International Conference on Advances in Functional Materials and Applications

February 20 – 22, 2025

Venue: BITS PILANI K K BIRLA GOA CAMPUS

BOOK OF ABSTRACTS

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About AFMA - 2025

- ## Goals of the Conference:

The primary aim of this conference is to provide a common platform for eminent national and international scientists as well as young researchers to discuss the current state of the art, generate novel ideas, and trigger collaborations in the seminal areas of research in structural and functional inorganic, organic and materials chemistry. Topics will range from catalysis, energy storage, environmental remediation, sensors, therapeutics to smart materials. The conference aims to provide a common platform for young researchers and eminent scientists alike for the dissemination of the most recent important discoveries and developments in the aforementioned areas and to foster discussions and trigger collaborations between research groups from across India and abroad.

- ## Themes of the Conference:

The conference will focus on (but is not limited to) the following key topics:

  - Structural Inorganic, Organic, Organometallic and Materials Chemistry
  - Catalysis
  - Energy Storage and Conversion
  - Environmental Chemistry
  - Sensors and Smart Materials
  - Therapeutics
  - Computational Chemistry and Materials Design

- ## Structure of the Conference:

The conference will be divided into several sessions; each session will focus on a specific theme. There will be plenary lectures (40 mins), keynote lectures (30 mins), and invited lectures (15-20 mins) in each session. In addition, poster sessions will give ample opportunities to research scholars for the presentation of their recent results. There will be poster competitions, and the selected posters of research scholars will be awarded best poster awards in recognition of their research achievements.

Convenors

Prof. Saurav Bhattacharya

BITS-Pilani K K Birla Goa Campus

Prof. Sukhendu Mandal

IISER Thiruvananthapuram

Co-convenors

Prof. Uttara Basu

BITS-Pilani K K Birla Goa Campus

Prof. Debajit Sarma

IIT Patna

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High-Entropy Oxide and Alloy Nanoparticles Synthesized by Continuous Supercritical Hydro/Solvothermal Flow Process

Hiroshi Kitagawa

Kyoto University, Sakyo, Kyoto, 606-8502, Japan

Email: kitagawa@kuchem.kyoto-u.ac.jp

Abstract:

High-entropy oxide nanoparticles (HEO NPs) have been intensively studied because of their attractive properties, such as high stability and enhanced catalytic activity. In this work, for the first time, denary HEO NPs were successfully synthesized using a continuous supercritical hydrothermal flow process without calcination.[1] Interestingly, this process allows the formation of HEO NPs on the order of seconds at a relatively lower temperature. The synthesized HEO NPs contained 10 metal elements, La, Ca, Sr, Ba, Fe, Mn, Co, Ru, Pd, and Ir, and had a perovskite-type structure. Atomic-resolution high-angle annular dark-field scanning transmission electron microscopy and energy-dispersive X-ray spectroscopy measurements revealed homogeneous dispersion of the 10 metal elements. The obtained HEO NPs also exhibited a higher catalytic activity for the CO oxidation reaction than that of the $LaFeO_3$ NPs.

Platinum-group-metal (PGM) high-entropy alloy nanoparticles (PGM-HEA NPs) have been also investigated as catalysis.[2,3] Among the types of alloys, solid-solution alloy NPs have the advantage of being capable of continuously changing their properties by tuning their composition. However, synthesizing PGM solid-solution alloy NPs with any combination and composition is not an easy task due to the metallurgical aspects. We have focused on PGM-based solid-solution alloy NPs, and particularly those with immiscible alloy systems.

Key words: *Catalysis, High-entropy materials, Solvothermal flow process*

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Prof. George Shimizu

Computational Modeling of Semiconducting Materials for Catalytic and Thermoelectric Applications

Swapan K Pati

Theoretical Sciences Unit, School of Advanced Materials (SAMat), Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur Campus, Bangalore 560064, India.

Email: pati@jncasr.ac.in

Abstract

In this lecture, I shall discuss our computational modeling approach on semiconductors for their applications in energy technology, namely, in electrocatalytic and thermoelectric applications. While, the bifunctional (OER & ORR; oxygen evolution and reduction reactions) electrocatalysts can be used as either Zn or Al-air battery and the water splitting electrocatalysts (HER; hydrogen evolution reaction) as green H_2 fuels, the thermoelectric materials convert directly the waste heat into the electricity at varous temperatures.

To model materials for electrocatalytic oxygen evolution reaction (OER) & oxygen reduction reactions (ORR), I shall discuss our computational approach on three systems: (a) three metal (Fe/Co/Mn)-fluorophosphates synthesized by an experimental group, (b) one Co-pyrophosphate synthesized experimentally and (c) (Co/Rh/Ir) and N co-doped graphene systems with varying N concentrations [1-3]. We also have modelled electro and photocatalysts for splitting water to generate hydrogen on tetrazine-based covalent organic framework in acidic media and on a heterojunction, which was synthesized by an experimental group, which shows HER activity at all pH values due to charge transfer [4, 5].

To compute thermal conductivity and thermoelectric efficiency, we have developed computational codes based on Boltzmann transport equations. We have computed the thermoelectric efficiency of a few interesting materials, namely, n-type ternary Ag_2Se systems with S and Te doping and 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf and Y: Co, Rh, Ir) [6, 7]. I shall also talk on our recent calculations of thermal conductivity in glass like material, TlAgSe, which was in collaboration with an experimental group [8]

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Helically Chiral and Conformationally Locked Anthracene and Indolocarbazole Incorporated Macrocycles

Gokulnath Sabapathi

Department of Chemistry
Indian Institute of Science Education and Research, Thiruvananthapuram
Email: gokul@iisertvm.ac.in

Abstract:

Enantiopure helical systems have potential applications in circularly polarized luminescent materials (CPL), nonlinear optical materials, spin filters, circularly polarized organic light emitting diodes (CP-OLEDs), and bio-imaging applications. Chirality in porphyrinoids is an emerging field recently realized with large and flexible macrocycles with appropriate linking subunits. The optical resolution of these macrocycles is often difficult to achieve owing to their dynamic interconversion between two conformers. In the first part of my talk, the synthesis, structure, and chiroptical properties of a conformationally stable, helically locked, and twisted Cyclo[2]Dipyrrins **1** containing two dipyrrin units separated by anthracene subunits will be presented. Macrocycle **1** is a non-planar, crystallizes as a racemic mixture and adopts a highly twisted non-planar conformation. High racemization energy barrier enabled facile optical resolution. The (***P,P***) and (***M,M***) enantiomers show moderate chiroptical properties, such as absorption dissymmetry factors in the order of 10^{-3} and luminescence dissymmetry factors of 3.8×10^{-3} and 2.9×10^{-3} at 702 nm respectively.

Next, we synthesized a *'figure-eight'* helical chiral macrocyclic system embedded with dihydroindolo(2,3-a)carbazole. The crystal structure revealed the presence of both ***P,P*** and ***M,M*** enantiomers within the crystal packing. Hydrogen bonding interactions stabilize this '*figure-eight*' conformations, and further rigidification was achieved through BF_2 complexation **2·BF₂** and subsequent fusion led to **2·BF**. The rigid chiral framework of **2·BF** complex facilitated the chiral separation of enantiomers ***P,P*** and ***M,M***, which showed a chiral response in the near-region with $\Delta\varepsilon$ of up to 150 M^{-1} cm^{-1} at 692 nm.

Key words: *Macrocycle, conformation, helical chirality,*

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Enhancing the Resistive Switching *WORM* Memory Behavior of D- π-A-based Ester-flanked Quinolines

S. Nagarajan

Department of Chemistry, Central University of Tamil Nadu, Thiruvarur-610 005.
E-mail: snagarajan@acad.cutn.ac.in

Abstract:

Organic small molecule-based electronics are the most demanding area of research due to their alteration of bandgaps by simple alterations in the molecular structure, simple synthetic routes, easy purification, and solution processability. Organic molecules in a donor-acceptor (D-A) architecture especially gain more importance in electronics due to the push-pull within the system, which can induce a better charge transfer and facilitate efficient charge transport. Organic memory devices are one such area of electronics that has been admired in recent years through the incorporation of D-A systems. This work constitutes the design, synthesis, and characterization of functionalized ester-flanked quinolines for their application in non-volatile resistive random-access memories (RRAMs). All the compounds were synthesized in a D-A architecture, with quinoline as the acceptor molecule, and the donor molecules were changed to obtain different memory behaviors. These compounds were synthesized through Pd-catalysed Suzuki and Sonagashira cross-coupling reactions, yielding the targeted compounds. The memory device fabrication and characterization were performed on an ITO-coated glass plate, above which the compounds were spin-coated, and then the electrodes were placed. All the compounds exhibited Write-Once Read-Many (*WORM*) memory behaviour with the triarylamine attached quinolines in D-A and D-A-D architecture, giving rise to a binary WORM memory with an on/off ratio of 10^3-10^4 and very low threshold voltages of ~ 1 V under ambient conditions. The ferrocene end-capped quinolines exhibited a ternary WORM memory with a threshold voltage of -0.58 V. For the molecules studied the mechanism includes charge transfer, charge trapping, geometrical change, and redox behavior.

Keywords: *Organic Electronics; Memory Devices; WORM memory; Quinoline; D-A System.*

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In quest of synergy: Understanding the entropy effect in disordered materials for enhanced energy applications

Sourav Laha
Department of Chemistry, National Institute of Technology Durgapur, Mahatma Gandhi Avenue, Durgapur-713209, West Bengal, India
Email: slaha.ch@nitdgp.ac.in

Abstract:

Disordered bimetallic and multi-metallic materials are known to exhibit superior electrochemical performances than their mono-metallic counterparts. A series of new disordered materials are being systematically investigated to understand the synergistic/ entropy effect arising from improved electronic coupling between different constituent elements.

In the solar rechargeable aqueous Na-ion batteries, the power density and cyclability of PBAs ($Na_2MFe(CN)_6.xH_2O$; M = 3d transition metal) significantly improves as the number of constituent of 'M' increases from one to five (high entropy PBA).[1-5] (Mn,Co,Ni)-PBA delivers promising capacity (>120 mA h g^{-1}) enhancement. Full cells have been fabricated with different TM oxide-based materials (NaV_3O_8, $Na_xFe_2O_3$, $NaTi_2(PO_4)_3$, $H_2V_3O_8$) as anodes. This led to the development of 5 V/ 5 mA h Na-ion battery prototypes which successfully illuminate 5 V/ 250 mW light emitting diode setup.

On the electrochemical HER, OER and OWS, a bimetallic MOF comprised of Ni(II) and Co(II) metal centers, nicotinate (NA), N-nicotinoyl glycinate (N-NG) ligands outperform (η_{10} = 120 mV) the mono-metallic Ni derivative (η_{10} = 150 mV)[6] in HER activity whereas the MOFs with BTC exhibit increasingly better activities towards HER, OER and OWS with increasing the number of metals,[7] from one to five (high entropy).

On transition metal oxide nanosheets, $H_yMn_{0.8}Co_{0.2}O_2$ demonstrate promising HER activity but limited OER performance.[8] On the other hand, the incorporation of Pd NPs onto the nanosheets establishes a strongly coupled metal/metal oxide hybrid system, enabling robust and efficient bi-functional catalytic activity. The Pd/$H_yMn_{0.8}Co_{0.2}O_2$ hybrid achieves the current density (*j*) of 10 mA cm^{-2} in 1.0 M KOH with applied overpotentials of 210 mV for HER, 390 mV for OER and retains stable performance for ~24 h.[9] A two-electrode Pd/$H_yMn_{0.8}Co_{0.2}O_2$||Pd/$H_yMn_{0.8}Co_{0.2}O_2$ electrolyzer efficiently performs OWS at a cell voltage of 2.00 V, operating continuously for ~120 h without significant change in *j* highlighting a cost-effective and scalable electrolyzer fabrication.

Therefore, this talk will shed some light on the complex relationship between entropy effect in materials chemistry and practical application from the perspective of materials-to-device development.

Keywords: *Energy materials, Aaqueous Na-ion battery, solar energy storage, electrocatalysis, device fabrication*

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Noble Metal-Oxo Cluster Chemistry: Synthesis, Structure and Catalysis

Ulrich Kortz

School of Science, Constructor University, Campus Ring 1, 28759 Bremen, Germany
Email: ukortz@constructor.university

Abstract: Polyoxometalates (POMs) based exclusively on Pd^{II} ions (polyoxopalladates, POPs) were discovered in 2008.[1] The area of POP chemistry has developed rapidly ever since due to the fundamentally novel structural and compositional features of POPs resulting in unprecedented electronic, spectroscopic, magnetic, and catalytic properties. [2] In recent years efforts were made to modulate the POP structures along with their associated charges so as to control the structure-property relationship. This pursuit has led to the preparation of neutral palladium(II)-oxo clusters (POCs),[3] followed by the synthesis of the first examples of cationic POCs.[4] Here we provide an overview of the synthesis, structural characterization (in solution, solid state, and gas phase) and catalytic properties of POPs and POCs.[5]

Key words: *Polyoxometalates, Polyoxopalladates, Palladium-Oxo Complexes, Catalysis*

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Functional Molecular Vessels

Partha Sarathi Mukherjee

Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore - 56012

Email: psm@iisc.ac.in

Abstract:

Due to the restricted degree of freedom of chemical entities in confined nanospace their physical and chemical properties are expected to be different from their conventional properties in the bulk medium. Metal ligand dynamic coordination bonds have been extensively used to design discrete metallosupramolecular architectures. My lecture will focus on the design of a few water-soluble Pd(II) discrete molecular architectures that have hydrophobic confined nano-pockets. My lecture will focus on our recent observation on the role of the shape of reaction vessels on the fate of a chemical reaction (Figure 1). By changing the shape of Pd_6 aqueous molecular cages the oxidation of anthrone in presence of water gave different products under the identical reaction conditions. Introduction of flexibility/functionality into the ligands to design unusual functional architectures for selective photocatalytic oxidation and separation of isomeric polyaromatic hydrocarbons by aqueous extraction will also be presented in my lecture.

Figure 1. Cavity-shape dependent divergent synthesis.

Key words: *catalysis, self-assembly, isomers separation*

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Bio(in)organic Activation of Nitrite: Modelling Bioregulatory Routes for NO and H_2S Signalling

Subrata Kundu

School of Chemistry, Indian Institute of Science Education and Research (IISER),
Thiruvananthapuram 695551, India
Email: skundu@iisertvm.ac.in

Abstract:

Though nitric oxide (NO) and hydrogen sulfide (H_2S) are known as notorious toxins, both of them serve as gasotransmitters, thereby assisting various physiological activities including vasorelaxation, neuro-transmission, and anti-inflammation.[1] Biochemical processing of NO and H_2S occurs through a set of tightly controlled complex transformations involving a wide array of reactive sulfur, oxygen, and nitrogen species (RSONs). Our recent works outline new molecular pathways for the generation of elusive (per)thionitrite (S_nNO^-) and nitroxyl (HNO) species,[2] and thus showing how nitrite (NO_2^-) may play pivotal role in modulating the chemistry of RSONs. Furthermore, this talk aims to highlight the reductive transformations of NO_2^- in the presence of biologically relevant redox cofactors.[3] Employing a set of structurally characterized metal(II)-nitrite model complexes, our recent works illustrate the role of proton-coupled electron-transfer (PCET) versus proton-transfer (PT) in NO generation from nitrite.

Keywords: *Bioinorganic Chemistry, Nitrite, Nitric oxide, Reactive intermediates, Mechanism*

Reference:

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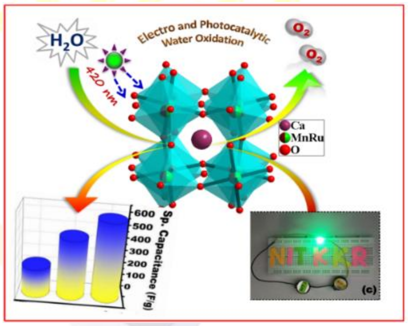
Effect of 3*d*-Transition Metal-ions in Ruthenate Perovskite Materials for Sustainable Energy Generation and Storage Applications

Avijit Kumar Paul

Dept. of Chemistry, NIT-Kurukshetra, Haryana-136119.
Email: apaul@nitkkr.ac.in

Abstract: The design and exploration of advanced material as a durable multifunctional electrocatalyst towards sustainable energy generation and storage development is the most perdurable challenge in the domain of renewable energy research. Solids unveiling structural variation, electronic phenomena and energy related properties are of great interest to investigate by chemist, physicist and engineer. The tuning of structure-property correlation can be performed by permutation of transition (*d*-block) elements in the materials. Double perovskites ($A_2BB'O_6$) are the finest candidates to investigate as they can accommodate minimum three transition (in *A*, *B* and *B'* position) in their structure. The combinations of *3d*- and *4d*-transition metal in ruthenates are more exciting as *3d*-transition metal shows pronounced electronic ordering and *4d*-transition metal introduces anomalies in electronic properties due to the spin-orbit coupling. Ca_2ScRuO_6, $CaSrScRuO_6$, $CaLaScRuO_{6+\delta}$, Ca_2FeRuO_6, $CaSrFeRuO_6$, Ca_2MnRuO_6 are the recent developed perovskite materials in our group.

Energy storage and conversion driven by electro- or photocatalyst is a highly exciting field of research in an environmentally benign discipline. The present materials work as efficient and robust trifunctional electrocatalyst for ORR/OER/HER followed by four electrons transfer pathway in a strong alkaline medium. Interestingly, the material proficiently works for OER via visible-light driven water splitting at neutral pH in an eco-friendly manner. The dual natures of the designed structural and chemical flexible perovskites are the rare examples of heterogeneous catalysts for the trifunctional activity, accomplished with electro- and photo-chemically. The detail structural, electronic and energy related properties of various perovskites will be explained in the presentation.



Scheme1: Schematic view of energy conversion and storage behavior for present perovskite materials

Keywords: *Double Perovskite; Electrocatalysis; Photocatalysis; Supercapacitor*

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Inversion Symmetry Breaking and Magnetoelectric Properties Induced by Chemical Ordering

A. Sundaresan

Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur Campus, Bangalore 560064, India.

E-mail: *sundaresan@jncasr.ac.in*

Abstract: Combining ferroelectricity and magnetism within a single material remains challenging due to the intricate crystal chemistry and strict symmetry requirements. In conventional ferroelectrics, polarization typically arises from the second-order Jahn–Teller effect, driven by cations with a d^0 or s^2 lone-pair electronic configuration. In contrast, magnetism is usually associated with cations possessing partially filled *d* or *f* electron orbitals. While materials that integrate these two types of cations in distinct crystallographic sites can exhibit multiferroic properties, the coupling between their magnetic and ferroelectric behaviors is often weak. However, certain spin structures can induce weak ferroelectricity below the magnetic ordering temperature in some materials, leading to stronger cross-coupling between magnetism and ferroelectricity. Recent research has explored hybrid improper ferroelectricity, where the interplay between ferroelectricity and magnetism yields promising magnetoelectric properties. In this talk, we introduce a novel class of multiferroics in which polar distortions arise from chemical ordering. These polar oxides exhibit pyroelectric behavior across a broad temperature range and demonstrate magnetoelectric coupling below their magnetic ordering temperatures.

Key words: *Ferroelectricity, Inversion symmetry, Magnetoelectric, Chemical ordering*

Reference:

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Porous Organic Photocatalysts for Energy Conversion

Samrat Ghosh

Inorganic and Physical Chemistry Laboratory, Council of Scientific and Industrial Research
(CSIR), Central Leather Research Institute (CLRI), Chennai – 600020, India.

E-mail: samrat@clri.res.in

Abstract:

Tapping solar energy as chemical energy or fuel is an essential technology for the sustainable society and economy. Solar energy, as an ideal sustainable resource, has significant potential to contribute to the goal of net-zero carbon emissions, if effectively harnessed and converted into a reliable and storable energy carrier. Photocatalysts are the key materials to directly convert sunlight into chemical energy carriers. Fundamentally, photocatalysts are semiconductors with tunable bandgaps, that can absorb light of different wavelengths and drive chemical reactions. In general, photocatalysis is a surface reaction and the reaction rate increases with the increase in the surface area of the photocatalyst.[1] As a result, porous organic photocatalysts have received significant attention due to their high surface area with tunable pore-size, functionality, band gap and band positions. Specifically, covalent organic frameworks (COFs) are one of the emerging porous organic photocatalysts, that are crystalline materials composed of π-conjugated building blocks with micro- and mesopores.[2] Recently, COFs showed promising photocatalytic performance for the hydrogen evolution, carbon dioxide reduction and hydrogen peroxide generation.[3] Typically, COFs are light weight insoluble powders and challenging to process as films. We have developed a relatively easy method to process COFs as thin film photocatalysts.[4] In comparison to suspended powders, thin films of photocatalysts offer inherent advantages such as low light scattering, scalability, easy recovery, and reusability, making them more suitable for practical applications. Additionally, film photocatalysts can provide consistent, quantifiable, and reliable results. As a proof of concept, the COF films were tested for the photocatalytic hydrogen evolution, and it showed significant enhancement in the photocatalytic activity.[5] The mechanistic details were investigated using various analytical and time-resolved spectroscopic method.

Key words: *Photocatalysis, Covalent Organic Frameworks, Green Hydrogen*

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Understanding Ionic Transport and Oxidative Stability of Solid Electrolytes for Solid State Batteries

Ananya Banik[a]* and Wolfgang G. Zeier[b]

[a*] *Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology (TCG-CREST). Sector - V, Salt Lake, Kolkata. India.*

[b] *Institute of Inorganic and Analytical Chemistry, University of Münster, Correnstrasse 30, 48149 Münster, Germany.*

Email: ananya.banik@tcgcrest.org

Abstract:

Solid electrolytes with high ionic conductivity and expansive electrochemical stability windows are central to developing solid-state batteries. In my presentation, I will focus on the critical aspect of solid electrolyte design concerning the (electro)-chemical stability and structure-transport correlation, which can help to understand solid-state battery failure and hence can help designing high-capacity solid-state batteries with long cycle life. Specifically, I will discuss the (electro)-chemical stability of argyrodite solid electrolyte, one of the most explored solid electrolytes in solid-state batteries, by understanding chemical bonding, which can shed light on the solid-state battery failure mechanism associated with (electro)-chemical degradation of the solid electrolyte. Next, I will focus on the structural understanding of lithium halide ionic conductors, a potentially stable alternative to argyrodite solid electrolyte as catholyte. Understanding the structural complexity of halide electrolytes along with the (electro)-chemical stability of argyrodite solid electrolytes will advance the solid electrolyte design for solid-state battery development.

Key words: *Solid state batteries, solid electrolytes*

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Miracle of Impurity Level Doping to Design Ultralong Afterglow Materials

Dr. Bibhisan Roy

Department of Chemistry, HNB Garhwal University (A Central University), Uttarakhand

Email: bibhisanroy90@gmail.com

Abstract:

Room-temperature phosphorescence (RTP) materials have been an attention gainer, owing to their potential applications in various fields such as information storage, encryption, organic light-emitting diode (OLED), sensing, biological imaging, and more. Traditionally, the RTP materials often incorporated platinum, iridium and other heavy metals for boosting the spin orbital coupling (SOC) for populating the triplet states and achieving efficient phosphorescent emission. However, the toxicity of the heavy metals, and their higher production cost pose a significant challenge in realizing their triplet energy for real life application. Purely organic RTP materials are widely recognized as the modern alternative to heavy metal-based phosphors. The organic RTP molecules, especially that are smaller in dimension, are relative cheap, easier to fabricate and are often compatible with the green visions of the current age. Various strategies are employed to rectify the poor SOC and stabilizing the unstable triplet excitons of organic molecules, and thereby activating the long persistent phosphorescence emission. Among the numerous endeavors to achieve organic phosphorescence emission, the host guest doping and co-crystallization techniques are intriguing. In the **Host-guest doping**, the target guest molecule is embedded within a stable host matrix in minimal concentrations. **Co-crystallization**, another effective method in which target molecule is co-crystallized with a donor or acceptor partner molecule. Both these techniques are highly effective in stabilizing the triplet excitons by creation of a rigidified environment through various intermolecular interactions. Such rigidification isolates the phosphors from quenching elements, thereby enabling the room temperature applications. Intriguing involvements of the host matrix or the donor or acceptor partner species are often observed in enhancing the phosphorescence emission or even activating a radiative triplet pathway of a non-phosphorescent molecule. By utilizing these strategies and careful molecular engineering, we are motivated in development of organic RTP systems with high energy blue shifted phosphorescent emission and Near Infrared region (NIR) phosphorescent emission that are rarely observed. The pursuit of blue shifted and NIR-emitting organic RTP systems holds promise for revolutionizing various technological applications.

Key words: *Phosphorescence, triplet states, afterglow etc.*

Reference:

[1] Dr. Bibhisan Roy, Dr. Iván Maisuls, Jianyu Zhang, Dr. Felix C. Niemeyer, Dr. Fabio Rizzo, Dr. Christoph Wölper, Dr. Constantin G. Daniliuc, Prof. Dr. Ben Zhong Tang; *Angew. Chem. Int. Ed.* doi.org/10.1002/anie.202111805

Inorganic Nanomaterials for the H_2 Generation and Storage

Minyoung Yoon

KNU G-LAMP Research Center, KNU Institute of Basic Sciences, Department of Chemistry,
Kyungpook National University, Daegu 41566, South Korea.

E-mail: *myyoon@knu.ac.kr*

Abstract:

Due to global climate change, using non-carbon sources as an energy source is required, and H_2 can be a candidate to replace fossil fuels. Considering the full cycle of H_2 technology, production, delivery/storage, and utilization are critical issues to tackle. Considering production, current production is mainly dependent on fossil fuel-dependent technology. For the efficient generation of H_2, new catalytic materials should be developed. In this work, we will present two novel strategies: 1) incorporation of organometallic catalysts in metal-organic frameworks (MOFs) for confinement effect and 2) hybridizing a conventional nanocatalyst (NiS) in a porous scaffold for utilization of synergetic effect of hybrid nanocatalyst and porous support (diatom). The novel strategies allow for increasing the catalyst's long-term stability and efficiency compared to conventional materials. In addition, new technology should be developed to facilitate the delivery and storage of H_2. Unlike the generation of H_2, the storage process requires the development of storage media (liquid organic hydrogen carrier; LOHC) and hydrogenation/dehydrogenation catalysts. A novel organic media, methylbenzyl naphthalene (MBN), was newly prepared on a large scale (> 10 g). For the storage and extraction of H_2, new Pt and Ru nanocatalysts were developed for hydrogenation and dehydrogenation, respectively, was developed. The MBN showed the lowest dehydrogenation enthalpy among homocyclic LOHC media, which allows facile dehydrogenation of the media. In addition, further works will also present the doping of sulfur elements on Pt on TiO_2 for efficient and selective dehydrogenation of MBN. Despite the fundamental understanding, the new materials may provide a unique opportunity for H_2 energy utilization.

Keywords: *Metal-organic frameworks, Breathing, CO_2 adsorption, Pollutant removal, Direct air capture*

Buckling and Defects in Two - Dimensional Atomically Thin Monolayers

Ayan Datta

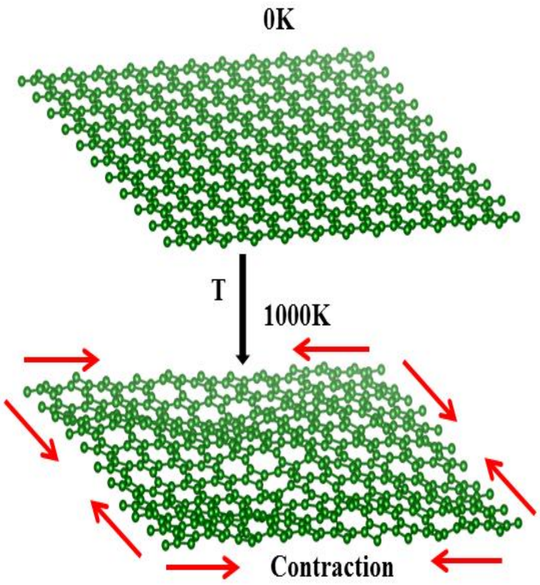
School of Chemical Sciences, Indian Association for the Cultivation of Science (IACS), Kolkata – 700032, India.

Email: *spad@iacs.res.in*

Abstract:

Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, MoS_2, germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold particularly in its local reactivity to halogens and hydrogens along the more ~sp^3 atoms. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture.

Keywords: *Inorganic Graphene; Vibronic effects; Excited States; DFT.*



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Paired Electrocatalysis with Functional Heterostructures: Simultaneous Generation of Fuels and Value-added Chemicals

C. Retna Raj

Functional Materials and Electrochemistry Lab, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur-721302

Email: crraj@chem.iitkgp.ac.in

Electrocatalyst plays a vital role in electrochemical energy conversion technologies. Studies on most of the existing electrocatalytic reactions including hydrogen evolution, oxygen reduction, carbon dioxide reduction, etc. focus on the cathode half-cell. Due to sluggish electron transfer kinetics at the anode half-cell reaction, the cathode reactions largely suffer from a high energy barrier. Pairing the cathodic reaction with a thermodynamically readily accessible anode reaction is a promising approach to decreasing the cell voltage and increasing the energy efficiency. Such pairing has the additional advantage of producing value-added chemicals at the anode when the anode counterpart is rationally selected. We synthesized electrocatalytically active functional heterostructures based on transition metal phosphide, sulfides, etc., and demonstrated their electrocatalytic performance towards hydrogen evolution and ammonia generation at the cathode. The half-cell reaction at the cathode is paired with the anode half-cell reaction to simultaneously generate hydrogen/ammonia and value-added products and increase energy efficiency.

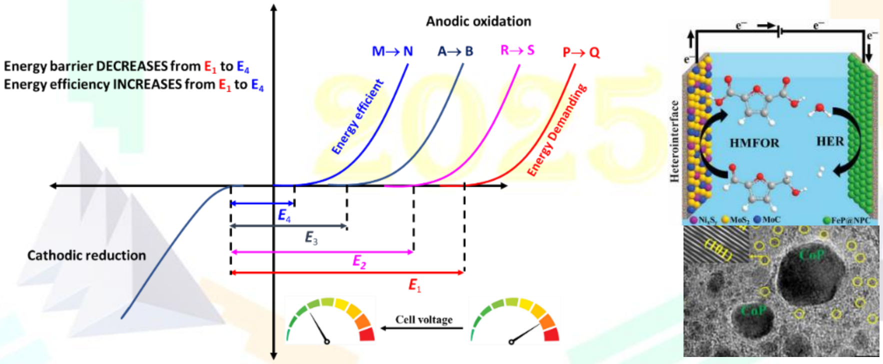

Fig. 1. Schematic illustration of paired electrocatalysis showing the energy-demanding and energy-efficient reactions. Inset: TEM image of the functional heterostructure (CoP@NC-Ru).

Keywords: *Electrocatalyst; Heterostructure; Transition metal phosphide; Energy efficiency*

Reference:

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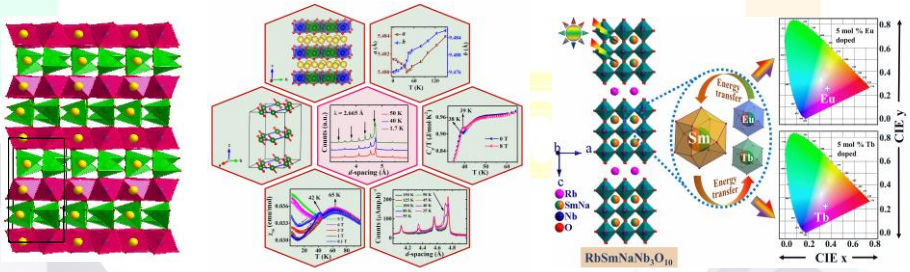
Functional Inorganic Solids Built on Solid-State Concepts

Professor S. Uma
Senior Professor, Materials Chemistry Group, Department of Chemistry, University of Delhi, Delhi-110007
E-mail: *suma@chemistry.du.ac.in*

Abstract:

Synthesis of novel solids by a variety of approaches combined with careful structural evaluation is the essential step to understand the structure property relationship, in order to target the materials for various applications. The search for functional materials ranges from electrodes, electrolytes for the various rechargeable batteries, for second harmonic generation, dielectric, ferroelectric, inorganic pigments, catalysts, and photocatalysts that are necessary to provide a cleaner, greener energy, and environment. We have been focusing on the exploratory approach by systematically screening the phase diagrams along with the careful cationic and/or anionic modifications in the existing structures. The identification of new phase formation and confirmation of their structures is a rigorous exercise and, in several instances, unusual results are obtained and will be presented in this talk. Alternately, synthesis of the solids by rational designing is possible in certain cases and appropriate examples will be shared to emphasize the significance of the alternate preparative methods. The broader materials aspects of these materials particularly based on a variety of mixed metal oxides will be presented as shown by various application-oriented characterization techniques.



Key words: *Mixed metal oxides, X-ray diffraction, honeycomb ordering, layered perovskites, polar materials.*

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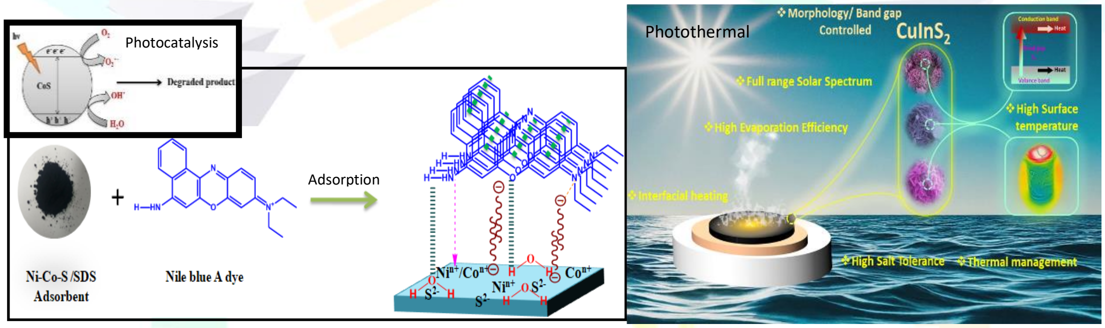
Metal Chalcogenides with Tunable Phase, Bandgap and Surface Properties for Adsorption, Photocatalytic and Photothermal applications

Sahid Hussain

Department of Chemistry, Indian Institute of Technology Patna, Patna 801 106 and
Email:sahid@iitp.ac.in

Abstract: Adsorption photocatalysis and photothermal effect are of great interest due to their applications in environmental and energy issues. TiO_2 was the first semiconductor photocatalyst which was applied and was only active under ultraviolet light due to its wide band-gap.[1] In order to utilize the solar spectrum, tailoring of band-gap is invoked as one of effective techniques. On the other hand, the surface properties may be tuned with the ratio of precursors, ligands, surfactants and reaction conditions. One of the current challenges is to synthesize photocatalysts, adsorbents and photothermal materials with desired band-gap, phase and surface properties via novel and benign protocol with controlled shape and size.



Herein, we report the environmentally benign route for the synthesis of binary and multinary chalcogenides like NiS, CoS, Bi_2S_3, Ni-Co-S, $ZnIn_2S_4$, $CuBiS_3$, $CuInS_2$with tunable, phase, band-gap and surface properties.[2-6] The band-gap was evaluated and found to be in the range of energy of visible and NIR. The absorption of light leads to the generation of electron and holes leading to generation of reactive species and heat due to nonradiative relaxation. While evaluating zeta potential, it was found that the materials showed both positive and negative charge on the surface which makes adsorption possible for cationic and anionic dyes. Thus, these chalcogenides can find practical application in adsorption and degradation of organic dyes, and photothermal interfacial water evaporation.

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Manipulating Copper Homeostasis with Small Molecules and Light to Control

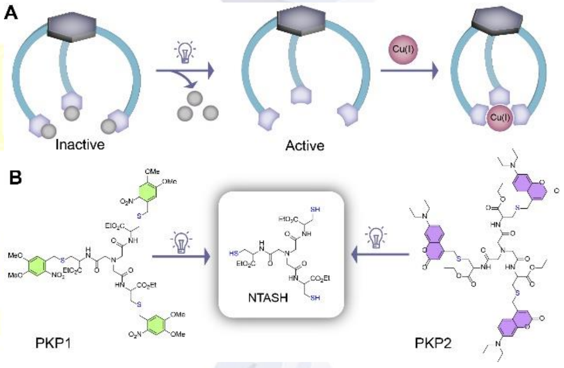
Dr. Debasish Manna

Department of Chemistry, IISER Bhopal.

Email: dmanna@iiserb.ac.in

Abstract: Copper is an essential trace element that plays important roles in various cellular processes, such as enzyme activity, protein folding, and cell signaling. To maintain the proper concentration of Cu(I) inside cells, cells have evolved a complex system of transport proteins and chaperones that tightly regulate the uptake, distribution, and efflux of Cu ions. Copper ions enter cells through specific copper transporters, such as CTR1 (Copper Transporter 1) and ATP7A (Copper Transporter ATPase 7A), which are localized at the plasma membrane. Once inside the cell, copper ions bind to chaperones, such as Atox1 and CCS (Copper Chaperone for Superoxide Dismutase), which then transport the copper ions to the specific enzymes that require them. To prevent the accumulation of toxic levels of copper ions, cells also have efflux transporters, such as ATP7B) and ATP7A, which pump copper ions out of the cell, and back into the extracellular space.

Failure to maintain the optimum copper concentration sometimes occurs and may lead to fatal pathological disorders. Change in Cu concentration in either direction can lead to various disease states. For example, accumulation of excess copper can lead to Wilson's disease, induces cuproptosis via aggregation of lipoylated proteins, and loss of iron–sulfur clusters resulting in proteotoxic stress and ultimately leading to cell death. On the other hand, deficiency of copper, leads to Menkes disease. Copper-specific chelators are used for the treatment related to copper accumulation. Copper accumulation, being organ specific, necessitates the development of a new generation of Cu chelators having tissue specificity or organ selectivity. We have developed a photocaged chelator which can chelate copper and remove the excess copper from the system only after exposure to a suitable wavelength of light. This gives us an additional layer to control to activate the chelator in a spatiotemporal manner and to gain tissue specificity. In addition, we have also designed a photocleavable copper complex to induce cuproptosis upon light exposure.



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Multi-stack dye oligomers and their folding behavior

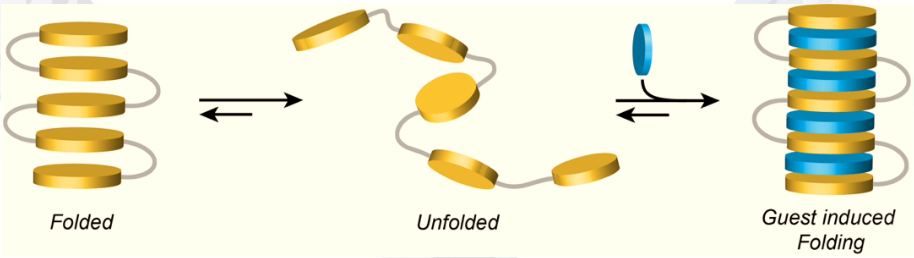
Bappaditya Gole

Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence Deemed to be University, Greater Noida, Uttar Pradesh 201314, India.
Email: bappaditya.gole@snu.edu.in

Abstract:

The cofacial stacking of planar π-conjugated molecules through π–π interactions is crucial for the structural integrity and functions of biomacromolecules such as DNA and proteins. It also plays a key role in dye assembly and the development of supramolecular self-assembled materials. Notably, it underpins the performance of optoelectronic organic devices, where close stacking of aromatic π-systems facilitates effective charge carrier mobility through significant orbital overlap, resulting in high-performance conductive materials. Most often, the long-range organization of the dyes is impacted by weak dispersion interactions, which are less suitable to drive specific arrangements among the monomers, therefore limiting extended intermolecular electronic communication. As an alternative, chemists have developed strategies such as dye aggregation,[1] incorporation into oligonucleotide backbones,[2] and covalently linked dye oligomers that fold and self-assemble via noncovalent interactions.[3] Among these, discrete dye oligomers with a defined number of stacked aromatic units have drawn significant interest due to their well-defined folding behavior, enabling precise control over π–π interactions and tunable photophysical properties for functional applications.[4] In this presentation, I will introduce a synthetic strategy to obtain larger dye oligomers and control their folding behavior, which is sometimes influenced by guest molecules with complementary electronic properties. Additionally, I will discuss some of their exciting photophysical properties.

Key words: *Foldamer, dye assembly, oligomers, optoelectronic materials*



Scheme 1. *Schematic representation showing folding and unfolding behavior of dye-oligomers induced by guest interaction.*

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Insights into Catalyst Development for Liquid-Organic Hydrogen Carriers in Hydrogen Energy Storage

Purna Chandra Rao, Younghu Son, Minyoung Yoon*

KNU G-LAMP Research Center, KNU Institute of Basic Sciences, Department of Chemistry,
Kyungpook National University, Daegu 41566, South Korea.

E-mail ID: purna@knu.ac.kr

Abstract:

Hydrogen is a clean energy carrier with a high energy storage density of 120 MJ Kg^{-1}, significantly higher than gasoline's 44 MJ Kg^{-1}. It can protect the environment with zero emissions, contributing to mitigating global warming. Hydrogen storage and transportation through liquid-organic hydrogen carriers (LOHCs) is potentially safer than conventional or other material-based storage methods and is also compatible with existing fuel infrastructure. LOHCs are liquid-phase, unsaturated molecules that can store and release H_2 through catalytic hydrogenation and dehydrogenation reactions. Compared to exothermic hydrogenation reactions, the endothermic dehydrogenation process plays a key role as it requires a high heat demand to release the hydrogen.[1] To implement this technology, the scientific community is highly focused on two major parameters: 1) designing suitable homocyclic and heterocyclic LOHC media that meet the required characteristic properties, and 2) developing efficient single catalysts on heterogeneous supports, considering ease of synthesis, sustainability, catalytic activity, and production cost for practical purposes. In this work, we present, for the first time, a novel methylbenzyl naphthalene (MBN), which is an example of a homocyclic LOHC medium with a high storage capacity of 6.49 wt.% and the lowest dehydrogenation enthalpy (<56 kJ mol^{-1} H_2^{-1}). The reversible hydrogen storage has been studied using freshly prepared Ru- and Pt-based heterogeneous catalysts. Additionally, theoretical calculations were evaluated to understand the dehydrogenation enthalpy and compare it with existing LOHC compounds.[2,3] Secondly, we present the development of a single Ni-Pd bimetallic catalyst on a silicon-carbon nitride (SiCN) support for quinoxaline and 2-picoline *N*-heterocyclic LOHC systems. The synthesis strategy, synergistic effect, and cost-effectiveness of Ni-Pd bimetallic nanocomposite catalysts were studied in *N*-heterocyclic LOHC media.[4]

Keywords: *Hydrogen storage, liquid-organic hydrogen carriers, heterogeneous catalyst*

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Atomistic Insights into Electrochemical Heterogenous Catalysis: A Potential-Dependent Model

Kalishankar Bhattacharyya

Department of Chemistry, IIT Guwahati, Assam-781039, India

Email: ksb@iitg.ac.in

Abstract: Modeling heterogeneous catalysts under electrochemical conditions presents significant challenges, particularly in unraveling the atomistic details of catalytic reaction mechanisms. In this talk, we introduce a novel methodology that explicitly incorporates the effect of potential to simulate structural changes in catalysts and their impact on reaction mechanisms under varying electrochemical environments. Using this approach, we demonstrate how Fe impurities influence the oxygen evolution reaction (OER) mechanism on cobalt (oxy)hydroxide catalysts, revealing that tuning the acidity of active sites can lead to diverse chemical pathways. Additionally, the role of Fe spin states in modulating the OER mechanism on 2D graphene-based structures will be discussed. This talk will highlight the broader applications of this methodology, offering new insights into the atomistic underpinnings of electrochemical reactions.

Key words: *Density Functional Theory*, *Heterogenous Catalysis*, *Electrochemistry*

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The Weyl Semimetals *M*IrTe$_4$ (*M* = Nb, Ta) as Efficient Catalysts for Hydrogen Evolution

Manisha Samanta

Department of Chemistry, IIT Gandhinagar, Palaj, Gujarat 382355, India
Email: manisha.samanta@iitgn.ac.in

Abstract:

The prevalent global energy crisis calls for searching viable pathways for generating green hydrogen as an alternative energy resource. Dye-sensitized photocatalytic water splitting is a feasible solution to produce green hydrogen. However, identifying suitable catalysts has been one of the bottlenecks in driving dye-sensitized photocatalysis efficiently. In this work, we report a new class of electrocatalysts based on the layered Weyl semimetals *M*IrTe$_4$ (*M* = Nb, Ta) for the Eosin Y (EY)-sensitized hydrogen evolution reaction (HER). NbIrTe$_4$ and TaIrTe$_4$ exhibit HER activities of ~18000 and 14000 µmol g^{-1} respectively, after 10h of irradiation with visible light. Time-dependent UV-Vis spectroscopy and high-pressure liquid chromatography coupled with mass spectroscopy analysis shed light on the reaction dynamics and enable a deeper understanding of the observed trend in hydrogen evolution rates for *M*IrTe$_4$. *M*IrTe$_4$ semimetals outperform transition metal-based Weyl semimetals in terms of catalytic HER activity using EY as photosensitizer and triethanolamine as the sacrificial agent. We hypothesize that the topology-related band inversion in *M*IrTe$_4$ Weyl semimetals promotes a high density of *M d*-states near the Fermi level, driving their high catalytic performance. This study introduces a new class of layered Weyl semimetals as efficient catalysts, and provides perspectives for designing topology-enhanced catalysts.

Key words: Hydrogen Evolution, Catalysis, Weyl Semimetals, Metal *d*-Band Density, Metal Chalcogenides

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Solvated Metal Atom Dispersion and Digestive Ripening – Duo *par excellence* for Diverse Nanostructured Materials

Balaji R. Jagirdar

Department of Inorganic & Physical Chemistry, Indian Institute of Science, Bangalore 560 012,
Email:jagirdar@iisc.ac.in

Abstract:

The properties of nanostructured materials strongly depend on their size, shape, interparticle distance, and the surrounding environment which could be tuned precisely by controlling the particle size of the material. Size dependent property of a polydisperse sample is an average effect due to the presence of different sized particles in the system. The property exhibited by a monodisperse sample however, could be ascribed as emerging from a single entity. Control over size and size distribution is indispensible for attaining a desired property. A lot of attention is focused on developing synthetic strategies leading to monodispersity and those that are simple to manipulate, easy to scale up and highly reproducible.

We have been using the Solvated Metal Atom Dispersion (SMAD) method for the synthesis of colloids of metal nanoparticles. The as-prepared colloid from this method consists of polydisperse metal nanoparticles. In a process termed as *digestive ripening*, addition of a surfactant to the as-prepared sample renders it highly monodisperse. This combination, SMAD and digestive ripening has recently been extended to obtain nearly monodisperse semi-conductor nanostructured materials as well. In this talk, the power of the SMAD and the (co)digestive ripening processes will be demonstrated toward the synthesis of highly monodisperse metal, core-shell, alloy, intermetallic, and composite nanostructured materials. Additionally, applications of some of the materials synthesized using this methodology in the fields of hydrogen storage and generation, magnetism, catalysis, and surface enhanced Raman scattering will also be discussed.

Keywords: *Nanoparticles, colloids, digestive ripening, Ostwald ripening, electron microscopy*

Phonon-Glass Electron-Crystal like High Performance Thermoelectrics

Kanishka Biswas

New Chemistry Unit & International Centre for Materials Science, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore 560064 (India)
Email: kanishka@jncasr.ac.in

Achieving glass-like ultra-low thermal conductivity in crystalline solids with high electrical conductivity, a crucial requirement for high-performance thermoelectrics, continues to be a formidable challenge. A careful balance between electrical and thermal transport is essential for optimizing the thermoelectric performance. Despite this inherent trade-off, the experimental realization of an ideal thermoelectric material with a phonon-glass electron-crystal (PGEC) nature has rarely been achieved. We demonstrated high thermoelectric performance with a near room-temperature figure of merit, zT ~1.5 and a maximum zT ~2.6 at 573 K by optimizing atomic disorder in Cd doped polycrystalline $AgSbTe_2$.[1, 2] Cadmium doping in $AgSbTe_2$ enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity via spontaneous formation of nanoscale (~2-4 nm) superstructures. Recently, we showed that isovalent Yb-doping induced enhanced atomic ordering decreases the overlap between the hole and phonon mean free paths and consequently leads to a PGEC-like transport in $AgSbTe_2$. A twofold increase in electrical mobility is observed while keeping the position of the Fermi level nearly unchanged and corroborates the enhanced crystalline nature of the $AgSbTe_2$ lattice upon Yb doping for electrical transport, which leads to zT ~2.4 at 573 K. These achievements highlight the potential of our approach in enhancing the thermoelectric performance of the material by tuning its inherent atomic disorder which can be applicable to other thermoelectric materials.[4]

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Factors Influencing Anodic Oxidation Reactions

Sounak Roy

Birla Institute of Technology & Science, Pilani Hyderabad Campus, Jawahar Nagar, Kapra Mandal, Dist.-Medchal-500 078, Telangana, India.

Email: sounak.roy@hyderabad.bits-pilani.ac.in

Abstract:

The transient quality of the primary feedstock has prompted the sustainable advancement of the H_2 economy. By means of an electrochemical process, water electrolyzers can transform water into the energy medium H_2. Nevertheless, the hindrance in this technology lies in the tardy anodic oxygen evolution reaction (OER), which is caused by significant kinetic energy barriers and resulting in high overpotentials. As a result, the pursuit for low-cost and durable anodic materials with high OER activity and low overpotential has gained greater scientific attention. The efficacy of OER reaction over metal oxides have been extensively studied and correlated with the descriptors like surface oxygen vacancy, metal–oxygen covalency vis à vis electrical conductivity, transition-metal *d*-electron count and the e_g occupancy. The field thus stands to benefit greatly from understanding the relationships among descriptors and identifying the most influential one(s). The presentation would address the recent development from our group on understanding the metal oxides towards Anodic Oxidation Reactions in light of the above descriptors. [1-4]

Key words: *Electrocatalysis, Descriptors, Oxygen Evolution Reaction*

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Rhodamine dyes as chemosensors for various metal ions

Partha Roy

Department of Chemistry, Jadavpur University, Jadavpur, Kolkata 700032, India and

Email: partha.roy@jadavpuruniversity.in

Abstract:

Detection of trace amount of metal ions is of great importance to the researchers of chemistry, biology, environmental science, industries, *etc*. as the cations play very important roles in different chemical and biological processes. They are beneficial for living being when they are present within a certain limit. However, they create various health related issues when they are present in excess and/or deficient amount. The metal ions are detected by different methods including by using fluorescent chemosensors. The chemosensors offer a number of advantages such as high selectivity, high sensitivity, simple analysis, low cost, *etc*. Designing of chemosensors from rhodamine fluorophore is of significant interest to the researchers because of their high molar extinction coefficient, good photostability, large quantum yield, and long excitation and emission wavelength, ease of signal modulation, *etc*.[1] Rhodamine derivatives are colorless and almost nonfluorescent when the spirolactam ring is in closed form. They become pink and highly fluorescent when the ring is opened upon interaction with the metal ions. Substitutions among different factors play crucial role in the metal ion selectivity. The focus of this talk will be on the various rhodamine derivatives[2] which are used in different metal ion sensing and applied in different fields.

Key words: *Chemosensors; Rhodamine: Fluorescence; Colorimetric*.

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An accelerated computational methodology to compute diverse varieties of finite temperature properties of solid materials

Pinku Nath[a], Yuki Ide[a], Jose. J. Plata[c], Yasuhide Inokuma[a], Masaharu Yoshioka[b]

[a] Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo001-0021, Japan

[b] Graduate School of Information Science and Technology, Hokkaido University, Kita 14, Nishi 9, Kita-ku, Sapporo, Hokkaido, 060-0814, Japan

[c] Departamento de Química Física, Facultad de Química, Universidad de Sevilla, Seville 41012, Spain

E-mail:* *pnath@icredd.hokudai.ac.jp

Abstract:

Accurate computations of the finite temperature properties are computationally intensive processes. Simultaneously calculating thermodynamic, mechanical, and thermal transport properties can greatly increase the computational cost. Usually, different computational setups are required to predict these three types of properties or domains. Moreover, the information generated while computing one domain is generally not utilized in the other two. Besides the high computational cost, traditional methodologies often overlook the need for incorporating high-temperature corrections that stem from the anharmonicity of the material. To tackle these challenges, an automated and accelerated computational framework has been developed to enable the computation of finite properties of the three above-mentioned domains simultaneously. This new approach utilizes interdomain data efficiently and combines accelerated methodologies such as machine learning regression for the extraction of high-order force constants and the quasi-harmonic three-phonon method to reduce the computational cost without compromising accuracy [1-4]. Temperature-dependent phonons are included in the calculation to include strong anharmonic effects. The methodology can be used with either classical interatomic potential or DFT-based codes.

Keywords: *quasi-harmonic, anharmonicity, elastic constants, thermodynamic, thermal conductivity*

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Mono-, Di- and Tetranuclear Lanthanide (III) Complexes as Molecular Magnets

Vadapalli Chandrasekhar
Tata Institute of Fundamental Research Hyderabad, Hyderabad-500 046, India
Email: vc@tifrh.res.in

In this talk we will present some synthetic strategies that allow a rational assembly of lanthanide complexes with varied nuclearity. Specifically, we will examine the synthesis of mono- di- and tetranuclear complexes (Figure 1). The ligand design and usefulness of specific ancillary ligands for the preparation of such complexes will be presented. The structural characterization and magnetic properties of these families of lanthanide complexes will also be discussed.

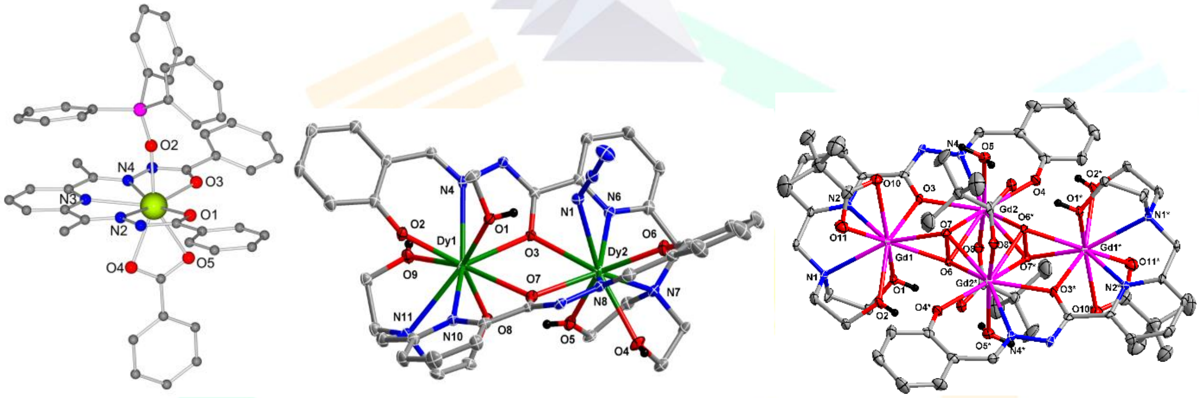

Figure 1. Molecular structures of representative examples of mononuclear (left), dinuclear (middle), and tetranuclear (right) lanthanide complexes.[1-3]

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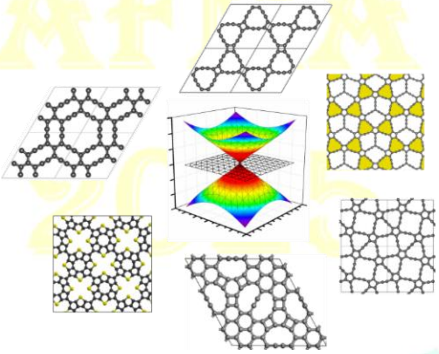
Computational Studies on the Design and Development of Carbon based Novel Two-Dimensional Dirac Materials

V. Subramanian

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600 036, India.

Email: *subramanianv@iitm.ac.in*; *subuchem@hotmail.com*

Abstract: In this study, we have proposed a series of novel 2D Dirac carbon allotropes with the aid of density functional theory-based first-principle calculations. The presentation gives a brief account on the different carbon allotropes, two-dimensional (2D) materials, Dirac materials[1,2] and their electronic prospects. Further, I will also discuss about the structural and electronic properties of some of the novel 2D Dirac materials which mainly include α-2 graphyne,[3] β-graphyne analogues, butterfly-graphyne, coro-graphene, circumcoro-graphyne,[4] cp-graphyne,[5] sulflower based quasi-planar 2D porous networks. In addition to these, another novel 2D material known as acetylene-mediated borophosphene and its potential as an anode material in lithium-ion batteries will be addressed.[6] In particular, the energetics of proposed 2D materials, structural properties, dynamical and thermal stabilities, mechanical stability, energetic favorability for the experimental synthesis, effect of the nanoconfinement, strain, doping and extremal electric field on the Dirac electronic dispersion will be addressed.



Key words: *2D Materials, Dirac Materials, Carbon allotropes and Anode Material*

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Confluence of Molecular and Nanomaterial Metal Phosphate Chemistry for Energy Applications

Ramaswamy Murugavel

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076

Email: rmv@chem.iitb.ac.in

Reaction of phosphonic acids and phosphate monoesters with a divalent metal such as Zn^{2+} in a donor solvent (L) leads to the isolation of tetranuclear metal phosphates $[(R)PO_3Zn(L)]_4$ (R = alkyl/aryl or alkoxy/aryloxy), whose inorganic core resembles the zeolitic D4R secondary building units (SBUs).[1,2] In recent times, we have unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions.[3] On the other hand, the reactions of phosphoric acid esters yield either 1-D or 2-D materials which thermally anneal below 300 ^{o}C to produce ceramic nanomaterials.[4,5] Rationalization of building principles along with the use of this class of compounds for energy applications will be highlighted in this lecture.

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Catalytic activity of phosphine ligated Pd complexes

Raja Mitra

School of Chemical and Materials Sciences, Indian Institute of Technology Goa, Goa-403401, India.
Email: rajamitra@iitgoa.ac.in

Abstract:

The appropriate tuning of ligand electronic and steric properties can effectively control product selectivity and enhance catalytic activity. Literature indicates that Ad_2P (where Ad refers to adamantyl) offers improved stability to the catalytic system, attributed to the steric bulk of the adamantyl groups. By maintaining the Ad_2P framework, we developed several innovative ligand systems based on P^N/P^C coordination modes. The newly synthesized ligands exhibit smaller bite angles compared to Xantphos. However, the catalytic activity of these complexes demonstrated that they were not suitable for C–N cross-coupling reactions. In contrast, all ligands proved to be effective in Pd-catalyzed C–C cross-coupling reactions.

During the development of a catalytic system for the C–N cross-coupling reaction, we discovered that the $Pd_2(dba)_3$/Xantphos catalytic system effectively promotes the exclusive formation of triarylamines from aryl bromides and $NaNH_2$ under optimized conditions. Aryl bromides with *para* or *meta* substitutions yield moderate to excellent amounts of triarylamine products, whereas *ortho*-substituted aryl bromides predominantly lead to diarylamine products. Mechanistic investigations and control reactions indicate that triarylamine formation occurs through three sequential C–N coupling reactions between the aryl bromide and $NaNH_2$.

Key words: *Catalysis, Pd, Phosphines, Mechanistic investigation*

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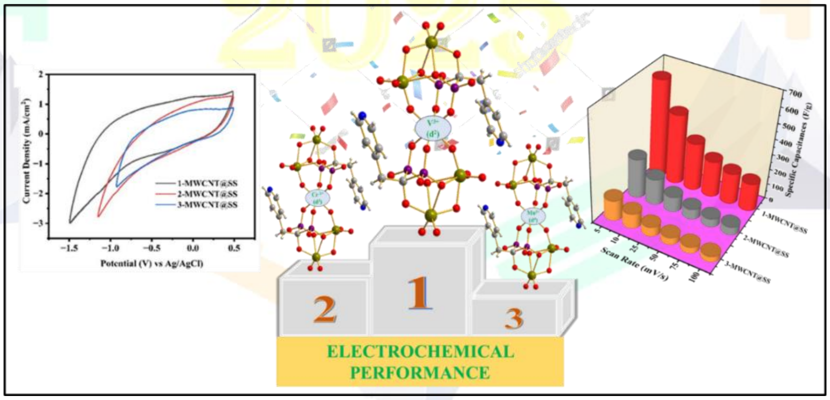
Investigations into the Electrochemical Energy Storage Properties of Diphosphonate derivatives of Oxo-vanadates: Experiment and Theory

Dr. Abhishek Banerjee

Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur
Email: abhishekbanerjee@chm.vnit.ac.in

Abstract: Electrochemical supercapacitors have become popular and pivotal as energy-storing devices; having immense potential along with remarkable properties, like excellent fast charging capacity, high power density, and long-lasting cyclic stability. Vanadates, with their unique redox and coordination properties, have also found important applications energy storage. Oxo-vanadates with diphosphonate ligands, are a relatively newer class of materials. Such ligands are observed to stabilize multiple oxidation-states of the metal in the same complex, making them extremely versatile electrochemically. From our studies with mixed-metal molybdate complexes, $[(\mathrm{Mo^{VI}}_2\mathrm{O_5})_2(\mathrm{MO_2})\{\mathrm{O_3P\text{-}C(O)(CH_2\text{-}4\text{-}C_5NH_4)\text{-}PO_3}\}_2]^{7-}$ [where M = V(III), Cr(III), Mn(III)], we have observed highest efficiency with the molybdenum-vanadium systems, exemplifying the better redox activity of vanadium. Our subsequent studies with mixed-valent vanadates $[(\mathrm{V^{IV}O_2})(\mathrm{V^{V}}_2\mathrm{O_5})_2\{\mathrm{O_3P\text{-}C(O)(CH_2\text{-}n\text{-}C_5NH_4)\text{-}PO_3}\}_2]^{10-}$ (n = 2, 3), and shows greater electrochemical efficiency with respect to the mono-valent vanadate complex $[(\mathrm{V^{IV}O})_3(\mathrm{O})\{\mathrm{O_3P\text{-}C(OH)(CH_2\text{-}4\text{-}C_5NH_4)\text{-}PO_3}\}_3]^{8-}$. Furthermore, presence of encapsulated guest molecules within the capsular assemblies of the complexes $[(\mathrm{V^{V}O})_2(\mathrm{V^{IV}}_4\mathrm{O_8})_2\{\mathrm{O_3P\text{-}C_6H_4\text{-}PO_3}\}_4]\subset 2\mathrm{H_2O}]^{10-}$ and $[(\mathrm{V^{V}O})_2(\mathrm{V^{IV}}_4\mathrm{O_8})_2\{\mathrm{O_3P\text{-}C_6H_4\text{-}C_6H_4\text{-}PO_3}\}_4\subset 2\mathrm{DMF}]^{10-}$ creates significant differences in their electrochemical performances.



Keywords: Oxo-vanadates, Supercapacitor, electrochemistry, energy storage.

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Supramolecular Liquid Crystalline Alkoxy Azopyridine Derivatives Showing Photoresponsive Property

Susanta K. Nayak

Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur,
Maharastra-440010, India

Email: sknayak@chm.vnit.ac.in

Abstract:

Liquid Crystals (LCs) are the family of soft materials that combine the anisotropy of crystalline solids and agility of liquids, which may show extraordinary technological potential. LCs have been used in display technology due to their sensitivity to electric field as well as magnetic field [1]. Azopyridine derivatives, in particular, have attracted interest due to their remarkable reversible *trans-cis* photo-isomerization under the influence of light. [2] The liquid crystalline behaviour of these materials can be fine-tuned through either covalent approach using different substitutions or by utilizing various non-covalent interactions. [3] Non-covalent interactions, such as hydrogen bonding (HB) [4] and halogen bonding (XB), [5] are widely employed in fabricating these materials because they can be prepared under ambient conditions with typically high yield. The hydrogen-bonded liquid crystalline materials have proven to be useful in tuning the mesomorphic phase transition by slightly modifying the hydrogen bond donors, resulting in various structural features. [6] In this context, alkoxyazopyridine derivatives have been synthesized by varying the alkyl chain length and complexed with hydrogen bond donor. The alkoxyazopyridine ligands were non-mesogenic whereas their hydrogen-bonded complex displayed liquid crystalline behaviour. Further, the photoresponsive property of the synthesized compounds was evaluated using UV-Vis spectroscopy.

Key words: *Photoresponsive, Liquid crystals, and supramolecular chemistry*

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The Fascinating World of Smart Materials (P-1)

Nerle Umadevi V[1]

Abstract:

Smart materials are suitable for harvesting biomechanical energies from human motions, environment or body heat, or shaping of biofuel powered devices. This will open up the horizon for Nano energy nanosystems that can themselves act as self-powered sensors or be utilized as power sources for other integrated transducers. Wearable and implantable technologies are contributing to a transformation in the mobile health era in terms of improving healthcare and health outcomes and providing real-time guidance on improved health management and tracking. Smart materials offer a significant role in on our lives covering various sensing and actuation applications in healthcare due to their responsivity to external stimuli such as stress, light, temperature, moisture or pH, and electric or magnetic fields. This work, gives an insight to the state-of-the-art micro/nano-systems that are proposed for implantable and wearable diagnostic, therapeutic and treatment applications. The unique property of these systems apart from the flexibility or conformability of the transducers (i.e. sensors and actuators) and the uniqueness of their building materials, is their integration with various types of energy harvesters that makes the whole system self-sustained or battery-free.

Key words: *Smart Material, Healthcare, Battery free.*

Reference:

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Physics, KLE Society's, *Shri Kadasiddheshwar Arts College & HSKotambri Science Institute*Vidyanagar, Hubballi-580031, Karnataka State, India

(Accredited by NAAC at 'A+' Grade with 3.28 CGPA in fourth cycle)
(KARNATAK UNIVERSITY DHRWAD)

([#]:Presenting Author; nerleuma28@gmail.com, [*]:Corresponding Author; nerleuma28@gmail.com)

Morphological Induced Control on Antioxidant Activity of Self-Assembled Cyclic Dipeptide of Tryptophan (P-2)

Vijay M[1], Shreya Pande[2], Priyadarshi Chakraborty[3], Jugun Prakash Chinta[1]*

Abstract:

Cyclic peptides are gaining attention as versatile building blocks in supramolecular chemistry due to their ability to self-assemble into diverse nanostructures with tunable properties.[1] These peptides exhibit remarkable stability, resistance to degradation, and unique structural features, making them ideal candidates for a range of applications in drug delivery, catalysis, and materials science.[2] This study focused on the self-assembly of cyclic dipeptides, particularly cyclo-Trp-Trp (cWW), as a model system to explore how solvent interactions and non-covalent forces like π-π stacking and hydrogen bonding influence structural transformations, with morphology transitioning from nanospheres to nanofibers in varying methanol-water ratios.[3,4] Spectroscopic results reveal that shifts in the H- to J- aggregation ratio, influenced by π-π stacking and hydrogen bonding, correlate with morphology-dependent optical properties and enhanced antioxidant activity linked to secondary structures and self-assembly. This work highlights the importance of solvent composition in regulating the self-assembly of cyclic dipeptides, offering insights into the design of nanostructures with specific properties. Additionally, the study underscores the potential of cyclic peptides in therapeutic applications, particularly in antioxidant-based nanomedicine, where their tailored properties can be leveraged for effective drug delivery and other bioactive functions. This research bridges structural organic chemistry, material chemistry, and therapeutics, shedding light on the design and application of cyclic dipeptides in supramolecular systems.

Key words: *Cyclic Peptides, Antioxidant, Self-assembly, Morphological Transformations, Nanostructures*

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[1] Department of Chemistry, National Institute of Technology, Warangal, Telangana – 506004.
[2] Department of Biomedical Engineering, Indian Institute of Technology, Hyderabad, Telangana – 502285
[3] Department of Chemistry, Indian Institute of Technology, Hyderabad, Telangana – 502285
E-mail: jugun@nitw.ac.in

Title of Poster: Red emissive small molecule with aggregation induced emission (AIE) and solvatochromism characteristics (P-3)

Name of Presenters/Authors*: Jupitara Das, Peddaboodi Gopikrishna, and Parameswar Krishnan Iyer*

Abstract:

A novel small molecule with a D-π spacer-A framework was synthesized using bithiophene and 1,8-naphthalimide as donor (D) and acceptor (A) respectively. A facile four-step synthesis strategy produced the red emissive luminogen with aggregation induced emission (AIE)[1] characteristic. The molecule is soluble in most of the common organic solvents and in an aggregated state it showed a higher fluorescence quantum yield (Φ=31%). In the aggregated state nanoparticles were formed and confirmed by Transmission electron microscopy (TEM). One additional property exhibited by this molecule is solvatochromism[2]. Accordingly, DFT and TD-DFT method was used to calculate the excitation energies of the luminogen.

Keywords: *AIE, Luminogen, Solvatochromism.*

Reference:

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*Presenter/Author Address and E-mail ID:

Dr. Jupitara Das; Department of Chemistry; IIT Guwahati; Guwahati-781039;
jupitaradas@yahoo.co.in, jupitara_16@rnd.iitg.ac.in

Upcycling of Waste PET via Reprocessable Thermoset-like Covalent Adaptable Networks (P-4)

Vatsalya Gupta and Ramkrishna Sarkar*

Department of Chemistry, IIT Kanpur

Abstract:

The linear economic consumption of polymers has resulted in enormous energy loss and polymer waste accumulation which causes pollution. Efficient chemical recycling methods with apt economic viability and sustainability are highly desirable to address this concern. To this end, we have developed a strategy to upcycle the polyethylene terephthalate (PET) waste via internally catalyzed transesterification-based covalent adaptable networks (CANs), which though being thermosets, can be reprocessed and chemically recycled owing to the presence of dynamic covalent bonds. Two CANs were developed using the monomers, bis(2-hydroxyethyl) terephthalate (BHET), a triol crosslinker, and pyromellitic dianhydride (PMDA) wherein, BHET was derived from the commercial PET waste. Furthermore, one of the two internally catalyzed CANs were prepared from a crosslinker derived from a bio-source, further enhancing sustainability. The CANs were fully reprocessable at higher temperatures and exhibited noteworthy thermal and mechanical properties. After achieving the desired properties, the closed-loop recyclability of the networks was demonstrated wherein the network degradation and subsequent monomer recovery with high purity is shown. To the best of our knowledge, this is the first report that describes the degradation and closed-loop recyclability of a polyester-based CAN derived from waste plastic. As per our exploration, the presented research leads the way in upcycling commercial polymer waste using a simple and one-step method employing easily derivable, and cheap materials to a special class of recyclable thermosets using dynamic covalent chemistries.

Key words: *Thermosets, Covalent Adaptable Networks (CANs), Upcycling, Sustainable polymers, Closed-loop recycling*

Reference:

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***Presenter/Author Address and E-mail ID:** vatsalyag22@iitk.ac.in

Address: Department of Chemistry, IIT Kanpur, Uttar Pradesh, PIN-208016

Facile fabrication of doped α-MoO_3 ultra-thin based memristors (P-5)

Ayushi Tyagi*, Tanushree H. Choudhury[1]

Abstract:

Purpose: Today, our technology faces a challenge to meet the human demands for faster and smaller memory devices. It is due to excessive time and power consumption as a consequence of the physical separation between memory and processing unit[1]. To address this issue, researchers took inspiration from the most efficient technology, i.e., the brain, where the fundamental idea is to process and store the data simultaneously. A memristor seems to be the perfect choice to realize this concept[2]. This is due to their simple structure, high operating speeds, and ultra-low-power operation[3]. However, reproducibility in memristor performance remains a significant challenge due to uncontrolled filament formation. α-MoO_3 has emerged as a promising candidate to resolve this issue due to the low formation energy of oxygen vacancies, which give memristive properties via the formation of conductive filament[4]. Its thermal stability, makes it well-suited for withstanding the repetitive switching cycles required in memory devices. However, uncontrolled pre-existing oxygen vacancies often lead to inconsistencies and premature device failure. This led to this work where defect engineering will be explored to control the oxygen vacancies via scalable, energy-efficient, and rapid processing.

Research methodology and results: Using a facile liquid-phase precursor-assisted synthesis, we have developed a limited thermal exposure process to synthesize undoped and copper-doped α-MoO_3 coalesced films. Fig.1 highlights the process and the properties of the films. Fig. 1(a) shows the process schematic, which results in coalesced films on an area of 3×1 cm^2 Si/SiO_2 substrate shown in Fig. 1(b). Ammonium molybdate tetrahydrate and copper nitrate trihydrate are dissolved in ethylene glycol and spin-coated onto a plasma-treated substrate. Annealing is done in a tubular furnace at 400°C - 3 min in an oxygen (O_2) ambient. Successful doping of Cu is confirmed by x-ray photoelectron spectroscopy (XPS) shown in Fig. 1(c).

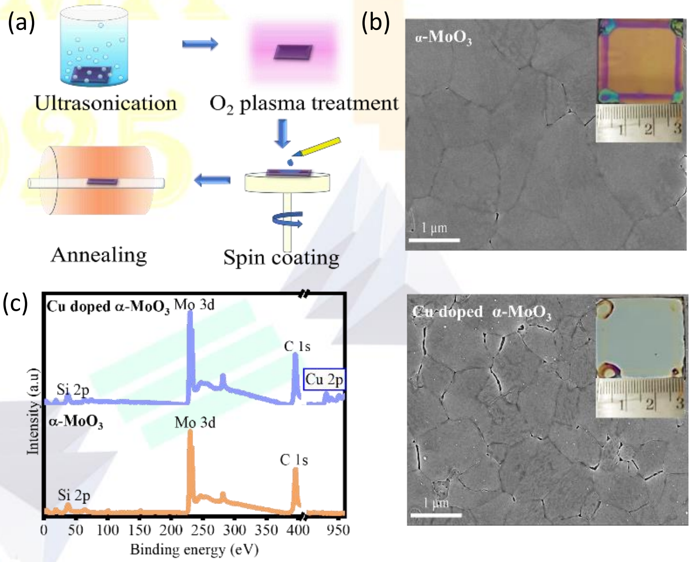

***Fig.1 (a)** Schematic of the liquid-precursor phase-assisted method **(b)** SEM images showing coalescence of undoped and doped films (in inset) **(c)** XPS showing elements present in the films*

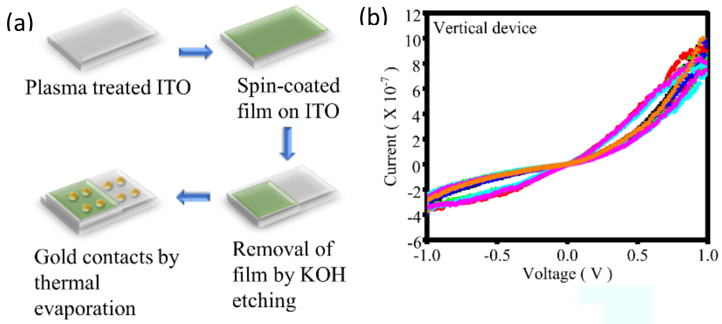

Fig.2 ***(a)*** *Schematic of the metal-semiconductor-metal (MSM) structure device fabrication* ***(b)*** *Current-voltage (I-V) measurements on the cu-doped α-MoO$_3$ film showing hysteresis, an indication of memristive property of the film*

Vertical devices are fabricated on doped and undoped films by shadow mask technique as shown in Fig. 2(a). The electrical measurement of I–V in Fig. 2(b) reveals bipolar resistive switching in the doped films and the results confirmed that the enhanced resistance switching property of Cu doped device contributed to the Cu doping effect in the formation of conducting filament in the device. Also, I-V is repeated 10 times on the same device and overlapped to show that devices are giving repeatable results.

Detailed structural characterization by XPS, Raman spectroscopy, low-temperature photoluminescence spectroscopy (PL), x-ray diffraction (XRD), conductive atomic force microscopy (c-AFM), and electrical characterization on doped α-MoO$_3$-based memristors will be discussed at the conference.

Key words: *ultra-thin films, low-power memristors, liquid-phase precursor-assisted synthesis, doping*

Reference:

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***Presenter and E-mail ID:** Research scholar, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology Bombay, Mumbai, 214110019@iitb.ac.in

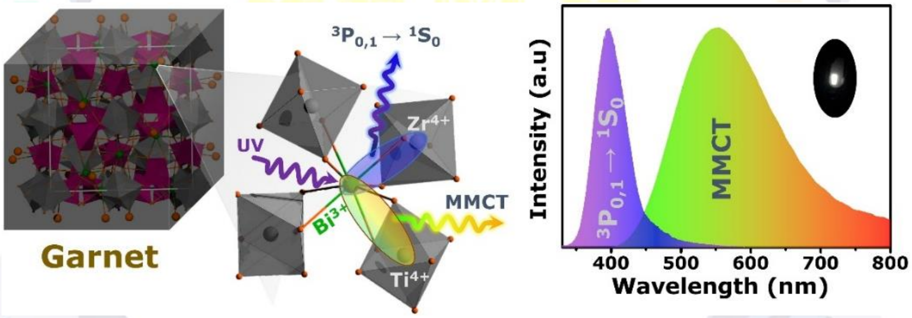
^{1}**Author Address and E-mail ID:** Assistance Professor, Department of Metallurgical Engineering and Material Science, Indian Institute of Technology Bombay, Mumbai, tanuhc@iitb.ac.in

Engineering A-band and D-band Emissions in Bi^{3+}-Activated Garnets for WLED Applications (P-6)

<u>Gurusamy Sivakumar</u>, Akkarakkaran Thayyil Muhammed Munthasir, Pakkirisamy Thilagar, Srinivasan Natarajan*

Abstract:

Mineral-based materials, particularly garnets, have long been explored for their diverse structural and optical properties, making them ideal candidates for phosphor applications. Herein, we report the high-temperature solid-state synthesis and intriguing optical features of Bi^{3+}/Ln^{3+} doped $Ca_2YTi_2Ga_3O_{12}$ (**CYT**). The optical behavior of **CYT** was tuned by substituting Zr^{4+} at Ti^{4+} sites and Bi^{3+}, Ln^{3+} at Y^{3+} sites. All compounds crystallize in a cubic *Ia*-3*d* (no. 230) space group. Bi^{3+} doping in **CYT** produced a yellow-orange photoluminescence (PL) band (~552 nm) from a metal-to-metal charge transfer state (MMCT). Co-doping with Tm^{3+} yielded excitation-dependent, white-light emission (**$CYT:Tm_{0.02}Bi_{0.012}$**). Substituting Zr^{4+} for Ti^{4+} resulted in **$CYZ:Bi^{3+}$**, which emitted violet-indigo light (395 nm, λ_{ex} = 315 nm) via the $^3P_{0,1} \rightarrow {}^1S_0$ transition. Further co-doping **$CYTZ:Bi^{3+}$** with Sm^{3+} produced white-light emissive **$CYTZ:Bi^{3+};Sm^{3+}$**. Notably, **$CYT:Bi_x$** showed slower PL decay (microseconds) compared to **$CYTZ:Bi_x$** (nanoseconds). Structural, optical, and time-resolved studies, supported by semi-empirical calculations, rationalize the unique optical features of these compounds.



Key words: *Garnets · Bi^{3+} emission · s-p transitions · MMCT transitions · white-light emission*

Reference:

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***Corresponding Author Address and E-mail ID:** Solid state and Structural Chemistry Unit, Indian Institute of Science, Bangalore; snatarajan@iisc.ac.in

Discovery of Novel, potent anticancer agent against Solid tumors (P-7)

Rahul Sawant, V H KrishnaPrasad, Vijayashree Nayak, Sanjay Kumar*

Abstract:

Cancer remains one of the most formidable global health challenges, with its emergence and increasing resistance significantly impacting life expectancy and treatment outcomes. The development of resistance to existing therapies has further complicated cancer management, necessitating the discovery of highly potent novel molecules to combat both cancer progression and drug resistance. In this study, we report the design, synthesis, and biological evaluation of a novel, potent anticancer molecule targeting solid tumors. The compound demonstrated significant cytotoxic activity in patient-derived oral cancer cell lines, with ongoing investigations in other solid tumors.

Keywords: *Cancer*, *Cytotoxicity*, *Drug resistance*

Reference:

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*Presenter/Author Address and E-mail ID:

Professor Sanjay Kumar, sanjaykumar@goa.bits-pilani.ac.in

Professor Vijayashree Nayak, vijayashree@goa.bits-pilani.ac.in

Rahul Sawant, p20240009@goa.bits-pilani.ac.in

V H KrishnaPrasad, p2022003@goa.bits-pilani.ac.in

Terpyridine Ligand-Based Transition Metal Complexes for CO_2 Reduction (P-8)

Shriya Saha* and Raja Mitra

Abstract:

Reducing carbon dioxide (CO_2) in the presence of a proton source is currently a significant challenge in homogeneous catalysis[1]. The problem of product selectivity can be tuned by designing a ligand framework, as Lehn showed in 1984[2]. For the Lehn complex, *fac*-Re(bpy)$(CO)_3$Cl, the selectivity towards CO_2 reduction over proton reduction was observed as the bpy ligand stabilizes the negatively charged intermediate [3], which is selective towards CO_2. Since then, the ligand designing has been one of the major research paths to get selective CO_2 reduction. Attaching a hydrogen□bond donor to the bipyridine system showed improved efficiency for CO_2 reduction [4], which is reported with various donors, such as amines, thiourea, hydroxyl, and imidazolium[5].

In this work, the bipyridine was replaced by terpyridine (tpy) with □^{2}□NN coordination, leaving a free pyridine ring as a hydrogen□bond donor. Five rhenium complexes were synthesized and characterized with varying substituents on the 4□position of the tpy[6]. DFT studies showed that the complexes attain distorted octahedral geometry. All the derivatives showed selective CO_2 reduction over proton reduction, and the role of pendant pyridine in overall reduction was also studied under acidic conditions. Further study of electrocatalytic CO_2 reduction with tpy ligand and different earth-abundant metals, such as cobalt, was also conducted to develop more sustainable catalysts.

Key words: *CO_2 reduction, electrocatalysis, rhenium catalyst, terpyridine ligand, spectroelectrochemistry*

Reference:

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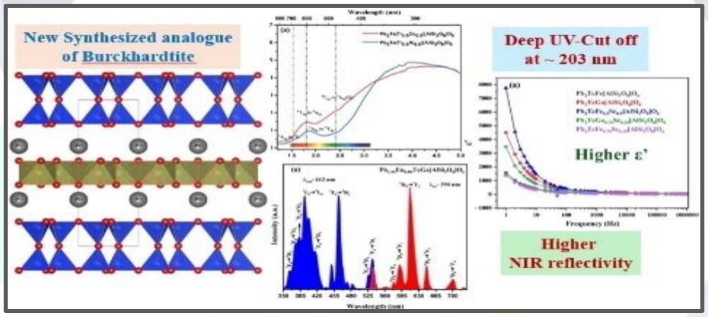
*****School of Chemical and Material Sciences, Indian Institute of Technology Goa, Farmagudi, Ponda – 403401, Goa, India; shriya19251103@iitgoa.ac.in

A New Synthetic Analogue of the Burckhardtite Mineral, $Pb_2TeGa[AlSi_3O_8]O_6$: Synthesis, Structure, and Properties (P-9)

Diksha Malik, and Srinivasan Natarajan*

Abstract:

The mineral, Burckhardtite, $Pb_2TeFe[AlSi_3O_8]O_6$, is synthesized and characterized. A new analogue, $Pb_2TeGa[AlSi_3O_8]O_6$, is successfully prepared for the first time under laboratory conditions. The substitution of Ga^{3+} by $Ti_{0.5}M_{0.5}$ ($M = Co^{2+}$, Ni^{2+}) results in new compounds with the Burckhardtite mineral structure. The transition metal-containing compounds exhibit interesting new colors, partly resulting from d-d transitions and metal-to-metal charge transfer (MMCT) transition. The Ga compound shows a deep UV cut-off (~ 86%), which is one of the better known values of deep UV cut-off compounds. The compounds exhibit good dielectric behavior with low dielectric loss. The Eu^{3+} - substituted samples show deep red emission with a long lifetime of ~0.89 ms. The magnetic behavior of the transition metal-containing compounds indicates anti-ferromagnetic interactions. The successful synthesis of the naturally occurring mineral along with newer analogues with interesting properties suggests that it is profitable to investigate compounds of mineral origin.



Key words: *Burckhardtite mineral, High dielectric constant material, Red Photoluminescence, Anti ferromagnetism, Deep UV Cutoff material, Metal-to-metal charge transfer*

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****Presenter/Author Address and E-mail ID:*** Diksha Malik, Inorganic and Physical Chemistry Department, IISc Bangalore, Karnataka 560012, India. *dikshamalik@iisc.ac.in*
S. Natarajan, Solid State and Structural Chemistry Unit, IISc Bangalore, Karnataka 560012, India snatarajan@iisc.ac.in

Exceptional performance in near ambient NO_2 sensing utilizing vertically aligned ultrathin MoO_3 nanorods synthesised through pulsed laser deposition (P-10)

Shivam Singh, J.P Singh*

Abstract:

Nitrogen dioxide (NO2), a notable global pollutant, necessitates precise and prompt monitoring to ensure the protection and well-being of public health. Metal oxide semiconductors (MOS) have been extensively utilized for their chemiresistive gas sensing applications historically; however, the elevated operating temperatures present challenges for practical implementation. This study utilizes an ultrathin vertical α-MoO3 nanorods film as the gas sensing material for the sensitive detection of NO2 under near-ambient conditions. This study presents an uncommon case of an α-MoO3 based gas sensor demonstrating a p-type response at temperatures approaching room temperature. The process of pulsed laser deposition (PLD) was conducted at a growth pressure of 8 Pascal and a substrate temperature of 550°C, resulting in the synthesis of high-quality, vertically aligned ultrathin one-dimensional α-MoO3 nanorods on silicon dioxide (SiO2) substrates. The MoO3 nanorods exhibit a notable sensitivity to NO2, achieving a response value of 19.7 for a concentration of 50 ppm at a temperature of 35°C. Furthermore, the sensor exhibits an exceptionally low detection limit of 500 ppb at this temperature, highlighting its appropriateness for low-temperature, high-performance gas sensing applications and advancing the field of environmental monitoring technology.

Key words: *Pulsed laser deposition (PLD), α-MoO3 nanorods, Gas sensing, near room temperature gas sensing, Response and Recovery time.*

Reference:

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***Presenter/Author Address and E-mail ID:** Shivam.singh@physics.iitd.ac.in

Design and Synthesis of ph-responsive, Water-dispersible N, S-doped Red Emissive Carbon Dots for Bacterial Imaging (P-11)

A. A. Pinheiro[*] **M. Banerjee**[*] **and A. Chatterjee**[*]

***** Department of Chemistry, BITS-Pilani, K.K. Birla Goa Campus, Sancoale, Goa, 403726
E-mail: p20220047@goa.bits-pilani.ac.in

Abstract:

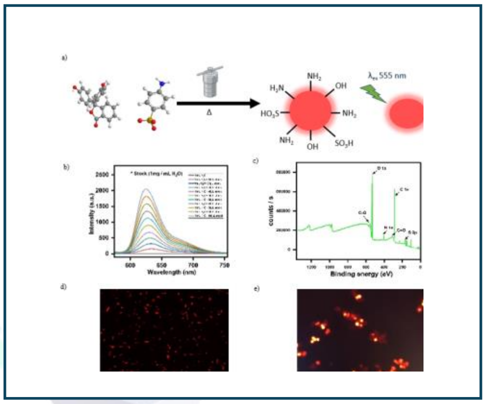

Figure 1. a) Graphical representation of synthesis of CDs. b) Fluorescence response of R-CDs in water. c) XPS data of the R-CDs d) E. coli staining using CDs e) S. aureus staining

Carbon dots (CDs), fluorescent carbon nanoparticles smaller than 10 nm, have been extensively used in sensors, bioimaging, catalysis, light-emitting (LEDs), and photoelectronic devices [1]. This is due to their unique characteristics, including low toxicity, biocompatibility, high photostability, ease of surface modification, and up-conversion fluorescence. Carbon dots (CDs) have proven effective in revealing the 3D structures of biological samples, distinguishing between normal and cancer cells, and detecting various analytes inside cells [2]. Most of the carbon dots are blue-green emitting CDs. The practical use of blue-green-emitting carbon dots (CDs) is limited by their shallow penetration, photobleaching, and autofluorescence issues [3]. The synthesis of red-emissive carbon dots (CDs) is highly sought after for sensing applications, but challenges remain in precursor preparation and product purification. Red-emissive carbon dots (RCDs) have been developed to address these issues. They offer deep tissue penetration, reduced photodamage, low autofluorescence, and high imaging contrast. Herein, we designed and synthesized RCDs with high water dispersibility, low toxicity, and excellent optical properties using the hydrothermal method. These features make them ideal for a range of biological applications.

Key words: *Carbon Dots (CDs), Fluorescent, Red-Emissive, Bioimaging*

Reference:

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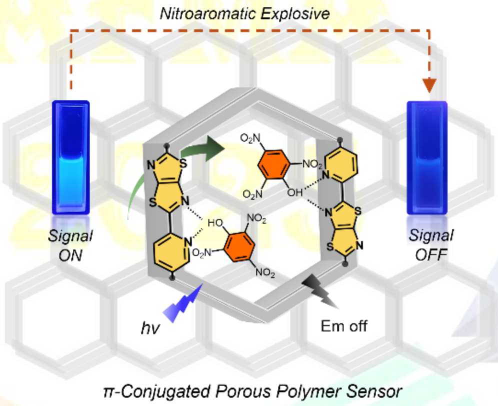
***Presenter/Author Address and E-mail ID:** p20220047@goa.bits-pilani.ac.in

Thiazolothiazole Porous Polymers for Nitroaromatic Explosive Sensing (P-12)

Saurabh Kumar Rajput*, Atul Kapoor and Venkata Suresh Mothika
Department of Chemistry, Indian Institute of Technology, Kanpur-208016, Uttar Pradesh, India
Contact details: saurabhkr22@iitk.ac.in , smothika@iitk.ac.in

Abstract. Nitroaromatic explosive sensors ensure human safety and help to assess the environmental impact of post-war scenarios.[1] Over the past few decades, extensive research has led to the development of numerous fluorescent materials aimed at detecting explosives with exceptional sensitivity, selectivity, and rapid response time.[2] In this study, we synthesized π-conjugated porous organic polymer nanosheets, NTzCMP and TzCMP, to achieve selective detection of picric acid (PA) among various nitrophenol explosives. The interaction between PA and the pyTTz moiety in the CMPs resulted in hydrogen bonding, where the hydroxy group of PA formed weak H-bonds with the pyridine and TTz units. This interaction caused significant fluorescence quenching in the CMPs, indicating the formation of a ground-state complex. This conclusion was supported by linear Stern-Volmer quenching plots, unchanged excited-state lifetimes, and detailed FTIR analysis of PA-exposed CMPs. Notably, both NTzCMP and TzCMP displayed superior responses to smaller analytes like 4-nitrotoluene compared to the less electron-deficient 2,4-dinitrotoluene. The CMPs exhibited high Stern-Volmer quenching constants (K_{SV}) of 9×10^3 M^{-1} and 2.1×10^3 M^{-1} for PA, with corresponding detection limits of 0.46 ppm and 1.6 ppm, respectively.



Keywords: chemical sensing, porosity, π-conjugation, electron transfer, dynamic quenching

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Presenter/Author Address: Saurabh Kumar Rajput, Dr. Venkata Suresh Mothika*
Lab No. 101H, Department of Chemistry,
Indian Institute of Technology, Kanpur (208016)
Email Id: saurabhkr22@iitk.ac.in , smothika@iitk.ac.in

Energy Storage and Conversion Properties of 3d-4d Transition Metal Double Perovskite Oxide (P-13)

Ankur Chakraborty

Abstract:
Toward achieving sustainable energy conversion and storage, ruthenium-based multinary metal oxides have emerged as promising materials due to their exceptional catalytic and electroactive properties. Herein, a Co and Ru doped disordered double perovskite oxide CCRO, and its application in energy-related processes are presented. The polycrystalline oxides demonstrated efficient electrocatalytic water oxidation and electrochemical supercapacitor performance, highlighting the influence of B-site elements. The CCRO oxide electrode achieved a specific capacitance of 210F g^{-1} at 1 A g^{-1} in 1 M H_2SO_4 with a remarkable capacitance retention after 4000 charge-discharge cycles. This study underscores the potential of double perovskite oxides for advancing green and efficient energy technologies.

Key words: Double perovskite, Electrocatalysis, Supercapacitor, Water oxidation

Reference:

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***Presenter/Author Address and E-mail ID:**

Ankur Chakraborty

National Institute of Technology Kurukshetra, Haryana - 136119

ankurkishore1@gmail.com

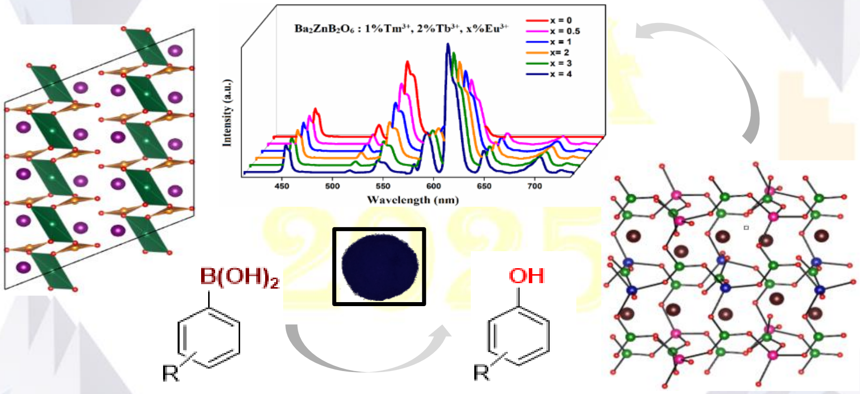
Synthesis, structure and properties of compounds derived from Kotoite-related structures towards white-light emission and catalysis (P-14)

Shreya Sasmal, Nainamalai Devarajan and Srinivasan Natarajan *

Abstract:

A series of compounds with the general formula $A_2MB_2O_6$ (A = Zn, Ba, Pb; B = Pb, Ba, Zn, Cu) related to the kotoite structure has been prepared employing high-temperature solid state methods. The substitution of transition elements in place of Zn^{2+} ions resulted in colored compounds. The optical absorption spectra could be explained based on Tanabe-Sugano diagram and allowed d-d transitions. Dielectric studies on $Ba_2ZnB_2O_6$, $(Ba_{1.5}Pb_{0.5})ZnB_2O_6$, $PbZn_2B_2O_6$, $Pb_{1.5}Zn_{1.5}B_2O_6$, $BaZn_2B_2O_6$ and $Pb_2CuB_2O_6$ at room temperature indicate reasonable values at low frequencies, which decrease on increasing frequencies. Magnetic study of synthesized single-phase compounds $BaZnCoB_2O_6$ and $Pb_2CuB_2O_6$ have been performed. The substitution of Eu^{3+}, Tb^{3+} and Tm^{3+} in place of Ba^{2+} in $Ba_2ZnB_2O_6$, gives rise to the expected emission of red, green and blue colors. Suitable modifications of the different phosphors in $Ba_2ZnB_2O_6$, resulted in white-light emission in $Ba_2ZnB_2O_6$. The $Pb_2CuB_2O_6$ compound was found to be a good catalyst in the ipso-hydroxylation of arylboronic acids.

Key words: Kotoite, • dielectric, • magnetism, • white light emission, • organic catalysis



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***Presenter/Author Address and E-mail ID:** shreyasasmal@iisc.ac.in, snatarajan@iisc.ac.in

Structural and electrical properties of textured $Bi_4Ti_3O_{12}$ prepared via molten salt method (P-15)

Dipankar Kundu[a,*], I Lakshmigandhan[a], A Sree Rama Murthy[a,b], V. Jayaraman[a,b] and K I Gnanasekar[a,b,#],

[a]Materials Chemistry& Metal Fuel Cycle Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India, [b]Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai,400094, India, [#]Corresponding author email: igsk@igcar.gov.in

Abstract:

The lead-free Bismuth titanate ($Bi_4Ti_3O_{12}$, BIT)) is one of the Aurivillius-type layered perovskite oxides with a piezoelectric coefficient, d_{33} of 30 pC/N with a Curie temperature of 948 K provides the scope for operations in high temperatures. It also finds applications in photocatalysis, transducers, CO_2 reduction, NO_x removal, memory devices, etc. Being an anisotropic compound, the d_{33} is high along the c-axis which demanded 'c' texturing for enhanced piezoelectric coefficient. Most of the solution chemical routes/solid-state synthesis offer randomly oriented grains. Literature review shows molten salt synthesis offers preferential texturing. In this work, we have adopted this method to explore the formation of preferential texturing of BIT using an eutectic mixture of NaCl (44 wt%) and KCl (56 wt%). NaCl-KCl eutectic composition was mixed with a stoichiometric amount of Bi_2O_3 and TiO_2 with a salt-to-precursor ratio of 3:1 and the mixture was heated at 1073 K for 2 h in air and cooled to room temperature [1]. The resultant product was washed using distilled water to remove the salts and dried. Powder XRD pattern showed preferential texturing along (00l) direction and the structural refinement was carried out using Full Prof software, confirming the phase purity of the compound crystallized in S.G. Fmmm(69). SEM study showed plate-like morphology. EDX and elemental mapping show that the ratio of Bi/Ti is as expected and that the distribution of Bi and Ti is homogenous across the sample respectively. The prepared sample was made into pellet form and sintered at 1323 K for 4 h for conductivity measurements over a temperature range of 373 - 823 K using impedance spectroscopy.

Key words: *molten salt synthesis, piezoelectric material, high Curie temperature, Structural Refinement, electrical conductivity*

References:

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***Presenter/Author Address and E-mail ID:** Dipankar Kundu, Scientific Officer/D, Material Chemistry division, Materials Chemistry and Metal Fuel Cycle Group, Indira Gandhi Center for Atomic Research, Kalpakkam, Tamil Nadu,603102

dipankar@igcar.gov.in, dipankarchem111@gmail.com;

Effect of La content on Structural, Spectroscopic and Magnetic Properties of $NiLa_xFe_{2-x}O_4$ ($0 \leq x \leq 0.3$) (P-16)

Rajshekhar Balagi and R. N. Panda*

Abstract:

Research on doped $NiFe_2O_4$ has become important owing to their various potential applications, such as: sensors, catalysis, biomedicine, energy storage, magnetic resonance imaging etc.[1]. Synthesis of lanthanum (La^{3+}) substituted nickel ferrite nanomaterial ($NiLa_xFe_{2-x}O_4$, $0 \leq x \leq 0.3$) has been achieved by using novel sol gel autocombustion technique. The synthesized materials crystallize in cubic spinel structure. Materials characterization were carried out using powder XRD, FESEM, Raman spectroscopy and magnetic measurements. The effect of increasing La substitution into the lattice structure of $NiFe_2O_4$ gave rise to increase in its lattice parameters; i.e. 8.3269 Å, 8.3288 Å, 8.3340 Å for La content, x = 0.0, 0.1 and 0.3, respectively. Variation in the calculated crystallite size is observed as there is a decrease from 42 nm for pure $NiFe_2O_4$ down to 22 nm for x = 0.1 and an increase to 29 nm when x = 0.3. FESEM studies confirm nearly spherical nature of the particles with particle sizes of 40 nm, 28 nm and 33 nm for x = 0.0, 0.1 and 0.3 in $NiLa_xFe_{2-x}O_4$, respectively. Surface morphology of these samples exhibit some agglomerations due to interactions between the magnetic nanoparticles. The compositions of the elements present in the materials were analyzed using EDX analysis which confirms the presence of desired elements (Fe, Ni, La, and O) in the samples with proper stoichiometry. Analysis of Raman spectra was performed within the range 900-100 cm^{-1} using an excitation source of wavelength 532 nm. Symmetric stretching of Fe-O at the tetrahedral site is represented by the Raman modes $A_{1g}(1)$ and $A_{1g}(2)$ which were observed at 680 cm^{-1} and 643 cm^{-1} respectively. The asymmetric bending and stretching of Fe(Ni)-O bonds at octahedral sites is represented by $T_{2g}(1)$ and $T_{2g}(2)$ modes at 547 cm^{-1} and 464 cm^{-1}, respectively. The energy bands $E_g(2)$ and $E_g(1)$ at 361 cm^{-1} and 313 cm^{-1} represent the spinel symmetric bending of the Fe(Ni)-O bond. The translation motion of the whole tetrahedron is represented by the Raman mode $T_{2g}(3)$ at 192 cm^{-1}[1,2]. There is a decrease in the observed saturation magnetization (M_s) values from 44.69 emu/g for x = 0.0 down to 25.18 emu/g in x = 0.3. The coercivity (H_c) values observed show an initial decrease from 155 Oe for x = 0.0 to 128 Oe for x = 0.1, following that an increase in value to 173 Oe for x = 0.3 is noted. This peculiarity can be attributed to the size and surface effect predominantly [3]. The remanent magnetization (M_r) values showed a progressive decrease from 9.33, 8.32, 6.97 emu/g for x = 0.0, 0.1, 0.3, respectively.

Keywords:*Chemical Synthesis, Magnetic property, Raman Spectroscopy, Ferrite, X-ray Diffraction*

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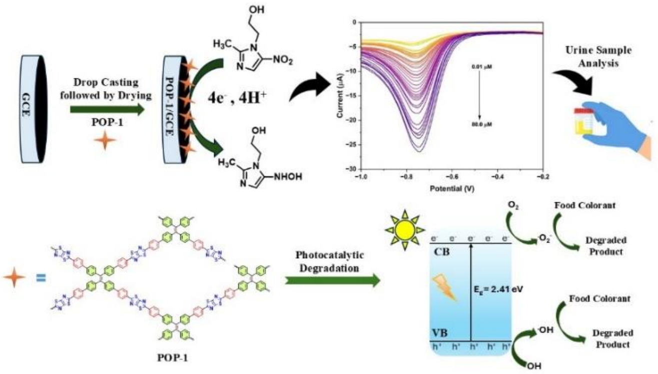
***Department of Chemistry, BITS Pilani K. K. Birla Goa Campus, Goa, India-403726, E-mail(s): Corresponding Author(RNP): rnp@goa.bits-pilani.ac.in / Presenting Author (RB): rajuibalagi1999@gmail**

Thiazolothiazole-Linked π-Conjugated Porous Polymer for Enhanced Metronidazole Detection and Photocatalytic Degradation (P-17)

Dr. Atul Kapoor, Nilojyoti Sahoo and Dr. Venkata Suresh Mothika*
Department of Chemistry, Indian Institute of Technology, Kanpur-208016, Uttar Pradesh, India
Contact details katul@iitk.ac.in, smothika@iitk.ac.in

Abstract. Strict quantification of metronidazole (MNZ) helps to control the overuse and its serious toxicity to human health.[1]. In this report, we demonstrate a highly selective electrochemical sensor based on thiazolothiazole (TTz) linked conjugated microporous polymer (TTz-CMP; $S_{\mathrm{BET}} = 331.8\ \mathrm{m^2 g^{-1}}$) for MNZ quantitation. TTz-CMP was prepared by condensation of tetrakis(4-formylphenyl)ethene and dithiooxamide and thoroughly characterized. TTz-CMP modified glassy carbon (GC) electrode showed a remarkable current response to MNZ in the range of 0.01–80 µM, and upon thorough optimization of the sensing response by changing the catalyst loading, pH of the solution, and accumulation time, the TTz-CMP allows the lowest detection up to 14.27 nM. Interestingly, the TTz-linear polymer (TTz-LP) showed a relatively less electrochemical response under optimized conditions. As evidenced by the electrochemical impedance spectroscopy (EIS), the lower interfacial resistance of TTz-CMP (259.84 $\Omega\mathrm{cm}^2$) compared to TTz-LP (360.41 $\Omega\mathrm{cm}^2$) and bare ITO (642.35 $\Omega\mathrm{cm}^2$), resulted in an enhanced electrochemical response of TTz-CMP to MNZ. Also, the TTz-CMP sensor exhibited excellent stability and reproducibility over several cycles indicating its high recyclability. In addition, the detection of MNZ in the urine sample was also demonstrated to illustrate the practical application of the TTz-MNZ sensor. Apart from electrochemical sensing properties, TTz-CMP also showed excellent photocatalytic properties due to its low band gap (2.41 eV)—degradation of several food colorants under direct sunlight conditions was demonstrated with degradation efficiency up to 98.25%. [2–3]



Keywords. Metronidazole detection, Conjugated Microporous Polymers, Electrochemical Sensor, Photocatalytic Degradation

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Pyrene and Anthracene-based Small Organic Fluorescent Probes for Sensing of Nitroaromatic Compounds (P-18)

Ritu Rani , Madhushree Sarkar*

Department of Chemistry, Birla Institute & Science, Pilani, Rajasthan, 333031, India

***Email:** msarkar@pilani.bits-pilani.ac.in

Abstract:

Two polyaromatic hydrocarbon-based fluorescent probes were investigated as chemosensors for the detection of nitroaromatic compounds. The probes showed selective sensing towards 4-nitroaniline (4NA) in homogeneous mediums such as acetonitrile (ACN) and DMSO. Detailed studies of the quenching mechanism showed the presence of dynamic quenching. Further the chemosensing response of the probes towards picric acid (PA) was also studies and a significant solvent effect on the sensing response was noted when the solvent was switched from ACN to DMSO to water. The detailed mechanistic investigation of their mode of action through spectral overlap, lifetime measurements, and density functional theory calculations reveals that resonance energy transfer and photoinduced electron transfer processes, and electrostatic interactions are the key aspects of the turn-off response toward nitroaromatics compound. Due to their insoluble nature of the probes in water, they were employed as heterogeneous chemosensors in an aqueous medium, where the probes showed excellent sensing response towards both 4NA and PA. The stability and recyclability of the probes after heterogeneous sensing studies were investigated by PXRD.

Keywords: Polycyclic aromatic hydrocarbons, Nitroaromatics compounds, Fluorescence quenching, Selective sensing

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Tuning Quantum States at Chirality-Reversed Planar Interface in Weyl Semimetals using an Interstitial Layer (P-19)

Eklavya Thareja*, Gina Pantano, Ilya Vekhter, Jacob Gayles

Abstract:

Topological features of the electronic band structure are robust against many types of disorder, which makes materials such as topological insulators and Weyl semimetals promising for low-power spintronics and quantum computing. Weyl semimetals possess topologically protected linear band crossings, called Weyl nodes, that always arise in pairs. The electronic excitations near these nodes have spin-momentum locking that can be characterized by a chiral charge, with individual nodes having opposite chirality [1]. While non-magnetic candidates for Weyl semimetals have been known for about a decade, their magnetic counterparts (typically having fewer Weyl node pairs) have only been identified recently [2,3,4]. Weyl semimetals, like other materials, have planar defects such as twin boundaries. Additionally, planar defects can be intentionally induced via an interstitial atomic layer. In this work, we show using a continuum model that a planar defect between chirality-reversed (due to magnetization-reversal) regions will host bound states, in agreement with Araki et. al. [5]. Moreover, we demonstrate the dispersion, and the spin texture of these states are highly tunable in the presence of a magnetic interstitial atomic layer at the planar defect. These properties have a periodic dependence on defect electrostatic potential, due to the emergent Weyl character of the electronic states, in agreement with similar result for topological insulators [6]. Another consequence of the Weyl character is that interstitial magnetic potential pointing out of the defect plane does not affect physical observables. Meanwhile, the in-plane magnetic potential parallel to the Weyl node split direction affects the spatial distribution of the states, and strongly blocks the bulk states from being transmitted across the defect. The other in-plane component perpendicular to the Weyl node split direction affects the shape of the fermi-arc-like bound states and spin selects the bulk states scattering off the defect. Hence, we provide a comprehensive picture of how electrostatic and magnetic potentials from the interstitial layer can tune chirality-reversed planar defect states in magnetic Weyl semimetals.

Key words:

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*Presenter/Author Address and E-mail ID:

Department of Physics, University of South Florida, Tampa, FL 33620, USA

ethareja@usf.edu

Colorimetric Sensor Array Coupled with Machine Learning Algorithms for On-site Detection and Discrimination of Pesticides and Herbicides (P-20)

Ranbir,* Narinder Singh[a]

Abstract:

Modern agricultural practice often depends on pesticides and herbicides to boost crop yields, but their residues pose risks to the environment and public health. To address these concerns, we developed a chromogenic sensor array using azodyes for detecting and distinguishing pesticides and herbicides in food and soil samples. This system leverages machine learning techniques such as Hierarchical Clustering Analysis (HCA), Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), and Partial Least Square Regression (PLSR). The sensor array combines azodyes with various metal ions, which exhibit unique photophysical properties, producing distinct response patterns for different pesticides and herbicides. These patterns are analyzed through automated multivariate techniques, enabling selective and sensitive identification of the target compounds. L0DA and PLSR were used for qualitative and quantitative analysis, showing a strong linear correlation (R^2 values of 0.89–0.96) with analyte concentrations, detection limits ranging from 5.3 ppm to 11.8 ppm. Additionally, the sensor array successfully identified and distinguished a binary mixture of the pesticide chlorpyrifos and the herbicide glyphosate.

Keywords: *Azodye-based receptor, Chromogenic Sensor array, Pattern recognition, Multivariate Analysis, Food safety.*

Reference:

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***Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar Punjab, 140001, India**

E-mail id: ranbir.20cyz0027@iitrpr.ac.in

Thermophysical and Spectroscopic Studies of Ternary mixture of Industrial Solvents with water (P-21)

Eshita Kakodkar*, Praseeda Nair, Rolee Verma, Ranjan Dey

Abstract:

The thermophysical properties of a ternary mixture comprising industrial solvents such as dimethyl sulfoxide (DMSO) and N-methyl-2-pyrrolidone (NMP) with water are crucial for understanding their behavior in various industrial and scientific applications. Due to their unique solubility properties, polarity, and ability to dissolve a wide range of compounds, these industrial solvents are commonly used in multifarious chemical processes, pharmaceuticals, and bioengineering. In this investigation, experimental determination of density has been carried out over the entire mole fraction range at varying temperatures (293.15 K-318.15 K). The excess molar volumes (V_m^E) have been evaluated and their graphical representations have been undertaken to gain an insight into the interactions between the components. Excess molar volumes provide critical information on the intermolecular interactions, deviations from ideality, and the structural changes occurring when the three components are mixed. Spectroscopic analysis using FTIR spectroscopy has been carried out to detect the presence of specific molecular interactions, such as hydrogen bonding to strengthen the excess volume findings. Understanding the thermophysical properties and the nature of these intermolecular interactions is essential for optimizing the use of this ternary mixture and consequently its sustainable and greener alternative in various applications, including drug delivery systems, solvent recovery processes, etc. while ensuring improved efficiency, safety, and performance in practical implementations.

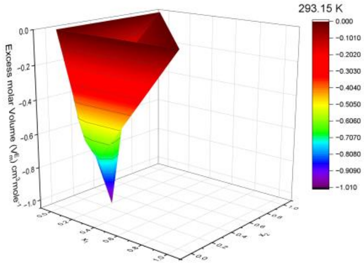

Figure 1. Plot of excess molar volume (V_m^E) vs mole fraction, of DMSO(x_1)+NMP(x_2)+Water(x_3) ternary mixture at T=293.15 K

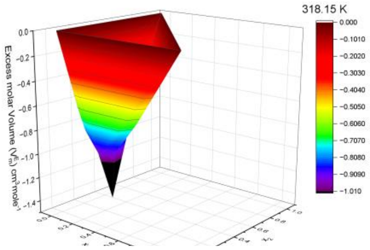

Figure2. Plot of excess molar volume (V_m^E) vs mole fraction, of DMSO(x_1)+NMP(x_2)+Water(x_3) ternary mixture at T=318.15 K

Key words: *Sustainable*, *Ternary*, *Thermophysical properties*

Reference:

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***Presenter/Author Address and E-mail ID: p20240010@goa.bits-pilani.ac.in**

Thermophysical properties Lab, Department of Chemistry, BITS Pilani K K Birla Goa Campus, Goa 403726, India

Synthesis of fused pyrrolo-napthridinone via ligand-free copper catalysed Ullmann (C-N coupling) type reaction (P-22)

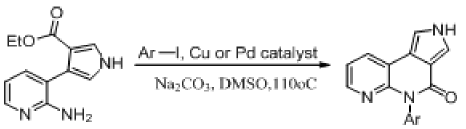
Mekala Ramesh[1] , Malempati Srimannarayana

Abstract:

A tandem approach of intramolecular lactamization and N-arylation using a copper catalyst to obtain a fused pyrrolo-naptharidinone has been developed. A ligand-free method for cyclization and Ullmann (C-N coupling) type reaction in a single step

Text Body

Fused pyrrole, pyridine with pyridinone components are shown to have many biological and pharmaceutical properties; fused pyrrole with naptharidinone also many potential components are active, such as 1-phenyl-1,8- naphthyridin-2(1H)-one derivatives act as Wee-1 kinase inhibitors, antitumor activity, antiallergy agents, CB2 receptor agonist, hedgehog(Hh) signalling inhibitors, gastric(H+/K+)-ATPase inhibitor, agents broncho dilating agents, 5-HT3 receptor agonist, antitubercular agent [1-3].



Scheme. Synthesis of fused pyrrolo-napthridinone via ligand-free copper catalysed Ullmann (C-N coupling) type reaction

Key words: *Pyrrolo-naphthyridinone, Ullmann reaction, Ullmann condensation, Ullmann-type reaction, Copper catalyst,*

Reference:

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*Presenter/Author Address and E-mail ID:

Mekala Ramesh

Department of Chemistry, School of Science, GITAM(Deemed to be University), Hyderabad
rameshvarma.mekala@gmail.com

Exploring Alkaline Oxygen Evolution Reaction on Ludwigite (P-23)

Indrani. G. Shanmugapriya, Srinivasan Natarajan*

Abstract:

The transition metals substituted ludwigite was investigated for the oxygen evolution reaction (OER) which showed superior electrocatalytic OER activity in the alkaline medium with a low overpotential value, lesser Tafel slope value, and excellent stability. We have explored a new way for the structural design of ludwigite (general formula $X_2YO_2[BO_3]$ where X = Co^{2+}, Ni^{2+}; Y = Fe^{3+}, Ti^{4+}, Sn^{4+}) to apply electrocatalytic water splitting. We probe the electroactivity of the oxide material based on linear scan voltammetry to find on-set potential, impedance for finding charge transfer resistance, chronoamperometry to know the stability of the electroactive material, and electrochemical surface area (ECSA) for finding the catalyst activity.

Key words: Tafel slope, on-set potential, impedance, ECSA.

Reference:

[1] Y. V. Knyazev, N. V. Kazak, V. S. Zhandun, J. Bartolomé, A. Arauzo, N. A. Belskaya, O. A. Bayukov, L. N. Bezmaternykh, S. G. Ovchinnikov, *Dalton Trans.*, **2021**, *50*, 9735.

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Presenter Address and E-mail ID: Frameworks Solids Laboratory, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru,560012. Email: igshanmuga@iisc.ac.in, igshanmuga@gmail.com

Efficient Nickel and Copper-Based Organophosphonate Frameworks for Electrocatalysis and Organic Transformations (P-24)

Poojita

Abstract:

Nickel- and copper-based organophosphonate frameworks have been explored as robust and sustainable catalysts for energy conversion and organic synthesis. Nickel compounds $[Ni(Hhedp)_2]\cdot 4H_2O$ (**I**) and $[Ni_3(H_3hedp)_2(C_4H_4N_2)_3]\cdot 6H_2O$ (**II**) exhibit distinct one-dimensional and three-dimensional architectures, with compound **II** demonstrating superior catalytic activity for OER (η_{10} = 305 mV) and HER (η_{10} = 230 mV), along with fourfold higher specific activity compared to **I**. Copper-based compounds $Cu_3[(Hhedp)_2(C_4H_4N_2)]\cdot 2H_2O$ (**III**) and $Cu_3[(H_3hedp)_2(C_4H_4N_2)_4(SO_4)]\cdot 2H_2O$ (**IV**) display layered and mixed-valent frameworks. Notably, compound **IV** excels in CO_2-to-CH_3OH conversion, driven by its optimized Cu^{1+} active sites, while both copper compounds effectively catalyzed solvent-free A^3 coupling and click reactions. These findings highlight the promise of hybrid phosphonate frameworks for next-generation catalytic applications.

Key words: Hybrid frameworks, Electrocatalysis, CO_2 reduction, Hydrogen evolution, Oxygen evolution

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***Presenter/Author Address and E-mail ID:** poojidhull@gmail.com

Spin-Selective Charge Transfer-SERS Driven Label-Free Enantioselective Discrimination of Chiral Molecules on Ag Nanoparticle-Decorated Ni Nanorod Arrays (P-25)

Lakshay Bhardwaj, Jyoti Yadav, Sarjana Yadav, J.P.Singh

Abstract:

Enantioselective discrimination is critical in several fields, particularly in pharmaceutics and clinical drug research. Chiral molecules possess unique charge transfer properties, showing an enantioselective preference for electron spin orientation when interacting with the magnetic surface. Here, we developed spin-selective charge transfer (SSCT)-based label-free surface-enhanced Raman scattering (SERS) achiral magnetic substrates for the enantioselective discrimination of chiral molecules without creating asymmetric chiral adsorption sites. The e-beam-based glancing angle deposition (GLAD) technique was utilized to construct achiral magnetic surface-enhanced Raman scattering (SERS) substrates by decorating Ag nanoparticles over Ni nanorods. SERS spectroscopy was carried out on significant enantiomers, including cystine, alanine, and DOPA (l-3-(3,4-dihydroxyphenyl) alanine). An external electromagnet was used to manipulate the magnetic substrate's spin polarization by altering the magnetic field's direction. Subsequently, SERS spectra were acquired. Based on the magnetic field's direction, there is a complementary variation in the intensities of SERS spectra of the enantiomers. The SSCT process between molecule–metal complexes synergized with the magnetic field direction to control the electron spin, leading to SERS-based enantioselective discrimination. This label-free, easy, yet practical approach offers a characteristic paradigm shift from the recent complex approaches for chiral detection and separation

Keywords: *glancing angle deposition, surface-enhanced Raman spectroscopy, magnetic shape anisotropy, chiral molecules, CISS effect.*

Reference:

[1] Lakshay Bhardwaj, Jyoti Yadav, Sarjana Yadav, and J.P. Singh, ACS Applied Materials & Interfaces 2024 16 (49), 67289-67301.

*Presenter/Author Address and E-mail ID:

Lakshay Bhardwaj

IIT Delhi, Hauz Khas, New Delhi, 110059, lakshaybhardwaj12@gmail.com

Development of Polyether Sulfone-Based Organic Nanoparticle-Embedded Membranes for Improved Detection and Purification of Amoxicillin from Wastewater (P-26)

Kamalpreet Kaur,* Narinder Singh[a]

Abstract:

Literature reveals the continuous release of pharmaceuticals and their metabolites into the environment from various sources, including urban domestic effluents, necessitating enhanced treatment methods to monitor and mitigate such contaminants in wastewater. This study presents the development of a self-assembled chemosensor utilizing an azodye-based imine-linked Co^{2+} complex ($R1.Co^{2+}$), demonstrating potential for ratiometric and colorimetric quantification of amoxicillin (AMX) in buffer/aqueous media with a limit of detection (LOD) of 0.717 μM and a limit of quantification (LOQ) of 4.14 μM. Additionally, electrochemical studies elucidate the mechanism of AMX detection, indicating selective oxidation of AMX by the $R1.Co^{2+}$ complex without interference from other analytes. FE- SEM analysis reveals analyte-induced self-assembly of the probe $R1.Co^{2+}$ upon interaction with AMX. Moreover, immobilization of the $R1.Co^{2+}$ complex onto polyether sulfone (PES) membranes demonstrates promising potential for AMX removal from environmental wastewater, exhibiting an adsorption capacity of 450.1 mg g^{-1} and removal efficiency of90%. Furthermore, the hybrid membrane serves as a solid-state colorimetric sensor for AMX, as evidenced by the hue, saturation, and value (HSV) parameter model, validated through a portable mobile-based prototype.

Keywords: *Chromogenic receptor, organic nanoparticles, Cyclic Voltammetry, Water Remediation, Environment Monitoring*

Reference:

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***Department of Chemistry, Indian Institute of Technology Ropar, Punjab 140001, India.**
E-mail ID: Kamalpreet.20cyz0015@iitrpr.ac.in

Numerical study for performance analysis of silicon carbide based porous radiant burner for the application of biomass cooking (P-27)

Prabhakar Zainith[1] and Niraj Kumar Mishra[1]*

[1]Department of Mechanical Engineering, National Institute of Technology Uttarakhand, Srinagar (Garhwal), 246174, India

Abstract:

For a biomass cooking stove, the combustion and emission analysis of a silicon carbide based porous radiant burner have been investigated in the present study. Numerical simulations have been performed with power inputs ranging from 1 to 3 kW and equivalence ratios (ERs) between 0.7 and 0.9. While the species transport model with finite rate/eddy-dissipation has been used to simulate the combustion process, a thermal equilibrium model has been used for the energy equations. This study's model, which includes discreate phase, energy, species movement, k-ε turbulence, and conventional radiation, has been applied to a biomass cook stove with a two-layer porous radiant burner. All combustion processes' chemical kinetics have been precisely captured by the species transport model in conjunction with a finite rate/eddy-dissipation technique [1]. The kinetics of eleven chemical reactions has been included in the species transport model to depict the combustion process [2]. Temperature distribution and emissions (CO and CO_2 composition) have been evaluated for different power inputs and equivalence ratios in this computational domain. In terms of radiation efficiency, the study found that the best operating range for domestic cooking falls within an equivalency ratio of 0.7 and 0.9 across various power inputs.

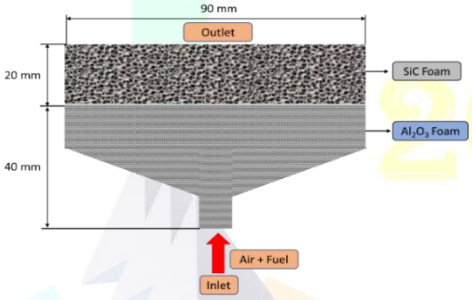

Figure 1 Schematic diagram of considered problem.

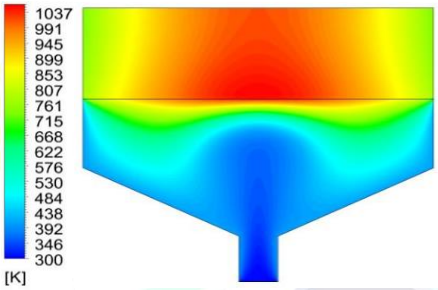

Figure 2 Temperature contour at 0.9 ER and 3 kw power input.

Key words: *Biomass cook stove, Equivalence ratio, Radiation efficiency, and Wood volatiles.*

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Acknowledgement: This work was supported by the Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Government of India [CRG/2021/007295]. *Niraj Kumar Mishra/Department of Mechanical Engineering, National Institute of Technology Uttarakhand, Srinagar (Garhwal), 246174, nkm@nituk.ac.in

Discovery of novel, potent JHAs and assessment of their larvicidal activities in *Aedes aegypti* and *Anopheles stephensi* (P-28)

Kartik Redkar*, Rahul Sawant*, Sanjay Kumar*, Tusar Saha*

Abstract

Mosquito borne diseases are a major contributor to the global burden of infectious diseases with nearly 300 million cases reported globally. To combat the rising global disease burden, there is a need to develop novel approaches that are relatively specific to vector species. Juvenile hormones (JH's) are structurally unique terpenoid growth regulators specific to insects. Regulated release of JH prevents transition of insect larvae into adults and perturbation in this homeostasis leads to abnormal development [1]. Juvenile hormone analogs (JHAs) are synthetic chemical moieties that agonistically exploit the growth regulating property and thus are widely used as insecticides [2]. Methoprene and pyriproxyfen are some of the most potent commercially available JHA's. Recent rise in resistance towards these molecules in target species and concerns over environmental toxicity has necessitated the development of novel JHAs. We herein report design and synthesis of novel and potent putative JHAs to combat the rising burden of mosquito borne diseases. Our findings indicate the disruption of the pupa-adult transition of mosquito larvae, leading to precocious development and an overall reduction in the emergence of adult mosquitoes. This developmental disruption highlights the potential of our putative JHAs as effective vector control agents. Future studies will focus on elucidating their precise mode of action, evaluating their environmental safety, and optimizing their formulation for large-scale deployment.

Key words: Mosquito-borne diseases, Juvenile hormone analogs (JHAs), Methoprene tolerant (MET).

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***Birla Institute of Technology and Science, K K Birla Goa Campus. Email ID: p20220041@goa.bits-pilani.ac.in**

Biphenylene-Graphene van der Waals Bilayer Heterostructure as an Anode Material for Li-ion Batteries (P-29)

Nidhi Duhan* and T. J. Dhilip Kumar

Abstract:

The quest to discover a top-tier electrode material for lithium-ion secondary batteries continues to advance for the past many decades in order to satisfy the surging power necessities. Pristine two-dimensional nanolayer electrodes often face challenges such as poor cycling efficiency, slow diffusion, and low lithium capacity. Fabricating heterostructure bilayers from different two-dimensional materials is a compelling approach to combine their inherent attributes while mitigating individual drawbacks of each material. Current research work showcases a thorough investigation of the biphenylene-graphene (BPN/G) van der Waals bilayer heterostructure through first-principles calculations, aimed at evaluating its viability in the role of lithium-ion battery anode. The BPN/G bilayer exhibits robust energetic and thermal stability, coupled with excellent electronic and ionic conductivity. The binding energy of lithium for BPN/G bilayer is calculated to be -0.97 eV, illustrating a significant improvement over that of the individual monolayers. Lithium atoms preferentially adsorb into the interlayer region initially and later occupy the outer surfaces. The bilayer achieves saturation to reach its maximum lithium storage capacity of 956 mAhg^{-1}, surpassing that of pure graphene. The diffusion energy barrier for lithium migration along various pathways varies from 0.47 eV to 0.26 eV. The low barrier and high diffusivity of 3.9 × 10−5 cm^2/s, points toward a high lithium mobility and excellent cycling efficiency. The BPN/G bilayer provides a beneficial operating voltage of 0.51 V, signifying stable cycling performance and safe operation. The outcomes indicate a high lithium storage capability, remarkable conductivity, smooth lithium mobility, and efficient voltage profile, validating the BPN/G bilayer as an ideal negative electrode component for lithium-ion secondary batteries.

Key words: *Biphenylene-Graphene Bilayer, van der Waals Heterostructure, Radial Distribution Function, Diffusivity, Open Circuit Voltage, Convex Hull.*

Reference:

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***Presenter/Author Address and E-mail ID:** Department of Chemistry, Indian Institute of Technology, Ropar, Rupnagar, 140001

E-mail: nidhi.20cyz0019@iitrpr.ac.in

Studies of Photophysical Behavior of Fluorescent Cationic Dye in Cubosomes: Their Use in Sensing Applications (P-30)

K. R. Khaparkhuntikar[a], A. Chatterjee[a], and M. Banerjee[a]

[a] *Department of Chemistry, BITS, Pilani- KK Birla Goa Campus, NH 17B Bypass Road,*
Zuarinagar, Goa, 403726, India

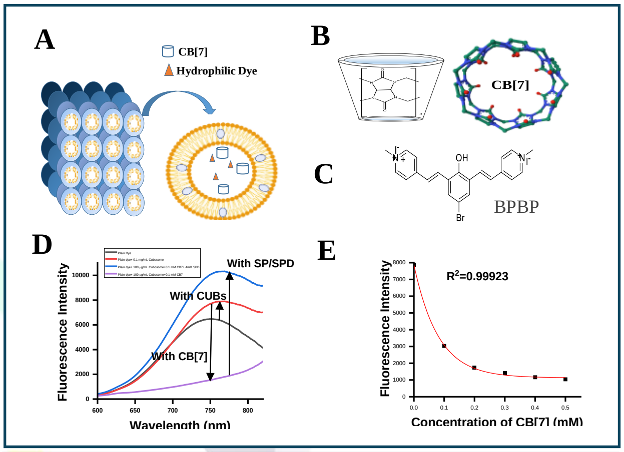

Figure 1. A) Representative structure of cubosome and possible interaction B) Structure of CB[7] C) Structure of cationic dye D),E) Fluorescence change upon the addition of each component of the supramolecular sensing system.

Cubosomes are biocompatible, nanostructured liquid crystalline carriers with a unique bicontinuous cubic phase morphology, formed through the self-assembly of amphiphilic lipids in specific ratios[1]. These nanoparticles exhibit reversed cubic phases and possess distinct physicochemical properties that render them a promising platform for drug and gene delivery[1]. Fluorescent molecules or materials are commonly employed for tracking cargo within drug delivery systems. The photophysical behaviour of fluorescent materials in cubosomes remains relatively unexplored. Cucurbit[n]urils, macrocyclic oligomers consisting of glycoluril units linked by methylene bridges, are recognized for their high affinity towards neutral and cationic species[2]. We have explored the unique affinity of Cucurbiturils (CB[6]) and (CB[7]) towards developing various supramolecular sensors for spermine (SP) and spermidine (SPD)[3,4]. In the current project, we intended to use a monoolein derived cubosome-CB[7]-cationic dye nanoenzyme for the supramolecular detection of SP and SPD. Upon the addition of CB[6] and CB[7] to a solution containing cubosomes and a fluorescent dye, a significant reduction in fluorescence intensity was observed. This quenching effect is likely due to the preferential interaction of the dye with the cationic binding sites of the CB[6] and CB[7] within the cubosomal structures. The host-guest conjugate remains non-fluorescent. Subsequently, the fluorescence is retrieved upon the introduction of spermine (SP) and spermidine (SPD) into the sensing system, suggesting that CB[6] and CB[7] preferentially release the cationic dye and bind to SP and SPD. Thus, a sensitive supramolecular sensor is developed in this manner.

Keywords: cubosomes, spermine, spermidine, supramolecular chemistry, dye

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Presenting Author: p20240801@goa.bits-pilani.ac.in (K. R. Khaparkhuntikar)

Conducting Polymers from Natural Fibers (P-31)

Nidhi Nitin Parmekar[#], Rashmi Chauhan*

Abstract:

Polymers are generally considered as insulating materials as their conductivities are below 10^{-10} S/cm in their neutral state. However, polymers with conjugated bond structures are organic polymers that act as intrinsic conductors. The emeraldine salt form of polyaniline (PANI), a conductive polymer, is widely utilized owing to its facile synthesis and superior environmental stability. In this work we report the synthesis and characterization of conducting polymers from natural fibers via copolymerization of keratin fibers (KF) with aniline. The copolymer formation was confirmed via FT-IR and SEM. In FT-IR the peak at 826 cm^{-1} corresponds to the vibration of C-C and C-H bond in the benzenoid structure of PANI. The characteristic peaks at 1556 cm^{-1} and 1478 cm^{-1} are due to the stretching vibration of the quinoid ring and benzenoid ring, respectively.[1] The peaks at 1654 and 1544cm^{-1} peaks correspond to the presence of amide I and Amide II functional groups of the KFs. [2]

The SEM images of the keratin fibers show distinct cuticle scales on the surface. On copolymerization of PANI the surface of fibers shows agglomeration of nanofibers of PANI. These copolymers exhibit conductivity in the range of 5.307×10^{-3} S/cm to 1.061×10^{-3} S/cm. To know the effect of dopants these polymers were de-doped with ammonium hydroxide and re-doped with dopants such as I_2, Br_2 and H_2SO_4. The measured conductivity obtained was 1.683×10^{-3} S/cm, 1.559×10^{-2}S/cm, and 1.061×10^{-3}S/cm respectively. The copolymers have also shown potential as sensor for ammonia gas at room temperature as their conductivities change significantly in the presence of ammonia vapors.

Key words: *Polyaniline, Copolymerization, Keratin fiber, Conductivity, Gas Sensor.*

Reference:

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#Presenting Author Address and Email id: Department of Chemistry, BITS Pilani K. K. Birla Goa Campus, p20230014@goa.bits-pilani.ac.in

*Corresponding Author Address and Email id: Department of Chemistry, BITS Pilani K. K. Birla Goa Campus, rchauhan@goa.bits-pilani.ac.in

Harnessing Microwave Irradiation and Water Surface for Efficient Synthesis of C-2 Functionalized Indolizines via Baylis-Hillman Reaction (P-32)

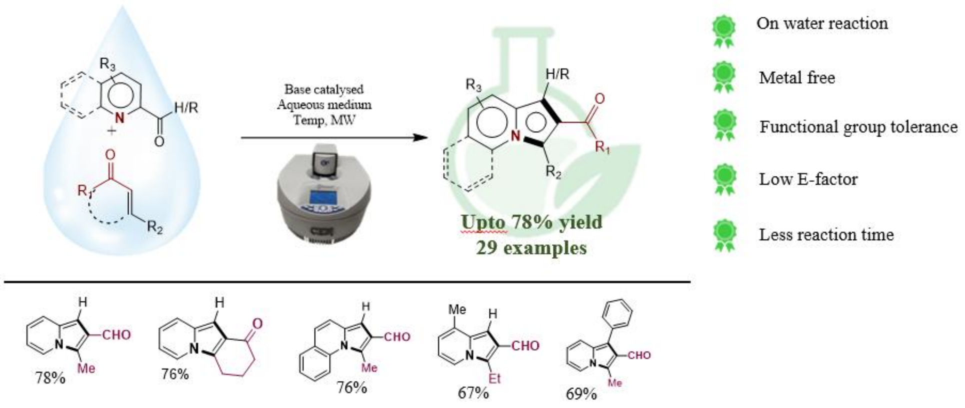
Soumik Saha,[a] Shravya B,[a] Shaurya Aneja,[a] Amrita Chatterjee[a]* and Mainak Banerjee[a]*

[a] Department of Chemistry, BITS Pilani, K K Birla Goa Campus, NH 17B Bypass Road, Zuarinagar, Goa 403726, INDIA

Abstract:

Indolizines, as nitrogen-containing heterocycles, are valued for their unique electronic and structural properties due to their fused bicyclic ring. These frameworks are found in many natural products and therapeutics.1 The "On-Water" platform enhances reaction sustainability, minimizing waste generation and aligning with green chemistry principles.2 Combining microwave irradiation with water as the reaction medium is a powerful tool for accelerating reactions.3,4 Herein, we present a sustainable method for synthesizing 2-acylindolizine scaffolds from 2-pyridinecarboxaldehyde and α,β-unsaturated compounds via a Morita-Baylis-Hillman (MBH) reaction, followed by microwave-assisted cyclization in water. We explored various scaffolds with different electronic properties in both pyridine and α,β-unsaturated compounds, observing minimal electronic effects.

Scheme:



Key words: *Microwave, Indolizine, Baylis-Hillman reaction, On-water*

Reference:

[1] V. Sharma, V. Kumar, Med. Chem. Res. 2014, 23, 3593–3606.
[2] A. Chanda, V. V. Fokin, Organic synthesis “on water”, Chem. Rev. 2009, 109, 725–748.
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Presenter/Author Address and E-mail ID:

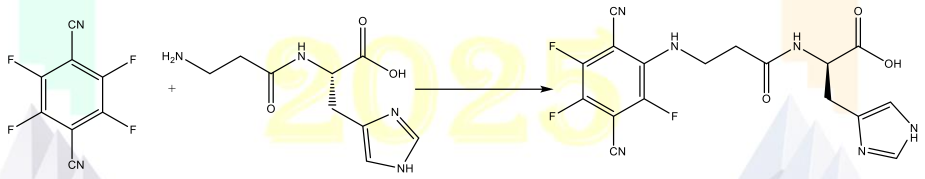
p20240015@goa.bits-pilani.ac.in; p20200049@goa.bits-pilani.ac.in; mainak@goa.bits-pilani.ac.in; amrita@goa.bits-pilani.ac.in

Mono-amino terephthalonitrile based single benzene fluorophores in selective fluorimetric detection of biothiols (P-33)

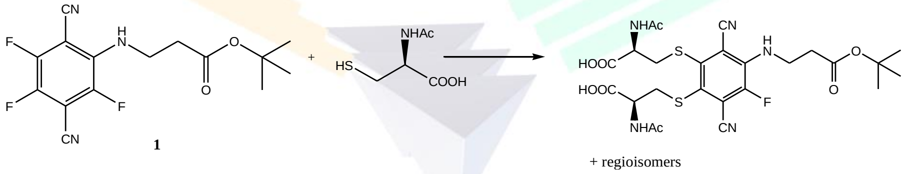
Ankita Sinha, **Subhadeep Banerjee***

Department of Chemistry, BITS Pilani, K K Birla Goa Campus, NH 17B Bypass Road, Zuarinagar, Goa 403726, INDIA

The selective detection of biological thiols and amines is crucial in bioanalytical applications. While tetrafluoroterephthalonitrile (TFTN) is known to react readily with primary amines,[1],[2] it has also been reported to undergo rapid nucleophilic aromatic substitution with thiols like cysteine.[3] We studied its reactivity with carnosine (Scheme 1), a biological dipeptide bearing a primary amine. Fluorescence spectral and LC-MS analyses confirmed the formation of a stable adduct, reinforcing TFTN's broad reactivity against all nucleophiles and thereby we may infer that TFTN would be an unsuitable candidate as a selective chemosensor only for thiols. To enhance selectivity, we evaluated the mono-aminoterephthalonitrile (AmTN) single benzene fluorophores (SBFs), particularly compound **1**, which demonstrated a preference for thiols over amines. This is due to its modulated S_NAr reactivity arising from its slightly less electrophilic nature, as compared to the parent TFTN, thereby preferring the more nucleophilic thiol unit. Fluorescence spectroscopic titration revealed a significant response to addition of N-acetyl cysteine (NAC) and glutathione (GSH), accompanied by red-shifted emission maxima (from 460 nm for **1** to 480 nm for the adducts). Additionally, ^{19}F NMR spectroscopy and LC-MS data confirmed selective thiol substitution in **1** with both NAC and GSH. We also tried the reaction between **1** and carnosine and we observed that the reaction proceeded very slowly. These findings highlight mono-AmTN SBFs as promising fluorescent chemosensors for thiol-containing bioanalytes.[4]



Scheme 1 Reaction of TFTN and carnosine.



Scheme 2 Reaction of **1** with N-acetyl cysteine (NAC)

Key words: *Fluorescence, single benzene fluorophores, amino-terephtalonitriles, bioanalysis*

Reference: [1] T. Raghava, A. Chattopadhyay, P. Bhavana, S. Banerjee, *Chem. Asian. J.* **2023**, *18*, e202201314. [2] T. Raghava, S. Banerjee, A. Chattopadhyay, *J. Org. Chem.* **2023**, *88*, 15708–15716. [3] H. Zhang, R. Liu, J. Liu, L. Li, P. Wang, S. Q. Yao, Z. Xu, H. Sun, *Chem. Sci*., **2016**, *7*, 256-260. [4] Manuscript under revsion with Asian Journal of Organic Chemistry

***Presenter/Author E-mail ID:** p20230412@goa.bits-pilani.ac.in

Exfoliated gC_3N_4-CdS-MXene as an Efficient Z-Type Heterojunction for Oxygen Evolution and Dye Degradation under Visible Light at Low Bias Voltage (P-34)

Darshana Anand Upar, Rajeshvari Samatbhai Karmur, Manash R. Das, C. Prathibha, Narendra Nath Ghosh*

*Nano-materials Lab, Department of Chemistry, BITS-Pilani K K Birla Goa Campus, Zuarinagar, Goa-403726, India.

*E-mail of presenting author: p20220049@goa.bits-pilani.ac.in *Corresponding author: naren70@yahoo.com*

Abstract:

The development of highly active catalysts for photo/electro/photoelectro catalytic reactions, such as oxygen evolution reaction (OER) and water treatment, is crucial for sustainable energy and environmental technologies. Catalysts that efficiently operate under solar light and have low external bias are especially valuable. This study introduces a novel all-solid-state Z-scheme g-C_3N_4-CdS-MXene heterojunction catalyst, which shows excellent performance in both OER and dye degradation, making it ideal for energy and environmental applications.

The g-C_3N_4-CdS-MXene heterojunction combines photocatalytic stability of g-C_3N_4, visible-light activity of CdS, and MXene's conductivity, forming a Z-scheme that improves charge separation and catalytic efficiency. The catalyst's photocatalytic performance was evaluated by degrading Methylene Blue (MB) under simulated solar light, showing excellent efficiency. In electrocatalytic tests for OER, the g-C_3N_4-CdS-MXene catalyst exhibited an early onset potential of 1.58 V, a low overpotential of 350 mV at 10 mA cm^{-2}, and a Tafel slope of 98 mV dec^{-1}, indicating its high electrocatalytic efficiency. In photoelectrocatalytic tests, the catalyst achieved 100% Methylene Blue degradation in 4 minutes under solar light at a low bias of 350 mV, showcasing its exceptional performance for environmental cleanup and dye degradation in textile wastewater.

Overall, g-C_3N_4-CdS-MXene heterojunction is a promising catalyst for simultaneous oxygen evolution and dye degradation, offering efficiency under visible light, low bias operation, and broad applicability for sustainable energy and environmental remediation.

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1. Upar, D. A.; Karmur, R. S.; Das, M. R.; Prathibha, C.; Ghosh, N. N., Exfoliated g-C_3N_4-CdS-MXene an efficient all-solid-state Z-type heterojunction serving as efficient photo/electro/photoeletro catalyst for oxygen evolution reaction and dye degradation under visible light at low bias voltage. *App. Surf. Sci.* **2024,** *677*, 161030.

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