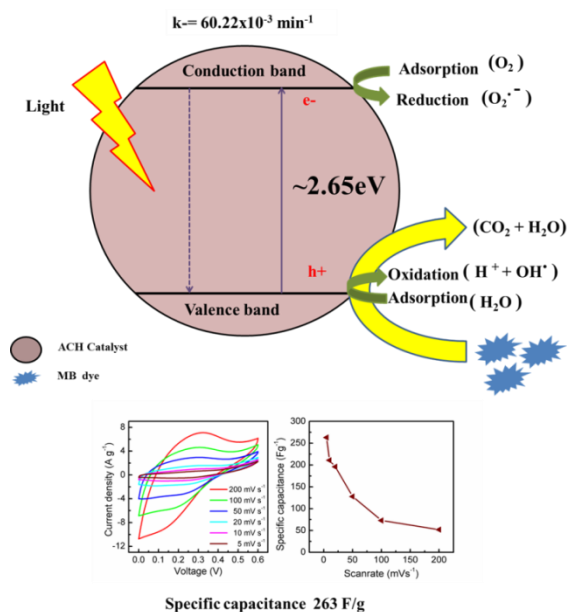
## PP-11

## Synthesis and characterization of alpha and beta cobalt hydroxide nanostructures for photocatalytic dye degradation and supercapacitor applications

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**Figure:** Represent Methylene blue dye degradation and the cyclic voltametric curve (two electrode configuration) using ACH catalyst

**Abstract:** Alpha and beta cobalt hydroxide nanocatalysts were synthesized by hydrothermal method. Both catalysts exhibited excellent catalytic activity in the Methylene Blue (MB) dye degradation. The alpha cobalt hydroxide catalyst shows 100% degradation efficiency within 60 minutes with a rate constant of  $60.22 \times 10^{-3} \text{ min}^{-1}$  (for 100ml  $3 \times 10^{-5} \text{ M}$  MB dye, 0.005g catalyst). The enhanced degradation rate by alpha cobalt hydroxide can be related to its unique structural characteristics. Electrochemical performance was also evaluated to explore energy storage applications. The electrochemical performance of alpha phase was superior compared to the beta phase. The Csp value of beta cobalt hydroxide obtained from

CV and GCD analysis was found to be 137 F/g and 2.4 F/g, respectively. But for the alpha cobalt hydroxide electrode, Csp values of 263 F/g and 80 F/g, respectively, along with an energy density of 6.85 Wh/kg and a power density of 601.46 W/kg. Findings suggest that alpha cobalt hydroxide nanostructures are more effective than the beta phase for catalytic and supercapacitor applications.

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## PP-12

**A theoretical study on the photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> for water splitting reaction****Dhilshada V N and Mausumi Chattopadhyaya***Department of Chemistry**National Institute of Technology Calicut, Kerala - 673601, India*

**Abstract:** Density functional theory was employed to calculate the photocatalytic activity of the g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> heterojunction. g-C<sub>3</sub>N<sub>4</sub> is a semiconductor and CoN<sub>4</sub> is a half metal, eventually the resultant heterojunction is half metallic in nature. The metallicity originates from the spin down channel of the g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> heterojunction while the spin up channel behaves as a semiconductor. The stability of the heterojunction was confirmed by calculating the formation energy from its isolated analogs. Charge density analysis and work function calculation suggests a substantial amount of charge transfer in g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> heterojunction and the direction of charge transfer was found to be from g-C<sub>3</sub>N<sub>4</sub> to CoN<sub>4</sub> unit. The optical absorption of the nanocomposite was found to be significantly enhanced in the UV-visible region in comparison to g-C<sub>3</sub>N<sub>4</sub> and CoN<sub>4</sub>. In g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub>, the valence band maximum (VBM)(+1.42V) exhibits a more positive potential compared to O<sub>2</sub>/H<sub>2</sub>O(+1.23V) on the NHE scale, while the conduction band minimum (CBM)(-0.38V) displays a more negative potential than that of H<sup>+</sup>/H<sub>2</sub>(0V) on the NHE scale. Consequently, this heterojunction can be effectively utilized for water splitting. Finally, details of band structure, density of states and band edge position determining calculations confirm that g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> composite forms type 1 heterojunction, making it a suitable photocatalyst for water splitting reaction. The state-of-the-art theoretical modeling of g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> heterojunction is the first theoretical study incorporating CoN<sub>4</sub> crystal.

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**PP-13****Fabrication of PPSU/  $\kappa$ -carrageenan nanocomposite membranes with copper immobilized zeolite for dye rejection applications****A. M. Vijesh<sup>1,2\*</sup>; P. V. Deepthi<sup>2,3</sup>**<sup>1</sup>*P.G. Department of Chemistry, Payyanur College, Payyanur,, Kannur University, Kerala - 670327, India*<sup>2</sup>*P.G. Department of Chemistry, Government College, Kasaragod, Kannur University, Kerala -673123, India*<sup>3</sup>*Department of Chemistry, Nehru Arts and Science College, Kanhangad, Kannur University, Kerala -671314, India**E-Mail: [vijeshnambisan82@gmail.com](mailto:vijeshnambisan82@gmail.com)*

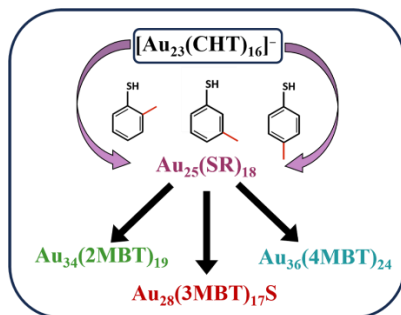
**Abstract:** Increased population in the last decade demands the requirement of new industries for fulfilling their daily needs. Many industries like textile, paper and dye industries produce large quantities of coloured effluents causing the pollution of soil and water resources, finally it may severely damage our environment and becomes a threaten to human life. Therefore industries must treat their effluents before discharging it to the water bodies and lands. Membrane technology holds a central position in numerous separation and purification procedures, and recent advancements in nanoscience have paved the way for augmenting membrane efficiency. High surface per volume compared with flat sheet membrane, makes hollow fiber membrane good choice for water refinement applications.

This abstract offers an overview of polysulfone/  $\kappa$ -Carrageenan composite membrane with nano additives, highlighting their characterisation and potential application in dye rejection studies. Phase inversion technique was adopted for the formation of well-defined nanocomposite membrane with enhanced structural and functional properties. Detailed characterisation techniques provide an insight into the morphology and chemical properties.  $\kappa$ -Carrageenan a potential pore-former increased the wettability and rejection efficiency. SEM, water uptake, contact angle, water permeability, porosity, antifouling capabilities and dye rejection experiments were carried out. The integration of nano additives upgraded the effectiveness of the novel membrane in eliminating the dyes Reactive black 5 and Reactive orange 16. The findings indicated that the additives have great potential to improve membrane properties while maintaining its rejection capabilities intact. The results of such studies will be discussed in this paper.

**PP-14****Role of isomeric methylbenzenethiols on the product determination in a ligand exchange reaction on  $\text{Au}_{23}(\text{SR})_{16}$  cluster****Eyyakkandy Nida Nahan, and Sukhendu Mandal\****School of Chemistry,**Indian Institute of Science Education and Research Thiruvananthapuram**Trivandrum, Kerala 695551, India.**Email: [nidanahanek19@iisertvm.ac.in](mailto:nidanahanek19@iisertvm.ac.in)*

**Abstract:** Metal nanoclusters (MNCs) are a class of ultras-small nanoparticles (1-3 nm) with potential applications in catalysis, bio-imaging, sensing, converting, etc., which originates from the atom precise nature and quantum confinement of the material<sup>1,2</sup>. Considering the unique nature of MNCs where they exhibit a change in their properties even with a slight variation in an atom, it is of paramount importance to tailor the structures of metal nanoclusters<sup>3</sup>. Ligand Exchange Induced Size/Structure Transformation (LEIST) method has been widely used as a post-synthetic strategy to obtain novel clusters and to modify the properties of the material<sup>4</sup>. Considering the existing challenge in designing a nanocluster of our interest, the LEIST strategy has gained the attention of material chemists owing to its ability to control the product formation in a ligand exchange reaction<sup>5</sup>.

In this work, we are concentrating on the LEIST on  $[\text{Au}_{23}(\text{CMT})_{16}]^-$  (CMT: Cyclohexanethiol) induced by isomeric methylbenzenethiols (SR) and the influence of these incoming ligands in directing the reaction pathway. The precursor is treated with o-methylbenzenethiol (2-MBT), m-methylbenzenethiol (3-MBT), and p-methylbenzenethiol (4-MBT) in identical conditions, and the reactions were monitored periodically with UV-visible spectroscopy as well as MALDI mass spectrometry. From the time-dependent mechanistic studies, it was revealed that the  $\text{Au}_{23}$  cluster has transformed to  $\text{Au}_{34}(\text{2-MBT})_{19}$ ,  $\text{Au}_{28}(\text{3-MBT})_{17}\text{S}$ , and  $\text{Au}_{36}(\text{4-MBT})_{24}$  with the respective ligands where  $\text{Au}_{25}(\text{SR})_{18}$  being the common intermediate behind each transformation. The way in which a subtle change in the incoming ligand has triggered the formation of entirely different clusters even after going through a similar intermediate is unlocking new methods to attain novel clusters and shedding light on the role of ligands in controlling the reaction pathway.



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**PP-15****Development and characterization of MPU/CA/nHA composite films as flexible tribo-piezoelectric nanogenerators****Gopika M, and G Unnikrishnan***National Institute of Technology Calicut, Calicut, 673601, India**E-mail: [unnig@nitc.ac.in](mailto:unnig@nitc.ac.in)*

**Abstract:** The development of polymeric piezoelectric composites for energy harvesting applications is considered as a significant research domain that offers the convenience of mechanical flexibility, lower manufacturing cost, and rapid processing compared to ceramic-based composites<sup>1,2</sup>. Here in this work, we propose the development of flexible tribo-piezoelectric polymer composite films based on a millable polyurethane (MPU)/cellulose acetate (CA) blend reinforced with nanohydroxyapatite (nHA) as a functional filler. Polymer-nanocomposite films have been fabricated through a solution casting technique and the effect of filler loadings has been studied. The morphology, mechanical strength, chemical features, and crystalline characteristics have been evaluated through SEM, UTM, FTIR, and XRD respectively. The butterfly-shaped amplitude curves from DC-EFM confirmed the piezoelectric nature of the composite films. Ferroelectric features have been studied through P-E hysteresis curves. Dielectric properties have been analyzed by an impedance analyzer. A device prototype has been fabricated and tribo-piezoelectric responses of the samples and resultant voltage generated to random finger tapping were evaluated by means of a digital oscilloscope. The results suggest a promising possibility of fabricating piezoelectric nanogenerators for a spectrum of applications<sup>3</sup>.

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## PP-16

**Predictive modeling of MAO-B inhibitory compounds: a machine learning-enhanced QSAR analysis****Jalala V.K, Muraleedharan K.***Department of Chemistry, University of Calicut, Malappuram, 673635, India*

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

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**PP-17****Fabrication of poly (lactic acid) nanocomposite membranes through phase inversion method for water purification application****Jeeshma R and Ranimol Stephen***St. Joseph's College (Autonomous), Devagiri, Calicut*

**Abstract:** Water contamination has evolved into an increasingly severe issue that demands eco-friendly solutions. Fabrication and utilization of biodegradable porous membranes have gained prominence in the field of water pollution control. The non-solvent induced phase separation method (NIPS) is found to be an efficient method to synthesis porous membranes, which enable the precise control over the membrane's pore characteristics by regulating the ratio of solvent outflow to nonsolvent inflow.[1] Various polymer membranes, exhibiting enhanced properties are prepared through phase inversion technique and find utility in diverse applications such as ultrafiltration, microfiltration,[2] pervaporation,[3] biomedical applications[4] etc. Environment-friendly, non-toxic, and cost-effective porous polymer membrane is fabricated using poly (lactic acid) (PLA), through the facile NIPS method. This membrane is effective in eliminating water pollutants such as organic dyes and oil. To enhance the properties of the PLA membranes, we have incorporated reduced graphene oxide as nanofiller into the PLA matrix. The resulting membranes exhibited exceptional dye absorption property, particularly with methylene blue and congo red. Furthermore, these membranes display remarkable oil absorption properties, with an impressive absorption capacity of approximately 12g/g for palm oil and 9.45g/g for castor oil respectively. Hence, these porous membranes are considered to be highly effective for the removal of organic dyes and oil from water sources.

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**PP-18****Enhancing stability and reusability of  $\text{Ag}_3\text{PO}_4$  nanoparticles through the introduction of a thin silica shell****Kavya P., Shanthil M.\****Department of Chemistry**Govt. Victoria College Palakkad, Kerala, India**E-Mail; [shanthilm@gmail.com](mailto:shanthilm@gmail.com)*

**Abstract:** A semiconductor photocatalyst, recognized for its potential and cost-effectiveness, shows promise in eliminating harmful organic contaminants from water.  $\text{Ag}_3\text{PO}_4$  has demonstrated high efficiency as a visible-light photocatalyst, aiding in water oxidation and dye degradation. This study successfully addressed the inherent limitations of  $\text{Ag}_3\text{PO}_4$  by applying a thin silica shell coating. The silica-coated  $\text{Ag}_3\text{PO}_4$  displayed sustained photocatalytic activity even after undergoing five cycles of photodegradation, while the uncoated  $\text{Ag}_3\text{PO}_4$  experienced a 50% decrease in photocatalytic efficiency. The research emphasizes the ability of the thin silica shell to improve photostability, preserving photocatalytic effectiveness across multiple cycles of dye photodegradation. XPS analysis revealed a higher formation of  $\text{Ag}^0$  on the surface of uncoated  $\text{Ag}_3\text{PO}_4$  compared to silica-coated  $\text{Ag}_3\text{PO}_4$ , contributing to the decline in photocatalytic activity after five cycles of photodegradation. Electrochemical studies identified crucial intermediates, such as  $\text{OH}^\cdot$  and  $\text{O}_2^\cdot$ , formed during water oxidation, playing a pivotal role in dye photodegradation. This investigation provides valuable insights for designing core-shell semiconductor nanostructures tailored for reusable photocatalytic applications.

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**PP-19****Removal of crystal violet using mahogany fruit pod powder****Mehar Al Minnath, Joshima Chandran, Hayah Rafeek, Jyothi Krishna***Dept of Chemistry, MES Mampad College*

*Abstract:* In this study, the removal of crystal violet dye from the aqueous medium using Mahogany fruit pod was investigated by adsorption method. The physico-chemical properties of the powder was studied using SEM and FTIR. Batch adsorption experiments were carried out to investigate the effect of different operational parameters on CV adsorption.

Experimental data were analyzed by adsorption isotherm models. Study results revealed that dye adsorption increased with biochar dosage, contact time, initial dye concentration, and solution pH. The effects of parameters on the adsorption process such as initial CV concentration, biosorbent dosage and contact time were investigated. The suitability of the obtained adsorption data to the Langmuir, Freundlich, Temkin and by Dubinin

Radushkevich isotherm models was investigated. Interpretation of the adsorption equilibrium data of Crystal Violet on Mahogany fruit pod powder using different adsorption isotherm indicates that the adsorption is endothermic and the mode of adsorption is physisorption. The adsorbent has high binding capacity on the dye. The results obtained show that Mahogany fruit pod powder can be used for the removal of textile dyes from waste water.

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**PP-20****Facile preparation and characterization of biodegradable biocompatible UV shielding transdermal patches based on natural rubber latex-dextrin****Mekha Mariam Mathew and Unnikrishnan Gopalakrishnapanicker***National Institute of Technology Calicut, Calicut, India**E-mail: unnig@nitc.ac.in*

**Abstract:** The physico-chemical and biological characteristics of natural rubber latex (NRL) along with its biodegradable and biocompatible features, makes it a potential material for generating transdermal patches for wound healing and drug delivery applications [1,2]. The ineffective resistance to environmental conditions of NRL has been addressed by blending with dextrin and has been explored as a potential system for fabricating transdermal patches; through the present work [3]. A systematic investigation has been done on the impact of different blend compositions on their physicochemical characteristics, encompassing mechanical properties, surface morphology, thermal stability, UV transmittance, biodegradability, and biocompatibility. Compatibility features and thermal characteristics have been assessed using FTIR, DSC, and TGA respectively. The blended polymers have been optimized for crystallinity, wettability features, and mechanical properties. Morphology characterization has been evaluated through SEM, and AFM techniques. Investigations into UV-visible absorption, cell viability, swelling, erosion, porosity, hemocompatibility and soil degradation properties, suggest a promising avenue for the development of high-quality transdermal patches from the NRL-DXT combination; the aligning with observations from the existing literature.

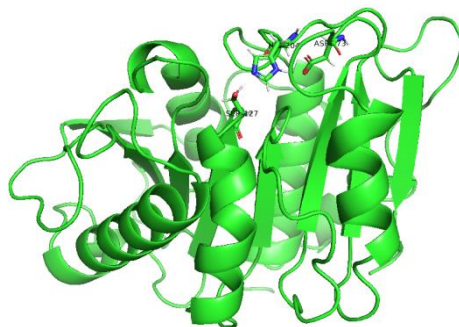
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## PP-21

**An atomistic insight into the temperature dependent variation on the structure and binding affinity of *Ca*PETase PET hydrolase****Dr. Muhasina P. V. and Dr. Susmita De\****Department of Chemistry, University of Calicut, Thenhipalam, Kerala, 673635*

**Abstract:** Enzymatic biodegradation of polyethylene terephthalate (PET) seeks efficient enzymes with high catalytic activity and robust thermostability traits. Rational engineering for PET hydrolases has primarily focused on the mesophilic *Is*PETase and thermophilic cutinases. Recently, a new PET degrading enzyme, *Ca*PETase, displaying properties of both mesophilic and thermophilic PET hydrolases has been reported to exhibit significant activity.<sup>1</sup> The PET hydrolysis of *Ca*PETase at 30°C–60°C temperature revealed a temperature dependent variation in the hydrolytic activity: superior activity at 30°C and 40°C but decreased activity at 50°C and 60°C in comparison with established PET hydrolases such as *Is*PETase, *Tj*Cut2, and LCC. This temperature dependent activity difference is attributed to the conformational changes of *Ca*PETase leading to differential PET binding with the active site residues. Here we attempt to investigate the effect of temperature on the conformational changes in *Ca*PETase and the molecular interactions of PET with *Ca*PETase that occur during the binding step. We have carried out molecular dynamic simulations at different temperatures on *Ca*PETase in its apo-form and the complexed form with tetrameric PET as substrate using the amber20 program. The binding free energies between *Ca*PETase and PET are calculated using the molecular mechanics-generalized Born surface area (MM-PBSA) method. This study will help to identify the role of important amino acid residues in the effective binding of PET.

**Figure 1.** Cartoon representation of *Ca*PETase with catalytic triad residues

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**PP-22****Easily separable, selective, and recyclable magnetic nickel spinel ferrite nanoadsorbent for the removal of malachite green dye pollutant****Nail Saleh Al Sailah<sup>a</sup>, Binitha N. Narayanan**

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**Abstract:** Hydrothermal technique is used here for successfully fabricating magnetic nickel ferrite nanoparticles in the presence of Tween 20, which showed an incredible degree of selectivity in the adsorption of malachite green (MG) from a solution containing malachite green and methyl orange (MO). The structural, magnetic, and morphological characteristics of these nanoparticles are studied by using X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), vibrating sample magnetometer (VSM), X-ray photoelectron spectroscopy (XPS), Brunauer-Emmett-Teller (BET) surface area measurements, and zeta potential ( $\zeta$ ). The effects of pH, initial dye concentration, and catalyst dosage on the MG adsorption are investigated in detail. The adsorption isotherms and kinetics of MG adsorption have also been investigated in batch studies. The monolayer adsorption capacity is 20.46 mg/g, and it fits the Langmuir model very well. A pseudo-second-order kinetic model followed the MG adsorption. The adsorbent is distinguished by a great ease of separation from water because of their high magnetic characteristics enabling the possibility of its repeated use.

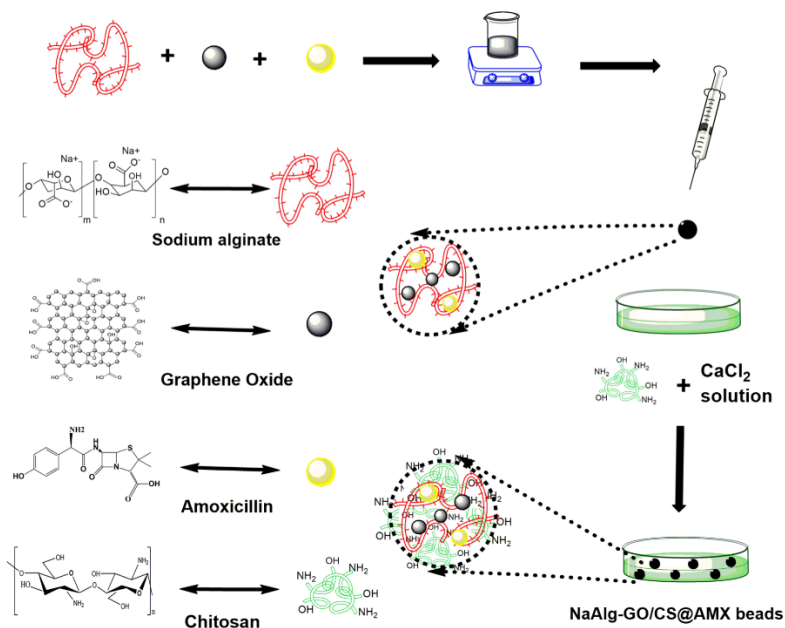
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**PP-23****Chitosan coated graphene oxide incorporated sodium alginate hydrogel beads for the controlled release of amoxicillin****Neethu Das P, Dr. K Govind Raj\****Department of Chemistry, Malabar Christian College, Calicut-673001*

**Abstract:** Biopolymers are crucial in pharmaceuticals, particularly for controlled drug release. In this study, we loaded the broad-spectrum antibacterial drug amoxicillin into sodium alginate, a wellknown biopolymer. Graphene oxide was incorporated into the composite, and the hydrogel beads were coated with chitosan for its mucoadhesive properties. Various composites were formulated by adjusting the weight percentage of graphene oxide (GO). The successful formation of the hydrogel beads (NaAlg-GO/CS@AMX) were explored via several characterization techniques.

The fabricated beads demonstrated controlled and sustained drug release, with 98% of the loaded drug molecules released over 24 hours at gastric pH. The antibacterial test using the disc diffusion technique confirmed the drug release, exhibiting greater effectiveness against the grampositive bacterium *S. aureus* than the gram-negative bacterium *E. coli*. The drug release data were optimized using zero order, first order, Higuchi, and Korsmeyer-Peppas models. The experimental data were best fit to the Korsmeyer-Peppas model with a relatively higher correlation coefficient value. Biocompatibility was evaluated through a cell viability test using mouse fibroblast cell lines (L929). The MTT viability assay confirmed high levels of cytocompatibility, even at higher concentrations (100 µg/mL), with 98.15% viable cells. These results highlight the potential of the fabricated beads as an effective amoxicillin drug delivery system with biomedical applications.



Proposed schematic illustration of the synthesis of NaAlg-GO/CS@AMX beads.

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**PP-24****Nanostructured silver formulation for biomedical application- Synthesis, characterization and optimization****Neethu George and Gayathri Devi D**

**Abstract:** New formulations of silver nanoparticles have been creating great concern if it retards the rate of carbohydrate digestion thereby explore an alternative strategy of reducing postprandial hyperglycemia in diabetic patients. This study proposes a value-added novel nanomaterial for multifaceted biomedical applications. This work explains a phyto-mediated approach to the synthesis of silver nanoparticles using the aqueous bark extract of *Terminallia bellerica* (TbAgNPs). The formation of TbAgNPs was assessed spectrophotometrically and characterized by X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy, Field Emission Scanning Electron Microscopy (FESEM). The thermal decomposition details were evaluated by Thermogravimetric analysis (TGA). TbAgNPs show potential antibacterial effects against gram-positive and negative strains. Antioxidant capacity was assessed by DPPH free radical scavenging assay. Furthermore, *in vitro* antidiabetic activity was analysed by evaluating the alpha amylase inhibitory activity of TbAgNPs. Hence TbAgNPs could act as an antidiabetic agent as a significant inhibitor of  $\alpha$ -amylase activity. Moreover, the growing number of infections among individuals with diabetes confirms the necessity of developing dual diabetes treatments. Therefore, the fact that TbAgNPs have an extra antibacterial capability is encouraging. This evidence proposes the development of a new nanostructured pharmaceutical formulation from *Terminallia bellerica* with a potent antioxidant, antibacterial and antidiabetic activity.



## PP-25

**Fluorescent carbon nanodots as efficient nitroaromatic sensor****Nidhisha V. and Renuka N.K \****Advanced Materials Research Centre, Department of Chemistry**University of Calicut, Kerala 673635, India**E-mail: [renuka@uoc.ac.in](mailto:renuka@uoc.ac.in)*

**Abstract:** Nitroaromatic compounds (NACs) constitute a class of industrially significant species which find various applications. Unfortunately, the extensive utilization of NACs raises significant concern about environmental pollution. Current treatment methods for NAC removal are often inadequate and unsustainable, resulting in their inadvertent release into the environment. As these compounds pose hazards to both human health and other living organisms, they have been included in the USEPA's priority pollutant group. Addressing the environmental impact of NACs requires more effective and sustainable treatment strategies to mitigate their potential adverse effects on ecosystems and public health<sup>1</sup>. Picric acid (2,4,6-trinitrophenol) is an environmentally deleterious substance among the NACs, that has been of pressing societal concern. Therefore, developing a convenient and reliable platform for its fast and efficient detection is of paramount importance from security point of view<sup>2</sup>. Here we have synthesized orange-red fluorescent carbon nanodots<sup>3</sup> (AM-CDs) for the selective, sensitive and rapid determination of picric acid. AM-CDs are adequately characterized using High Resolution Transmission Electronic Microscopy (HR-TEM), X-Ray Diffraction (XRD) Analysis, Fourier Transform Infra-Red (FT-IR) Spectroscopy, X-Ray Photoelectron Spectroscopy (XPS), UV-Visible Absorbance spectroscopy, Raman spectroscopy and Fluorescence spectroscopy. Luminescence quenching in carbon nanodots upon the introduction of picric acid paves the way to fluorimetric detection of picric acid at micromolar concentrations, with limit of detection 17.23  $\mu\text{M}$ . Additionally, a mechanism is proposed for picric acid induced luminescence quenching in carbon nanodots.

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## PP-26

## Microwave assisted synthesis of anisoin N(4)-methylphenylthiosemicarbazone and its Cu(II) complex

R. Jeevana<sup>a</sup>, K.K. Aravindakshan<sup>b</sup>

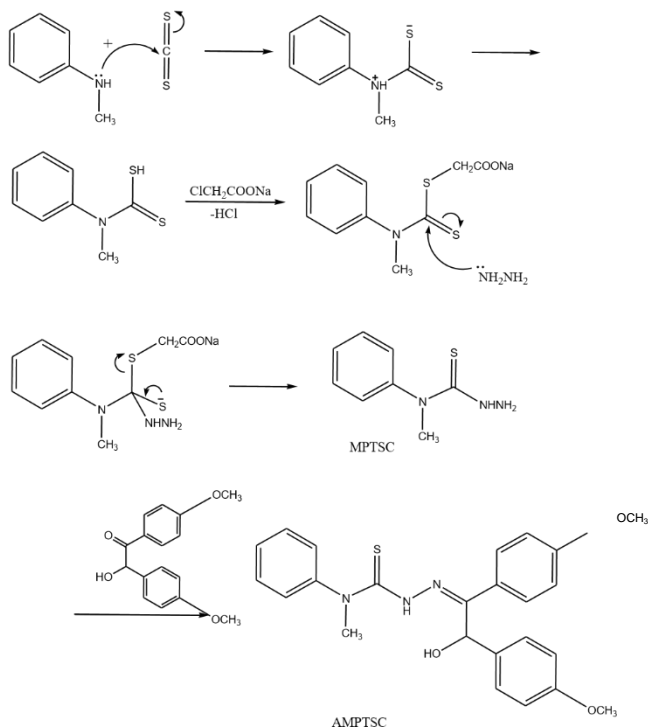
<sup>a</sup>Department of Chemistry, Gov.college Madappally

<sup>b</sup>Department of Chemistry, University of Calicut, Kerala673635, India.

**Abstract:** In recent years thiosemicarbazones and their metal complexes have received considerable interest because of their various biological activities<sup>1-5</sup>. Thiosemicarbazones show diverse bonding characteristics by virtue of the presence of several donor sites.

Thiosemicarbazide readily combine with carbonyl compounds to form thiosemicarbazones in alcohol medium. However, in recent times development of new synthetic routes for these types of compounds received great interest. In this paper we report the synthesis of anisoin-N(4)methylphenylthiosemicarbazone (AMPTSC), HL and its several transition metal complexes. Along with the conventional method of synthesis we have used the microwave irradiation technique for the synthesis of the ligand and some of its Cu(II) complexes

Following mechanism represents the formation of the ligand.



The reaction of anisoin with N(4)-methylphenylthiosemicarbazide (MPTSC) in ethanol under microwave irradiation leads to the formation of anisoinmethylphenylthiosemicarbazone (AMPTSC), HL, in just five minute and that too in high yields. We have synthesized Cu(II) complex of this ligand by microwave method. By using conventional method also we synthesized AMPTSC and its several transitional metal complexes. They were characterized by elemental analysis, magnetic susceptibility measurements, IR, <sup>1</sup>H NMR and electronic spectra. For Cu(II) complexes, five coordinated geometry were suggested.

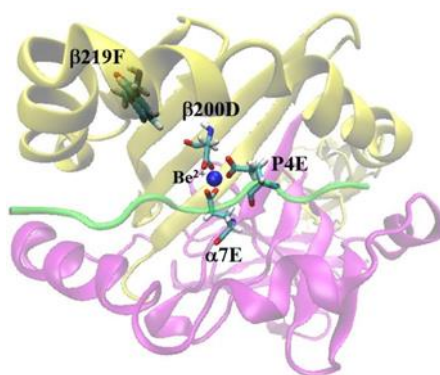
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## PP-27

**Identification of HLA-DR associated peptides involved in Beryllium hypersensitivity****Radhika Narayanan Nair, Susmita De***Department of Chemistry, University of Calicut, Malappuram, Kerala**E-mail: [radhikanarayananannair@uoc.ac.in](mailto:radhikanarayananannair@uoc.ac.in)*

**Abstract;** Beryllium exposure leads to beryllium sensitization and Chronic beryllium disease (CBD) which is a granulomatous lung disease caused by accumulation of Be-responsive CD4<sup>+</sup> T-cells in the lower respiratory tract.<sup>1</sup> Beryllium hypersensitivity and CBD is mainly associated with HLADP alleles having glutamate residue at 69<sup>th</sup> position of  $\beta$  chain.<sup>2</sup> In HLA-DP<sub>Glu69</sub> negative individuals, HLA-DR<sub>Phe47</sub> is the susceptible marker of beryllium hypersensitivity.<sup>3</sup> However, the potential Be<sup>2+</sup> binding site on the HLA-DR allele is unknown because the natural presenting peptide is unknown. Hence, molecular dynamics (MD) simulations combined with quantum mechanical/molecular mechanical (QM/MM) study were carried out to identify the appropriate peptide-Be<sup>2+</sup> ion combinations that can bind to HLA-DR3 protein. The binding free energies calculated using MM-GBSA method suggest the potential binding site of Be<sup>2+</sup> ion on the modelled protein-peptide complex.



**Figure 1.** Representative snapshot from MD simulation of the HLA-DR3\_peptide\_Be<sup>2+</sup> complex

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**PP-28****Studies of cure and mechanical properties of filled and unfilled NR/NBR blends****Rafna V. P.<sup>a, b</sup>, Ann Mary<sup>b</sup>, Fathima Murshida<sup>b</sup>, Sreenath Sreedharan<sup>b</sup>, Haris C.<sup>a\*</sup>**<sup>a</sup>Malabar Christian College, Calicut, Kerala, India<sup>b</sup>RAHS Innovation Centre, Technology Business Incubator,  
National Institute of Technology Calicut, Kerala, India.

**Abstract:** A comparative investigation on physicochemical properties of natural rubber (NR)/ nitrile butadiene (NBR) composite blend system was conducted with nanocarbon black and calcium carbonate as fillers. The blend ratio of 80:20, NR/NBR was selected to prepare different series of composite systems with and without the presence of nano-fillers. The composites were vulcanized at 150 °C using a hydraulic press. The cure characteristics such as T90 and scorch time were determined using rheometer. The physicochemical properties of the composites such as tensile strength, tear strength, elongation at break, hardness and specific gravity were also evaluated. The addition of calcium carbonate reduced the curing time and mechanical properties. However, the incorporation of nano-carbon black significantly improved the mechanical properties of NR/NBR blend system. The composite of 2% nanocarbon black showed an increment of 116% in tear strength, 13% in tensile strength and 32% in hardness when compared with pristine NR/NBR blend. The proposed system is suitable for new generation tyre blend applications.

**PP-29****Effect of hybrid fillers on the transport behaviour of natural rubber (NR) composites****Ranimol Stephen, Abhisha V.S***Department of Chemistry, St. Joseph's College (Autonomous), Devagiri**Affiliated to University of Calicut, Calicut, Kerala- 673 008, India.**E-MAIL: [ranistephen@gmail.com](mailto:ranistephen@gmail.com)*

**Abstract:** Polymer composites containing chemically modified fillers are promising materials for the production of highly efficient membranes for pervaporation, ultrafiltration, reverse osmosis and gas separation.(1–5).The role of natural rubber (NR) based polymer composites in the field of membrane technology demands the comprehensive understanding and in depth knowledge of transport behaviour of solvents in composite matrix. Transport properties of solvents in polymer composites are related to the distribution and reinforcement of fillers in the matrix. Modification of rubber matrix by the addition of conductive fillers such as, carbon nanotubes (CNT), conductive carbon black (CCB) and ionic liquid (IL) modified fillers generates changes in the transport properties of composites. NR/CCB composites resulted in a notable reduction in solvent uptake and swelling due to decreased free volume within the composite. Additionally, the inclusion of CNT further strengthened the composite, leading to lower solvent absorption and swelling. The combination of IL and CNT exhibited a synergistic effect, significantly reducing solvent uptake and swelling, modified hybrid systems exhibiting a remarkable decrease in solvent uptake. Empirical and semi-empirical mathematical models give theoretical perspective of experimental transport data. Experimentally obtained transport data are evaluated using different kinetic models such as first-order kinetics, Higuchi, Korsemayer-Peppas, and Peppas-Sahlin models. Peppas-Sahlin model fits well for the solvent diffusion of NR composites.

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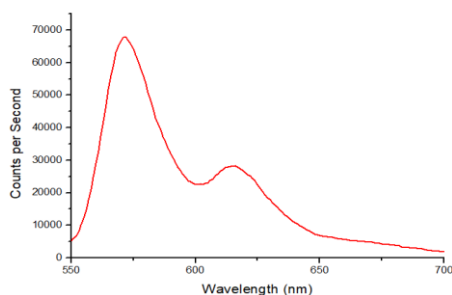
## PP-30

## A study on photoluminescent Ce(III) complex of hydrazone

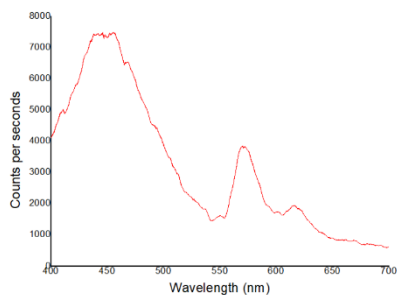
S.R. Sheeja

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Govt. College Madappally, Vadakara, Kozhikode 673102, Kerala, India

**Abstract:** In the present work, quinoline-2-carbaldehyde benzoyl hydrazone (HQb) and its Ce(III) complex were synthesized. The composition of these compounds was determined by the partial elemental analyses. For the characterization of these compounds, IR and UV-vis spectroscopic techniques were used. The emission spectrum of the complex was recorded in DMF. On excitation with 360 nm, the complex shows four peaks at 440, 457, 570 and 614 nm and on excitation with 521 nm, it displays two broad peaks at 571 and 614 ppm. The complex is applicable as blue-green light sources due to their  $4f-5d$  transition rather than conventional  $4f-4f$  transition of lanthanides



The emission spectrum of the complex on excitation with 521 nm



The emission spectrum of the complex on excitation with 360 nm

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**PP-31****The use of ethanolic extract of *Chromolaena odorata* flower as a natural and promising corrosion inhibitor for mild steel protection in acidic media****Dr. Shamsheera K O and Rahma Sinu C***Department of Chemistry,  
KAHM Unity Women's College, Manjeri, Kerala, India.*

**Abstract:** This work focuses on examining the corrosion inhibition properties of the ethanolic extract obtained from *Chromolaena odorata* flowers, known for their eco-friendly nature and rich phytochemical composition [1, 2]. Potentiodynamic polarization (PDP) and Electrochemical Impedance Spectroscopy (EIS) studies were in good agreement with the conventional weight loss method in concluding that the inhibition efficiency of *Chromolaena odorata* flower extract (COFE) inhibitor increase with increase in inhibitor concentration and decrease with increase in temperature from 303K to 323K. The optimum inhibitor concentration is shown by 3% (v/v) COFE in 0.5M HCl at room temperature. GC-MS studies of COFE showed the presence of DCarvone, Cyclooctasulphur, Elaol and Linoleic acid as major components. DFT calculations justify the corrosion inhibitive performance of flower extract on mild steel. Surface morphologies of mild steel in the presence and absence of inhibitor examined by FESEM and AFM techniques revealed that in the presence of the COFE, less damage occurs on the mild steel surface. The isothermal studies showed that the adsorption of COFE on the surface of steel was best fitted by the Langmuir isotherm.

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**PP-32****Surface functionalization of Zr based Metal Organic Framework with Polyvinylpyrrolidone for targeted and controlled drug delivery****Sneha Rajeev and G. Unnikrishnan***National Institute of Technology Calicut, Calicut, 673601, India**E-mail: unnig@nitc.ac.in*

**Abstract:** Metal Organic Frameworks (MOFs) with large surface area, high porosity and tunable functionalities have become one of the promising materials for effective drug delivery applications. Surface functionalization of these MOFs with biocompatible polymer polyvinylpyrrolidone can enhance the controlled and targeted drug delivery properties. The present study focuses on the synthesis of Zr based MOFs through a solvothermal method. Surface functionalization has been carried out by the physical mixing of the polymer polyvinylpyrrolidone. The crystallinity, chemical features, morphology, composition and thermal properties have been evaluated from XRD, FTIR, FESEM, EDX and TGA respectively. An anticancer drug has been loaded into the Zr-MOF/PVP system and the drug release study has been carried out with the help of UV–Visible absorbance spectrophotometer. The results obtained indicates the possibility of Zr-MOF/PVP as a promising drug delivery system.

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## PP-33

**Thermal analysis as a tool to address the effect of microplastics in soil****Suhada Kottakuth Matayil<sup>a,b</sup> and Yamuna Kunhi Mouvenchery<sup>a,c\*</sup>**<sup>a</sup>*Malabar Christian college, Calicut,*<sup>b</sup>*KAHM Unity Women's College, Manjeri,*<sup>c</sup>*N.S.S. College Manjeri**E-mail: [kmyamunanssmji@gmail.com](mailto:kmyamunanssmji@gmail.com)*

**Abstract:** Microplastics (MP) that are plastic particles of less than 5mm diameter are being increasingly attended by researchers across the world, owing to the pollution threat they pose, in all compartments of the environment including living organisms<sup>1</sup>. The nature of interactions that the MP particles induce within the environmental matrixes needs to be addressed since properties and hence processes are governed by structure-level interactions. This would help understanding and predicting the behaviour of MP in soil and water, leading to development of mitigation strategies, on long run.

This pilot study, therefore, aims at unravelling the influence of engineered microplastics – polyethylene (PE), polystyrene (PS) and polyvinylchloride (PVC) – on properties of a forest soil sample. Soil samples were spiked with polymers in batches, equilibrated and then assessed for various structure-relevant properties and processes. This part of the work shows results from thermoanalytical studies: low-temperature DSC and TGA-DSC analysis. These techniques would give implications on changes in soil matrix rigidity and thermal stability of different structural fractions, respectively, caused by the introduction of the three MP polymers<sup>2</sup>.

Results from thermal analysis as well as other chemical tests (water content, available C, etc.) show that chemical nature and abundance of polymer particles significantly affects the structural stability and hence related properties of soil. This is suggestive for that polymer microparticles induce notable interactions within soil matrix, instead of merely occupying the interparticle voids. This has serious consequences on structure and properties of soil matrix, bringing in additional concerns than sole effect of MP. This study is among the first ones to assess the structure-level consequences of MP particles in soils. Further studies on the effects of MP on various

environmental processes are being undertaken, which explore higher dimensions of MP pollution in soil.

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**PP-34****Synthesis and characterization of PVP/CMC ZnO nanocomposite hydrogel with enhanced antimicrobial properties****Suhaila T and Kavitha Manniledam***Department of Chemistry, Zamorin's Guruvayurappan College, Kozhikode, 673014, Kerala, India**E-mail: [kavitha236@gmail.com](mailto:kavitha236@gmail.com)*

**Abstract:** In the present study, ZnO nanoparticles were synthesised using coprecipitation method. The crystalline nature of ZnO nanoparticles was confirmed using XRD, morphological characterisations are carried out using SEM and TEM studies. Further PVP/CMC based ZnO nanocomposite hydrogel films were synthesised using solution casting method and morphological studies were evaluated using SEM studies. Mechanical studies demonstrated that PVP-CMC –Z3 composition has high tensile strength. The nanocomposite hydrogels found to have antibacterial effect against *Bacillus megaterium* and *Pseudomonas fluorescens*. The developed PVP/CMC ZnO nanocomposite hydrogels can be used effectively for biomedical applications

**Keywords:** Carboxymethylcellulose, Polyvinylpyrrolidone, Nanocomposite, Zinc oxide, antimicrobial.

**Acknowledgments:** The authors are thankful to University of Calicut for funding

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## PP-35

**Synthesis and photophysical properties of propyloxy substituted phenyleneethynylene carbaldehyde based charge transfer salts****Sumayya K and Reji Thomas\****Department of Chemistry, Farook College, Kozhikode-673632, Kerala, India**Email: reji@farookcollege.ac.in*

**Abstract:** Solid state luminescent materials have gained greater attention in recent years due to their wide applications in optoelectronics, sensors, light emitting diodes, cell imaging organic lasers etc. Luminescent properties of a single organic molecule with a donor and acceptor system can be tuned by incorporating different functional groups in the core structure for affecting  $\pi\cdots\pi$  interaction however the synthesis of such molecules is difficult. Crystal engineering can be used to obtain solid materials with diverse optical and electronic properties avoiding complicated synthetic procedures. In the present work, we have synthesized an oligo phenyleneethynylene (OPE) and co-crystallized with 2,3,5,6-Tetrachloroterephthalonitrile (TCTPN) and 1,2,4,5-tetracyano benzene (TCNB) to obtain crystals of charge transfer salts. The optical property of CT cocrystals was dependent on their aromatic stacking interactions in their crystal lattices. We explored the role of molecular packing and intermolecular interactions in determining the optical properties using single-crystal X-ray diffraction. The crystal structure of OPE with TCTPN showed two types of arrangement aggregates, namely, J-type and X-type aggregates. The OPE-TCTPN cocrystal showed a blueshifted luminescence maxima while the OPE-TCNB cocrystal showed a redshifted emission in comparison to that of pure OPE. The quantum yields of both OPE and its cocrystals were recorded, where the quantum yield of cocrystals showed decreased value attributed to the strong  $\pi\cdots\pi$  stacking interactions in the crystalline state.

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## PP-36

**Green Synthesis of Graphene for High-Performance Asymmetric Supercapacitors****Sumisha S, Binitha N<sup>\*</sup>***Department of Chemistry**University of Calicut, Thenhipalam, Malappuram, 673635, Kerala, India,**\*binithann@yahoo.co.in*

**Abstract:** The wide-reaching surface area and superlative conductivity of graphene ensure it as a promising electrode in supercapacitor applications. Asymmetric devices make use of two distinct electrode materials for expanding their working voltage window by overcoming the common obstacle of the thermodynamic breakdown of the electrolytes. Here graphene is prepared via a green, eco-friendly, ball milling method by avoiding toxic chemicals or corrosive oxidizing conditions. Graphite exfoliation is done with the assistance of a carbohydrate exfoliating agent, further leading to the edge functionalization of graphene. The electrochemical properties and thus the suitability of the material as an electrode material in supercapacitors are analyzed using cyclic voltammetry, galvanostatic charge-discharge measurements, and electrochemical impedance spectroscopy. The graphene /activated carbon asymmetric supercapacitor device showed a wide potential window and high specific capacitance in a neutral electrolyte. Two parallel devices connected in series could easily illuminate commercial light emitting diode (LED).

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## PP-37

**Development of a Supercapacitor Energy Storage Device based on a Metal-Free Graphene Nanocomposite Prepared via a High-Yielding In-Situ Green Strategy****Suvarna K. Subrahmanian<sup>1,2</sup>, Binitha N. Narayanan<sup>1,2\*</sup>**<sup>1</sup>*Department of Chemistry, University of Calicut, Malappuram (DT), Kerala - 673635, India*<sup>2</sup>*Department of Chemistry, Sree Neelakanta Government Sanskrit College, Pattambi, Palakkad-679306, Kerala, India*

**Abstract:** The hazardous nature of the graphite oxide-assisted preparation and the disturbed aromatic  $\pi$ -conjugative network of the resultant graphene demanded alternative strategies for graphite exfoliation, especially for applications where the conductivity of graphene is the major determining factor of its performance. Herein, a green and in-situ method is proposed for the synthesis of a graphene nanocomposite for supercapacitor applications via a carbohydrate-assisted graphite exfoliation strategy. The additional formation of nanostructured carbon in between the graphene layers is demonstrated from the FESEM and HRTEM analysis whereas the oxygen functionalities at the edges of graphene and on the nanocarbon are comprehended from the FTIR spectroscopy. The EDLC contribution from graphene along with the pseudocapacitance of oxygen functionalities delivered excellent energy storage properties for the graphene nanocomposite in terms of specific capacitance and life span. The superior supercapacitor performance of the nanocomposite resulting from the synergistic effects is further explored for the successful development of a symmetric coin cell supercapacitor. A series connection of four coin cells enhanced the potential window up to 4.5 V and the tandem device was exploited to light up a red light-emitting diode, which demonstrates the real-time application of the developed graphene-based supercapacitor as an energy storage device.

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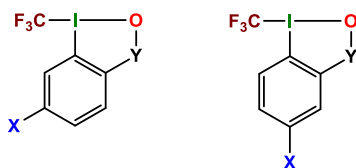
## PP-38

Quantification of the *trans* and *cis* Influences in Togni Type Reagents

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**Abstract:** Togni-type reagents, classified as hypervalent iodine (III) compounds, have been recognized for their potent trifluoromethylation capabilities. The *trans* and *cis* influences of various ligands in Togni type scaffolds are studied by using Molecular Electrostatic Potential at the carbon ( $V_C$ ) and iodine ( $V_I$ ) nuclei in the I–CF<sub>3</sub> moiety. The *trans* influences of atom (O/S) or group (NCH<sub>3</sub>), as well as the linker (Y), on the strength of the I–CF<sub>3</sub> bond is investigated. The impact of electron-donating and electron-withdrawing groups on the phenyl ring is explored to understand the *cis* influence. Through the utilization of  $V_C$  and  $V_I$ , the study effectively elucidates the combined effects of various ligands on both *trans* and *cis* positions on the bond dissociation energy (BDE) of the I–CF<sub>3</sub> bond. In general, our findings provide valuable insights into the influence of ligands and structural modifications on the trifluoromethylation capabilities and electronic properties of Togni reagents.



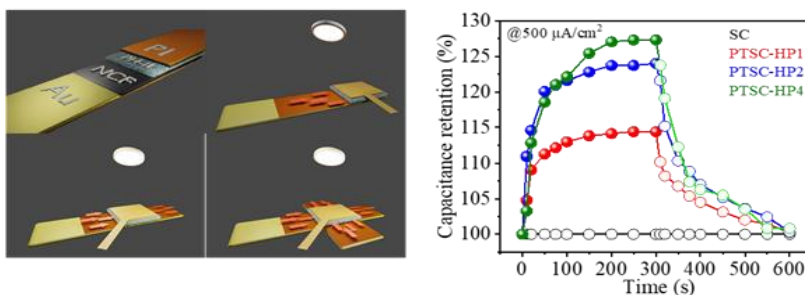
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## PP-39

**Photothermal modulating of ion-transport channels for solid-state, non-Faradic energy storage devices operable at sub-ambient temperatures****Mohammed Aslam Villan, Arnab Chowdhury, Chandramouli Subramaniam***Department of chemistry**Indian Institute of Technology-Bombay, Maharashtra, India.*

**Abstract:** Photothermal energy conversion promises transformative advancements in supercapacitor technology by synergizing energy storage with light-to-heat conversion. In this work, we elucidate a dual-functional material, nanostructured hard-carbon florets (NCFs) serving both as a photo-thermal converting material and as an electrode material for non-Faradic energy storage. The intrinsic micro- to mesoscale pore structures coupled with isotropically engineered conical cavities of NCF emerging as pivotal factors for robust energy storage and also facilitate broadband solar absorption (95% over 250-2500 nm). The short-range graphitic order within NCF facilitates photon thermalization through a phonon-driven process. NCF coatings on flexible electrodes, instantaneously generates surface temperature of  $120 \pm 5$  °C under solar illumination. The localised heat generated on NCF photo-thermal pads under illumination (power density =  $0.2 \text{ W/cm}^2$ ) is effectively conducted to enhance ionic conductivity of solid-polymer-ionic liquid electrolyte for achieving 40% improved energy storage ability. The resulting devices exhibit energy density 8.5 Wh/kg and power density 2.5 kW/kg with a relaxation time constant of 90 ms. Importantly, such photothermally operated flexible supercapacitors exhibit identical performance at sub-ambient temperature (10 °C) and ambient temperature (30 °C). Furthermore, the effect of electrode design in maximizing the performance of such photothermally driven devices is discussed, followed by the mechanistic insights of such systems, drawn from spectroscopic and microscopic techniques.



## PP-40

**Au<sub>9</sub> nanocluster-embedded UiO-66-NH<sub>2</sub> metal-organic framework for electrocatalytic hydrogen evolution reaction****Aparna Ravari Kandy, Sukhendu Mandal***Indian Institute of Science Education and Research, Thiruvananthapuram  
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**Abstract:** Atomically precise metal nanoclusters have gained immense popularity due to their amazing range of applicability in various fields, including catalysis.<sup>1</sup> Even so, their high surface energy emanating from the ultrasmall size (<3 nm) affects their stability under reaction conditions. Embedding nanoclusters in metal-organic frameworks, a class of crystalline porous materials, affords an effective strategy to overcome these limitations.<sup>2</sup> Herein, we synthesized a composite of atomically precise Au<sub>9</sub>(PPh<sub>3</sub>)<sub>8</sub>(NO<sub>3</sub>)<sub>3</sub> nanocluster incorporated in extraordinarily stable Zr-based MOF, UiO-66-NH<sub>2</sub>, using a bottle around the ship approach.<sup>3</sup> Characterization techniques, like PXRD, HR-TEM, XPS, etc., established the crystallinity and structural stability of the MOF as well as the size, distribution, and chemical composition of the nanoclusters. The composite was then used as a catalyst for electrocatalytic hydrogen evolution reaction (HER), which is envisaged as a powerful method for producing clean hydrogen.<sup>4</sup> This Au<sub>9</sub>@UiO-66-NH<sub>2</sub> composite delivered an impressive catalytic activity for HER in 0.5 M H<sub>2</sub>SO<sub>4</sub> with an overpotential of 65 mV at 10 mA/cm<sup>2</sup>. The Tafel slope of 41 mVdec<sup>-1</sup> also shows the potential of the material as an effective electrocatalyst. The catalyst offers excellent stability for more than 30 hours. This work may open up new avenues for the design and synthesis of nanocluster – MOF composite materials for energy-related applications.

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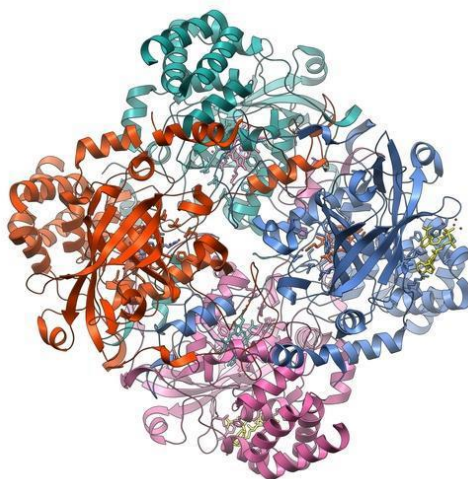
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## PP-41

**Kinetics of Enzyme Catalysed Decomposition of Hydrogen Peroxide****Mohammed Ziyad P. A., Hanna Fathima. P, Majidha Ameer, Muhammad Sibil. M P, Muhammed Fadheen Abdul Khader, Muhammed K K***Department of Chemistry, Farook College (Autonomous), Kozhikode, Keral, India*

**Abstract:** Catalases, heme enzymes which catalyze decomposition of hydrogen peroxide to water and molecular oxygen, are important members of the antioxidant defence system of cells of almost all aerobic organisms. However, recent studies suggest that catalase may be involved in various other processes in the cell. The work provides a review of reaction kinetics of catalases with their main substrate hydrogen peroxide. Potential biological significance of the reactions of mammalian as well as bacterial catalases with oxidizing species is discussed.



**Figure 1.** Schematic drawing of the polypeptide chain catalase subunit

The results of this study demonstrate that the kinetics of temperature-dependent enzyme-catalyzed decomposition of hydrogen peroxide are dependent on both temperature and hydrogen peroxide concentration. At 31°C, higher concentrations of hydrogen peroxide exhibited second-order kinetics, while lower concentrations showed first-order kinetics. Conversely, at 21°C, higher concentrations showed first-order kinetics, while lower concentrations exhibited second-order kinetics

## PP-42

**Cholesterol appended cyanostyryl thiophene positional isomers with multi stimuli responsive emission switching and liquid crystalline properties****Ramya N K, Athira P, Manoj Mathews and Reji Thomas***Department of Chemistry, Farook College, Kozhikode-673632, Kerala, India**Email: reji@farookcollege.ac.in*

**Abstract:** Solid state luminescent systems based on conjugated D- $\pi$ -A molecules find vast applications in different fields such as flat panel displays<sup>1</sup>, switches<sup>2</sup>, sensors<sup>3</sup>, organic light emitting diodes (OLEDs)<sup>4</sup> and anti-counterfeit materials<sup>5</sup>. Structural modification of the luminogens is used as a tool to generate a library of molecules that are highly emissive in the solid state. In addition to the structural modifications involving tedious synthetic steps, positional isomerism of functional groups also served as a strategy to achieve highly luminescent materials. Cyanostyrylbenzenes are a class of compounds with great research interest, owing to the possibility of generating versatile materials with tunable luminescence properties. The tunable optical properties in these molecules are achieved by the subtle control of the molecular conformation, packing, and intramolecular interactions in the solid state by suitably functionalizing the luminophore<sup>5</sup>. Herein we synthesized molecules with cyanostyryl thiophene as core structure functionalized by cholesterol to explore the role of positional isomerism on solid-state emission behaviour. The molecular design consists of a cholesterol moiety attached to the cyanostyryl thiophene fluorophore is favourable for stabilizing liquid crystalline phases.

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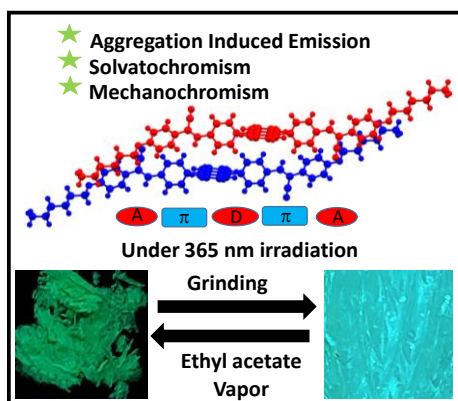
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## PP-43

**Anthracene appended cyanostilbenes with intramolecular charge transfer and aggregation induced emission****Cherumannil Femina,<sup>a</sup> M. Shanthil,<sup>b</sup> Pookkottu K. Sajith<sup>a</sup> and Reji Thomas\*<sup>a</sup>**<sup>a</sup>*Department of Chemistry, Farook College (Autonomous), Farook College P.O, Kozhikode-673632, Kerala, India*<sup>b</sup>*Department of Chemistry, Government Victoria College Palakkad-678 001, Kerala, India*  
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**Abstract:** Cyanostilbene systems obtained paramount interest among various  $\pi$ -conjugated systems owing to their fascinating fluorescence properties in the solid state.<sup>1</sup> The cyanostilbenes attached with various functional groups were explored for their aggregation induced emission (AIE) and multistimuli responsive nature.<sup>2</sup> Herein, we report the synthesis and photophysical properties of highly emissive donor-acceptor systems based on anthracene and cyanostilbene, carrying hexyl (**CSB-1**) and dodecyl (**CSB-2**) chains. The molecules are highly emissive in both solid and solution states owing to intramolecular charge transfer and AIE respectively. The molecule **CSB-1** showed stress induced emission switching and solvent induced recovery attributed to the change in crystallinity under applied stimuli. The observed photophysical properties of **CSB-1** is compared with that of **CSB-2** and substantiated with the structural and packing details obtained from single crystal X-ray diffraction and DFT calculations.



**Figure 1.** Anthracene-cyanostilbene based donor-acceptor systems with intramolecular charge transfer and Aggregation Induced Emission (AIE) properties.

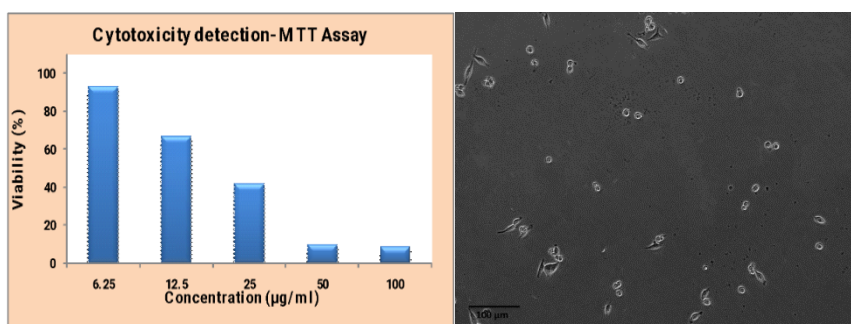
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## PP-44

**Antibacterial and anticancer activity of modified ZnO nanocomposite synthesized by novel approach****Shanavas Yoosuf and Shalina Begum T\****Department of Chemistry, Farook College, Kozhikode-673632, Kerala, India**Email: shalinat@gmail.com*

**Abstract:** This work intended to formulate nanocomposites of zinc oxide (ZnO), characterize their physical properties, and evaluate their antimicrobial and anticancer properties. X-ray diffractometer and SEM with EDX were applied to characterize the morphology and structure. To investigate the functional groups and visible light response of prepared nanocomposite, we used Fourier transform infrared analysis, UV–Visible diffuse reflectance and photoluminescence spectroscopy. Antimicrobial activities against bacterial strains were tested with agar well diffusion method. The MTT assay is used to measure cellular metabolic activity as an indicator of cell viability, proliferation and cytotoxicity. The modified nanocomposite had a high antibacterial activity towards two most important infectious bacteria ( *Escherichia coli* and *Staphylococcus aureus*) and anticancer activity against human colorectal carcinoma cell (*HCT-116*). Dose dependent reduction in cell viability was observed in cancer cells (*HCT-116*) administered with different concentrations of the sample. The maximum cytotoxicity was observed with 100 µg/ml (% viability: 8.34) of the sample.

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