Memorial Lectures

Prof. M. K. Rout Memorial Lecture

Three Component Dicarbofunctionalization of Unsymmetrical Alkynes

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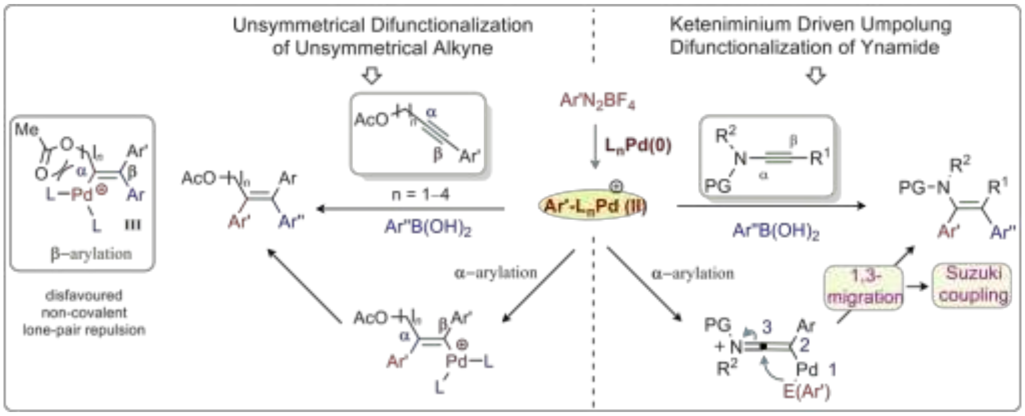
Presented here is the discovery of a regio- and stereoselective *syn*-1,2-dicarbofuctionalizationof unsymmetrical internal alkynes. A cationic Pd-catalyzed three-component coupling of aryl diazonium salts and aryl boronicacids (orolefins) with unsymmetrical alkynes enables access to tetra-substituted unsymmetrical olefins. Density functional theory (DFT) studies rationalize the selectivity of the reaction. Synthetic versatility of the carboxylate and amino bearing highly-substituted olefinsis also presented.



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Prof. S. R. Mohanty Memorial Lecture

Nanoscale materials for sensing and removal of hazardous substance

R.K. Dutta

Department of Chemistry and Centre for Nanotechnology, IIT Roorkee

Clean water is a necessity for sustainable growth of a society and a requirement for strengthening economy of a nation. In this scheme, rapid on-site sensing of hazardous substances e.g., toxic metal ions, dyes, phenols, pesticides, residual drugs, microorganisms, etc and their removal from water is a scientific challenge. Here we will discuss some possible solutions using three verticals of nanotechnology.

In the first part, we will discuss size dependent properties of inorganic quantum dots and crystalline carbon dots for detecting wide range hazardous substances. Though CdS quantum dots have been well explored as a probe for detecting wide range of metal ions, but till 2015 its application as a probe for detection of ultra-trace levels of uranyl ions was eluded. We will discuss our group's invention of a highly sensitive and selective method for detection of sub-ppb levels of uranyl ions by a novel strategy of double capped CdS quantum dots., via photoluminescence quenching. In addition, we will discuss a possibility of an alternative analytical signal comprising ratio of photoluminescence lifetime of a pristine probe and that of the probe treated with analyte. We will discuss this case using CdTe/CdS core shell type quantum dots for selective detection of nickel ions. Besides, metal-free probes based on amino acid mediated crystalline carbon dots as potential probes for analytical purposes.

In the second part, we will discuss on strategies for synthesizing different types photocatalysts with tunable band structure to produce highly oxidizing species which can potentially mineralize hazardous organic compounds. Semiconductor type nanoparticles upon interaction with light of suitable energy can trigger photoexcitation of electrons and holes. The inhibition of electron-holes recombination is a desirable phenomenon for producing reactive oxygen species (ROS). We will discuss the involvement of these reactive oxygen species towards lipid peroxidation and consequential antibacterial activity by destruction of the cell membrane. The production of ROS is involved in degradation of environmentally hazardous substances. We will discuss various photocatalytic degradation strategies by tuning the property of the materials, e.g., by doping, by making composites and by synthesizing heterostructures.

In the third and the final part, we will discuss about some specific cases for removal of uranyl ions by adsorption on chemically modified reduced graphene oxide. Here the emphasis is on synthesizing adsorbent with multifunctional groups to enhance the uranyl adsorption sites. Reduction of graphene oxide with adenosine monophosphate resulted into a highly efficient adsorbent for rapid adsorption of uranyl ions from aqueous medium. Details will be discussed in the talk.

Prof. P. L. Nayak Memorial Lecture

Circular Economy Driven Sustainable Polymeric Materials: Future is now in Mitigating Climate Change

Amar K Mohanty
Bioproducts Discovery and Development Centre
Department of Plant Agriculture & School of Engineering
University of Guelph, ON, Canada

The emission of the major greenhouse gas (GHG) CO_2 from human activities has reached the highest level in history. Our planet is in crisis! Plastic waste accumulation and plastic pollution are creating serious concerns to our health and environment. Plastic production and incineration pump ~900 million tons of greenhouse gases (GHGs) into the atmosphere annually and are projected to reach 3 billion tons by 2050. Of the 440 million tons of plastics the world produces annually, only about 9% is recycled. A more resilient, circular, and low-carbon economy is at the core of the world's waste plastic recovery plan. Plastic and composite materials are needed in our daily life, with uses spanning from packaging, auto-parts, electronics, to medical devices. By 2050, the annual production of plastics is projected to reach two billion tons globally. Around 300 million tons of plastic wastes are accumulated on our earth annually, equivalently to the weight of the entire population. Each second ~10,000 plastic bags and one garbage truck of textiles are thrown away. With the current trend, by 2050 there will be more plastic in the ocean than fish. Waste plastic creates micro-plastics (<5 mm in size), which can pose direct threats to human health as we consume them due to their presence in drinking water, fruits and fish. Their detection in human blood and even in human breast milk is shocking and alarming. The "Second Age of Plastic" is imminent to reduce and eliminate plastic waste concerns through "Sustainable Polymers". Sustainable materials comprise polymers and composites derived from wastes, recycled materials, bio-renewables and their combinations. Two types of materials, namely (a) bio-based biodegradable, and (b) bio-based non-biodegradable but recyclable materials can help create the circular economy of plastics. This lecture will highlight new sustainable composites developed for eco-friendly and compostable packaging as well as green and lightweight automotive parts and how they impact the resolution of environmental problems. A transition to a low C economy requires circularity. The use of bio C (new carbon) unlike petro-carbon (old C) will help reduce GHG emissions and accelerate the decarbonisation. Through innovation and disruptive technology development, we can combat climate change to secure a healthy economy and the environment for us all.

Prof. G. Sahu Memorial Lecture

Stability and Reactivity of Co-ordination Complexes in Solution

A.C. Dash
Professor of Chemistry, Utkal University, Bhubaneswar 751004

Metal–ligand interactions result in the formation of Coordination Complexes. This area is too extensive considering possible variations of metal ion, mono- and poly dentate ligand with different donor sites, different types of coordination complexes, medium and mechanistic aspects. This lecture is, therefore, not intended to project a comprehensive survey. It is primarily devoted to discussions on the stability and reactivity of select complexes of some first row transition metal ions investigated in our laboratory. The relevant kinetics and thermodynamic studies in aqueous, mixed solvent, and micellar media will highlight mechanistic aspects.

Award Lectures

Prof. Dayanidhi Patnaik Award Lecture

Exploring the Inclusion Complex Formation of 3-Acetylcoumarin with β-cyclodextrin and its Delivery to a Carrier Protein: A Spectroscopic and Computational Study

Nirmala Niharika Bhuyan[a], Ankita Joardar[a], Bhawani Prasad Bag [b], Hirak Chakraborty[a,*], Amaresh Mishra[a,*]

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Abstract

Drug solubility is an important parameter to determine the biological efficacy of a drug. To avoid the difficulties of drug insolubility, macrocyclic hosts like cyclodextrins (CDs)are used to enhance the solubility through the formation of inclusion complex. CDs are popular as drug-delivery vehicle as it dissociates the drug molecule at its binding destination, and has high biological tolerance. In this work, we report on the inclusion complex of 3-acetylcoumarin (3-AC) that induces apoptosis in breast cancer cells with β-CD exploiting steady-state and time-resolved fluorescence spectroscopyin tandem with molecular docking. We have further studied the transfer of 3-AC from its β-CDinclusion complex to BSA and determine the microviscosity of the β-CD cavity in presence of 3-AC. Spectroscopic and molecular docking results confirmed1:2 inclusion complex formationof3-AC:β-CD with high binding affinity. Moreover, the fluorescence resonance energy transfer and molecular docking results suggest that 3-AC partitions to the hydrophobic domain of BSA near the Trp 123. Our results demonstrate an efficient and convenient way of exploring bioavailability by increasing the aqueous solubility of biologically active 3-AC and its transfer to a carrier protein such as BSA.

Prof. R. C. Tripathy Award Lecture (Inside State)

Conformational Polymorphs and Fluorescence Chemosensor of 1-(6-aminopyridin2-yl)-3-phenylthiourea

B. R. Jali

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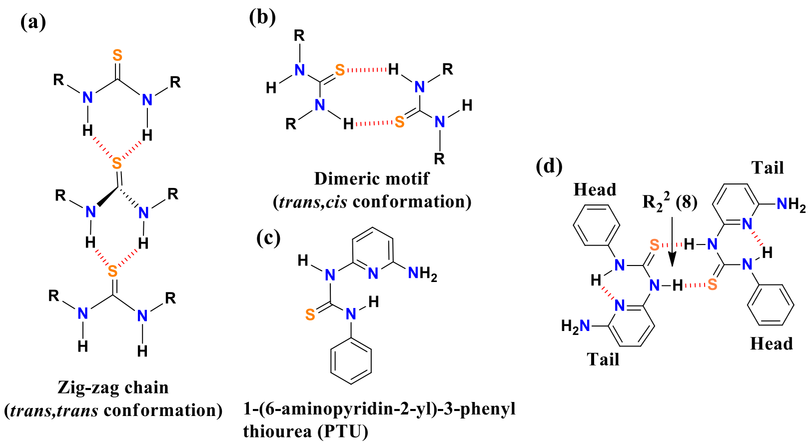
Three conformational polymorphs and two solvates of an asymmetrical N,N'-disubstitutedthiourea derivative namely, 1-(6-aminopyridin2-yl)-3-phenylthiourea (PTU) have been reported here. In all the polymorphs and solvates, the PTU molecules self-assemble into dimers in the solid state, via two complementary N-H···S bonds resulting the formation of $R_2^2(8)$-type of H-bond motif. The two PTU molecules in these dimers interact with each other in a head to tail fashion. Furthermore, the PTU molecule adopts trans, cis- conformation with an intramolecular N-H···N interaction in all the crystals. However, the orientation of the aminophenyl ring with respect to the phenyl ring plays crucial role in the solid state packing of the polymorphs and solvates. Additionally, three polymorphs are distinguishable by C-H···π, N-H···π and π···π interactions. The polymorph PTU-1 crystallizes in P-1 space group with Z'=2, whereas the polymorphs PTU-2 and PTU-3 crystallize~~s~~ in Pbcn and R-3 space group respectively, with Z'=1. On the other hand, the solvate PTU-DMSO crystallize in $P2_1/c$ with 1:1 host-guest ratio, and PTU-Morpholine exists in P-1 space group with 2:1 host guest ratio. Hirshfeld surface analysis was carried out to compare the intermolecular interactions in the three polymorphs and two solvates of the title compound. The 2D fingerprint analysis of each of the polymorphs reveals that besides the H···H interactions, C···H and S···H interactions contribute more to the generation of polymorphs. The contribution of C···H interactions in both PTU-2 (31.6%) and PTU-3 (32.1%) are much higher than that of any molecule in PTU-1 (19.8% and 23% for Molecule A and B respectively). Additionally, a tiny amount of π···π interaction was observed (C···C interaction, 4.5%) in polymorph PTU-1, which was absent in PTU-2 and PTU-3.

Key Words: Thiourea, Polymorphism, H-bonding, Hirshfeld Analysis, Finger Print plot.



Zig-zag chain (*trans,trans* conformation)

Dimeric motif (*trans,cis* conformation)

1-(6-aminopyridin-2-yl)-3-phenyl thiourea (PTU)

Figure 1: (a) and (b) Hydrogen-bonding motifs typically observed for disubstitutedthiourea in the solid state; (c) Structure of 1-(6-aminopyridin2-yl)-3-phenylthiourea (PTU); and (d) Formation of dimers through $R_2^2(8)$-type of cyclic motif via two complementary N-H···S interactions.

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Prof. G. B. Behera Best Ph.D. Thesis Award

Unravelling the Role of Heme in Bacterioferritin and Regulating Ferritin Self-Assembly: Implication towards Health and Diseases

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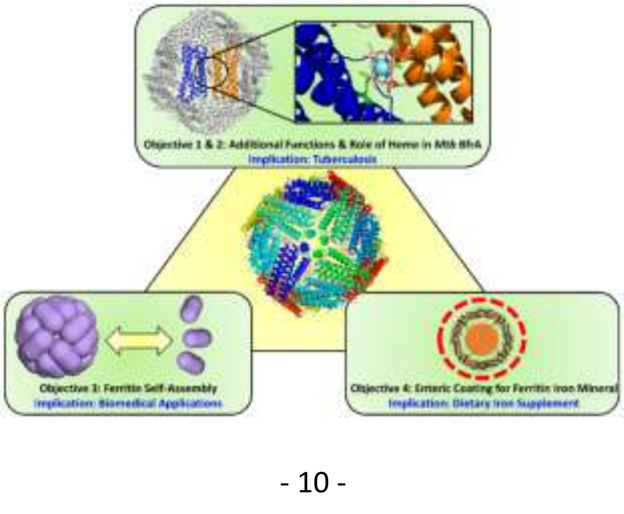
Iron behaves as a double-edged sword, i.e., beneficial as well as harmful, for both host and pathogens. During the host-pathogen battle for iron, host secretes H_2O_2 to kill pathogens but pathogens employ counter mechanisms/antioxidative proteins to detoxify it. *Mycobacterium tuberculosis* (*Mtb*), the causative pathogen of tuberculosis, expresses two maxi-ferritins: a heme binding bacterioferritin (BfrA) and a non-heme ferritin (BfrB) but not the mini-ferritin, i.e., Dps protein (which protects DNA from H_2O_2 induced oxidative stress). In the absence of Dps, *Mtb* must have evolved with other defensive strategies. Moreover, the expression of BfrA along with BfrB possibly suggests the existence of some additional functions for BfrA/heme. The current study on *Mtb*BfrA revealed its two new functions (catalase and Dps-like DNA protection activity) along with rapid ferroxidase activity. The presence of heme in *Mtb*BfrA contributes to its enhanced cage stability and reductive iron mobilization. Ferritin proteins are hollow, spherical, nanocaged structures, which are self-assembled from 24-polypeptide subunits and are capable of storing ~4500 iron atoms as ferrihydrite mineral. Although the factors that drive self-assembly process and control its kinetics are little investigated, the inherent reversibility of this phenomena has been recently exploited in cellular imaging and targeted drug delivery. The laser light scattering studies on ferritin self-assembly identified subunit monomers/dimers as starting materials and revealed the factors that altered the kinetics whereas electrostatics predicted the critical amino acid residues. In addition, the ferritin environment was modified by a biopolymer (guar gum) to repress iron mobilization by inhibiting the cage disintegration under acidic conditions, possibly suggesting its implication in oral iron formulations. Therefore, the current dissertation not only strengthens the understanding of the new functions of *Mtb*BfrA along with the role of heme, to possibly serve as a future platform to curb tuberculosis, but also provides insights on ferritin self-assembly to optimize the loading/unloading of drugs and nanomaterials for biomedical applications.



Prof. Donald S. Matteson and Prof. P. K. Jesthi Award Lecture

Recent Advancement on Decarbonylation Reactions Assisted by Ru-complexes: Synthetic and Mechanistic Approach

Rupam Dinda

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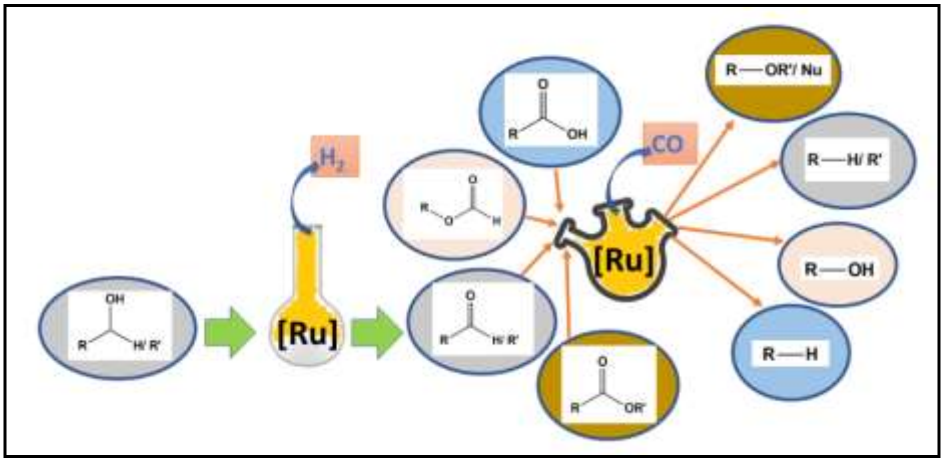
My talk in this frontier article will cover the recent advancements in the ruthenium complex catalysed decarbonylation reactions of different types of carbonyl compounds and provide a direction towards the mechanistic understanding involved in this.[1] The mechanistic pathways give the new strategies for the use of appropriate ruthenium-catalyst, increase the substrate scope and also help in the synthesis of new complexes having multiple functionalities. The content of the article is categorized on the basis of the use of the substrates. The new challenges of the decarbonylation reaction depend on the development of new ruthenium-catalysts[2] and the efficiency of the catalytic cycles. Therefore, this short review will give an overall idea about the progress in the field of ruthenium-complex catalysed decarbonylation, catalytic pathways, synthetic applications, and utilities of their products and side products.



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Prof. Sripati Pani Memorial Award

Bioinspired Assembly to Simultaneously Heterogenize Polyoxometalates as Nanozymes and Encapsulate Enzymes in a Microstructure for Peroxidase-Mimicking Activity.

Jayadev Nayak, Rakesh Chilivery, A. Kiran Kumar, Goose Begum, Rohit Kumar Rana*

Abstract

A polyamine mediated bioinspired strategy to assemble polyoxometalate (POM) (phosphotungstic acid (PTA)/phosphomolybdic acid (PMA)) nanoclusters and glucose oxidase (GOx) generating microsphere structures under very mild reaction conditions is demonstrated. The non-covalent interactions between multivalent anions (citrate ions) and polyamine chains (poly(allylaminehydrochloride), PAH) are key to the assembly process, which results in positively charged coacervates allowing the assembly of GOx and POM nanoclusters into microsphere structures. As observed in the process, in addition to have impact on the size, composition and textural properties of the spheres, the pH of the reaction medium has a pivotal role in safeguarding the enzyme. The enzyme assay shows that the activity of GOx is totally preserved during the assembly process and the enzyme loading is slightly improved with the increase in the pH of the medium. In contrast, a physical mixture of GOx and POM leads to inactivation of the enzyme retaining only ~50% GOx activity. The peroxidase like activity of PTA nanoclusters assembled in enzyme-nanozyme microspheres as indicated by maximal velocity (V_{max}) and catalytic constant (K_{cat}) values is improved by 3-5 folds with the increase in the pH, which in turn is attributed to the smaller size of the microspheres facilitating a better diffusion of reactants, intermediates and products. Importantly, the confinement and proximity of GOx and POM in the microspheres not only play crucial role in defining the peroxidase like activity of POM, but also endow high selectivity (by virtue of GOx) in detecting glucose at physiological pH conditions. Thus the microsphere-assembly while enables an effective heterogenization of the POM as nanozyme, simultaneously addresses the issues related to the high cost and instability associated with natural peroxidases.

Keywords: peroxidase, glucose oxidase, polyoxometalates, glucose sensing, microstructures.

Prof. Bimbadhar Nayak Memorial Award

Room temperature phosphorescence from phosphoramides: Photophysics unveiled by optical spectroscopy and DFT

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[2]Current address: Technical University Munich Campus in Straubing, Germany.

Room temperature phosphorescent (RTP) materials have attracted considerable research attention owing to their potential applications in organic light-emitting diodes (OLEDs), sensing, and time-gated bio-imaging applications. Recently, enormous research efforts have been devoted to developing metal-free organic phosphors because of their low toxicity and environment friendly nature. We report the design and synthesis of a series of room temperature phosphorescent phosphoramides with a donor-acceptor architecture.[1]All the compounds show structureless fluorescence with a nanosecond lifetime in dilute solutions. However, these compounds show dual fluorescence and room temperature phosphorescence (RTP) in the solid state. Both the intensity and energy of luminescence depend on the heteroatom attached to the phosphorus centre. The details of the photophysical studies will be presented in the talk.

References:

1. S. Jena, J. Eyyathiyil, Santosh K. Behera, MahoKitahara, Yoshitane Imai, P. Thilagar, *Chem Sci.,* 2022, 13, 5893-5901.

Prof. Manju Mishra Award

Energy Material development from Spent Lithium ion Battery: a pathway towards sustainable technology

Mamata Mohpatra[1,2]

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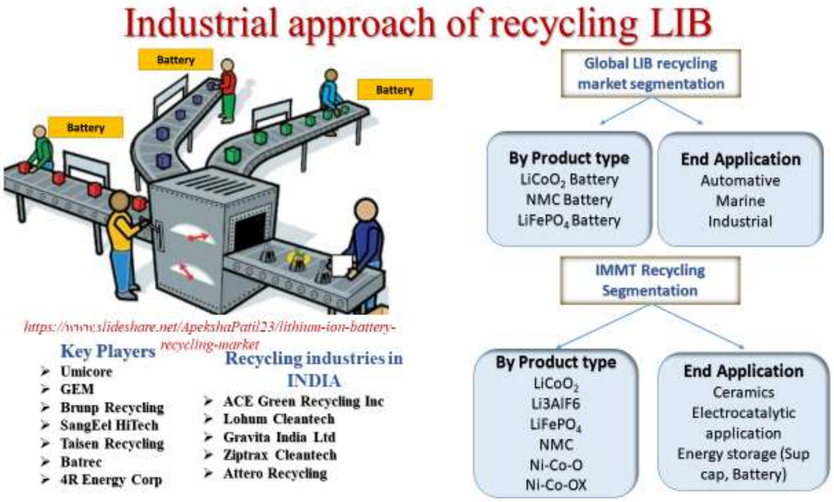
Lithium ion batteries are the family of rechargeable battery consisting of numerous cells connected to deliver the required voltage, power, and energy. The rechargeable lithium-ion batteries which supply majority of the world's energy needs are being produced at an accelerated rate which may eventually results in the enormous amount of battery-waste. [1]. The inevitable production reduced up-gradation and application of LIBs leads to the enormous amounts of spent LIBs due to their limited life expectancy (about 3 to 10 years) and charging-discharging of 1000 cycles [2]. As the electric vehicle sector is booming up, it is expected that around 1 million of the battery will reach their end-of-life (EOL) by 2025. To recover back the metal value from the exhausted batteries, trials are going on for the recycling of LIBs. It can diminish the effects of waste and eliminates the supply chain issue for the indigenous battery manufacturer. Existing solutions still have issues in the real world, despite the economic and environmental benefits of efficiently recovering raw materials from old batteries. At CSIR-IMMT, R&D efforts are going on for the development of energy materials along with the process based on close loop recycling through an innovative approach. For recycling of lithium-ion batteries based on heterogeneity of the starting materials, two processes have been developed. In contrast to more conventional processes, regeneration of electrode materials as products such as high crystalline graphite, graphene oxides, NMC and NCA types cathode materials, phosphate materials, aluminum based ceramic electrode material, oxide based electrocatalytic materials have been achieved[3-6]. Product purity evaluation and performance through coin cell testing is periodically evaluated by monitoring the impurities in the product. The feasibility of addressing gaseous emission during the process development has been taken up to minimize the environmental issues.



Industrial approach of recycling LIB

Global LIB recycling market segmentation

By Product type
$LiCoO_2$ Battery
NMC Battery
$LiFePO_4$ Battery

End Application
Automative
Marine
Industrial

IMMT Recycling Segmentation

By Product type
$LiCoO_2$
Li3AlF6
$LiFePO_4$
NMC
Ni-Co-O
Ni-Co-OX

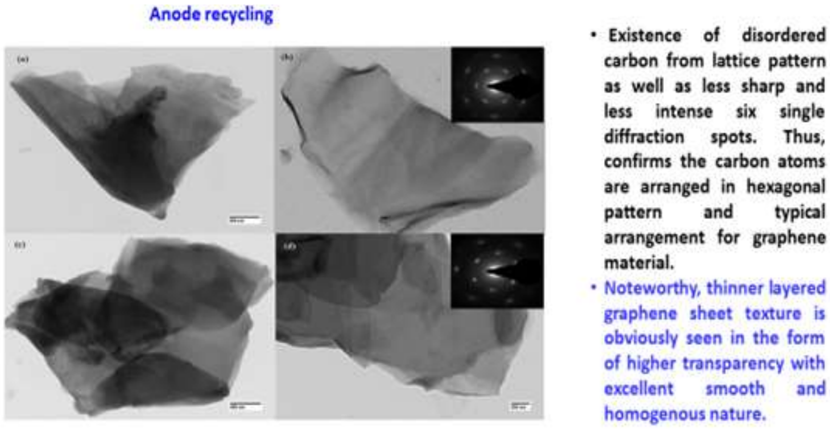
End Application
Ceramics
Electrocatalytic application
Energy storage (Sup cap, Battery)

https://www.slideshare.net/ApekshaPatil23/lithium-ion-battery-recycling-market

Key Players
- Umicore
- GEM
- Brunp Recycling
- SangEel HiTech
- Taisen Recycling
- Batrec
- 4R Energy Corp

Recycling industries in INDIA
- ACE Green Recycling Inc
- Lohum Cleantech
- Gravita India Ltd
- Ziptrax Cleantech
- Attero Recycling

Fig.1 : Global and CSIR-IMMT approach for the material development from Spent LIB



Anode recycling

- Existence of disordered carbon from lattice pattern as well as less sharp and less intense six single diffraction spots. Thus, confirms the carbon atoms are arranged in hexagonal pattern and typical arrangement for graphene material.
- Noteworthy, thinner layered graphene sheet texture is obviously seen in the form of higher transparency with excellent smooth and homogenous nature.

Fig.2 : Anode recycling at CSIR-IMMT from Spent LIB

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Oral Presentations

OP-01

Understanding the Role of Lipid Composition in Protein Trafficking: A Case Study with Apolipoprotein E Signal Peptide

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Soluble secretory and membrane proteins contain a short stretch of signal peptide (SP) at their N-terminal end, which gets cleaved after reaching the destination organelle. However, the importance of SP in protein trafficking is not yet clear. The lipid compositions of cellular organelles are highly heterogeneous, and the preference of SP toward a particular lipid composition might play a key role in the unidirectional trafficking of protein. To understand the preference of Apolipoprotein E (ApoE) toward the endoplasmic reticulum (ER), we have studied the interaction of its SP with membranes of varying lipid compositions. The importance of cholesterol is paramount as subcellular organelles contain a differential amount of cholesterol; the endoplasmic reticulum (ER) contains the least amount of cholesterol. We have utilized batteries of steady-state and time-resolved fluorescence techniques to understand the affinity of ApoE signal peptide toward membranes of varying lipid compositions. We observed that the ApoE signal peptide binds tightly with membranes devoid of cholesterol, and binding affinity reduces with increasing concentration of membrane cholesterol. Our results suggest the importance of membrane composition in the unidirectional movement of ApoE toward ER. This property of SP can further be utilized for the development of organelle-specific cargo delivery.

OP-02

Study of Thermal, Dielectric, and Sensing Properties of Gold Nanoparticle decorated functionalized Single-Walled Carbon Nanotubes reinforced Polyaniline Nanocomposites

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The current research is based on the improvement of the homogeneous dispersion of the nanofillers by decorating their surface with conducting polymers and studying their different properties. The gold nanoparticles (AuNPs) decorated functionalized single-walled carbon nanotube (f-SWNTs) hybrid nanofillers (Au@f-SWNTs) reinforced conducting polyaniline (PANI) nanocomposites (PANI/Au@f-SWNTs) are synthesized through in situ polymerization technique to analyze the effect of nanofiller on the thermal, dielectric, and sensing properties. Characterization of the polymer nanocomposites has been studied through different techniques, as the morphology of the nanocomposites is studied by scanning electron microscopy (SEM) and Field emission scanning electron microscopy (FESEM). The chemical interaction and nanostructural characteristic of the synthesized nanocomposites are characterized by employing ultraviolet-visible (UV-Vis) spectroscopy, Fourier-transform infrared (FTIR) spectroscopy, Raman analysis, X-ray diffraction (XRD) analysis, and X-ray photoelectron spectroscopy (XPS). The nanoparticle size distribution of the nanocomposite is analyzed by the dynamic light scattering (DLS) technique. The thermal and dielectric properties of the nanocomposite are investigated by thermogravimetry-differential scanning calorimetry (TG-DSC) and dielectric relaxation spectroscopy (DRS) techniques. The sensing properties of the nanocomposites are examined through UV-Vis analysis. The main objective of this research work is to modify the surface of AuNPs and f-SWNTs using PANI and as-synthesized Au@f-SWNTs hybrid nanofillers dispersed within PANI to enhance the materials properties (thermal, dielectric, and sensing properties) of the conducting nanocomposites.

Keywords: Single-walled Carbon Nanotube; Gold Nanoparticles; Polyaniline; Nanocomposites; Thermal, Dielectric and Sensing Property

OP-03

Optimization of Praseodymium-based Perovskite as Electrocatalyst for Oxygen Reduction Reaction

Bibhuti Bhushan Nayak, Purnendu Parhi*
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ABO_3-type oxides with flexible and adjustable A- and B- sites are ideal model catalysts to unravel the relationship between the electronic structure and electrocatalytic activity e.g.-oxygen reduction reaction (ORR). It has been well understood in our recent work that the secondary metal dopant at the A-site can regulate the electronic structure and improve the ORR activity. Praseodymium based perovskites $Pr_{1-x}Sr_xMnO_3$ (x=0.1, 0.2, 0.3, 0.4) denoted as PSM-0.9, PSM-0.8, PSM-0.7 and PSM-0.6 respectively

were prepared by sol-gel technique. The structural properties and morphology of the prepared catalysts are studied with the help of XRD, SEM, and XPS. Oxygen reduction reaction (ORR) activities of the prepared catalysts are reported in an alkaline medium. Among the prepared catalysts PSM-0.7 with an onset potential of -0.02 V is found to be the most active ORR catalyst. The Koutechy-Levich plot obtained from the rotating disk electrode shows a higher number of electron transfer “n” for the PSM-0.7 catalyst. Further, the lower Tafel slope of the PSM-0.7 catalyst justifies its higher catalytic activity. The higher catalytic activity is ascribed to the oxygen vacancies and Mn^{4+} concentration as confirmed by XPS analysis.

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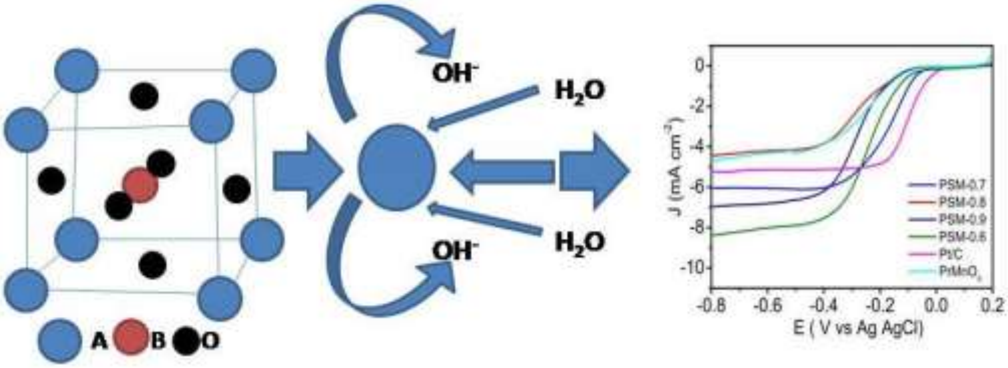

OP-04

Cu - Catalyzed Selective Hydroboration of Alkyne Enabling Synthesis of Allyl Vinyl Ethers

Minati Behera, Jaya Prakash Das*
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Alkynes are common functional existing reagents structurally diverse, shelf-stable, and readily available, consequently converting them to the borylation reaction which plays important role in different settings. Realizing the well-recognized borylation reaction, the chemical space of alkyne to vinyl boronic ester transformation possible via vinyl cuprate intermediate due to kinetic inertness of alkyne to strongly reducing diboron reagent bis-(pinacolato)diboron. However, copper (Cu) is a catalyst for this transformation to grow the area of research, promoted by a catalytic amount of ligand 1,10-phenanthroline. We are well grounded that both borylation (hydroborylation and carboborylation)

would require the presence of an electrophile and a base to reveal the stepwise formation of vinylboronic ester, inspire and encourage more invoking the synthesis of allyl vinyl ether to 3,3-sigmatropic Claisen rearrangement.

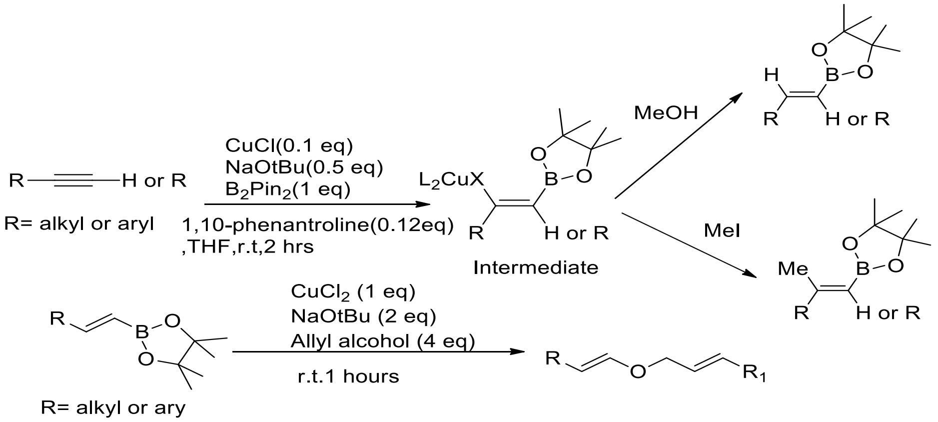

Figure 1: Synthesis of vinyl boron with allyl vinyl ether

Reference:

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OP-05

Adsorption performance of untreated silica towards some styrylpyridinium dyes in organic media - Influence of solvatochromism on adsorption capacity

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The dye adsorption performance of untreated silica surface towards the removal of some styrylpyridinium dyes was studied in some organic media of varying polarities. The dyes with different substituent groups and alkyl chains have been considered for the removal process. The adsorption phenomena have been tested by FT-IR, XRD, FESEM, and XPS techniques. The effects of optimum parameters like adsorbent dosage, sorbate concentration, temperature, and contact time have been studied on the dye removal process. The research outcomes have focused light on the exothermic nature of the adsorption process following the pseudo-second-order kinetic model. The isothermal analysis has shown a better correlation with the Freundlich model. D-R isotherm model has revealed the physisorption mechanism followed at the solid-liquid interface. The dye with the NMe_2 group and N-alkyl chain length has shown a maximum rate of adsorption with the highest spontaneity. Based on the experimental results, a suitable mechanism correlating the rate of adsorption with the solvation of dyes has been proposed for the organic-mediated removal phenomena on silica surfaces.

Keywords: Styrylpyridinium dyes, Silica, Solvation, Adsorption.

OP-06

Photoelectrochemical Characterization of CdPbS Thin films Engineered by SILAR Technique

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Because of the harsh environmental impacts of fossil fuels, harvesting of solar energy is extensively investigated as the cleanest and cheapest energy source. The fabrication of solar energy devices with superior quality and low cost requires the availability of inexpensive, non-toxic materials with potential application in solar energy conversion [1]. Chalcogenides of cadmium and lead are promising materials for designing of solar devices [2]. Herein CdPbS thin films are prepared by successive ionic layer adsorption and reaction method (SILAR). The synthesized CdPbS thin films are characterized by X-ray diffraction (XRD), scanning electron microscopy, and UV-VIS spectroscopy. The photoelectrochemical properties of the thin films prepared by 5cycles, 10 cycles, and 15 cycles are studied by fabricating photoelectrochemical cells of configuration;

Cr-stainless steel + CdPbS // S^{2-}/S_n^{2-}// graphite

by illuminating light of intensity 30 mW/cm^2. The power output (I-V) characteristic curves of fabricated photoelectrochemical cells show that the light to electricity conversion efficiency of CdPbS thin film prepared by 15 cycles is 1.07 with fill factor 39% , I_{SC} 3.1mA/cm^2& V_{OC} 0.26 V.

Reference:

1. F. Shao, J. Sun, L. Gao , J. Luo , Y. Liu , and S. Yang, Adv. Funct. Mater. 2012, 22, 3907–3913
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OP-07

Synthesis of 4-((2H-chromen-3-yl)/(2-phenyl-2H-chromen-3-yl)methylene)-3-``methylisoxazol-5(4H)-ones and evaluation of their antibacterial activity

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At present, progressive research for the development of new antibacterial drugs is highly required as the rise of multi- and pan-resistant bacteria (or, superbugs) has become a global concern for the healthcare system, which further escalated post-COVID-19 pandemic.[1]Lately, synthesis, and functionalization of N, O-heterocyclic compounds are gaining importance in drug discovery and development programs along with naturally available chromene derivatives to generate newer hybrid drug candidates.[2,3] In this regard, an efficient one-pot multicomponent reaction was developed for the synthesis of a series of 4-((2H-chromen-3-yl)/(2-phenyl-2H-chromen-3-yl)methylene)-3-methylisoxazol-5(4H)-ones via cyclo-condensation between ethyl acetoacetate, hydroxylamine hydrochloride, and 2H-chromenealdehyde, in presence of DABCO as organocatalyst in refluxing ethanol. The synthesized compounds were subsequently evaluated for in vitro anti-bacterial assay against Gram-negative (E. coli and K. pneumoniae) and Gram-positive (S. aureus and S. pyogenes) pathogenic bacteria in comparison to the standard antibiotic Gentamicin. Compounds **21f** and **21h** were found to have potent inhibitory activity against E. coli having ZI at 18 mm and 19 mm each corresponding to a MIC of 6.25 (μg/ml), respectively. SAR and molecular docking revealed compounds **21f** and **21h** having –Cl and –Br groups displayed improved halogen and hydrogen bond interaction with bacterial DNA gyrase of E. coli (PDBID:1KZN) having binding affinity of -8.8 kcal/mol respectively.

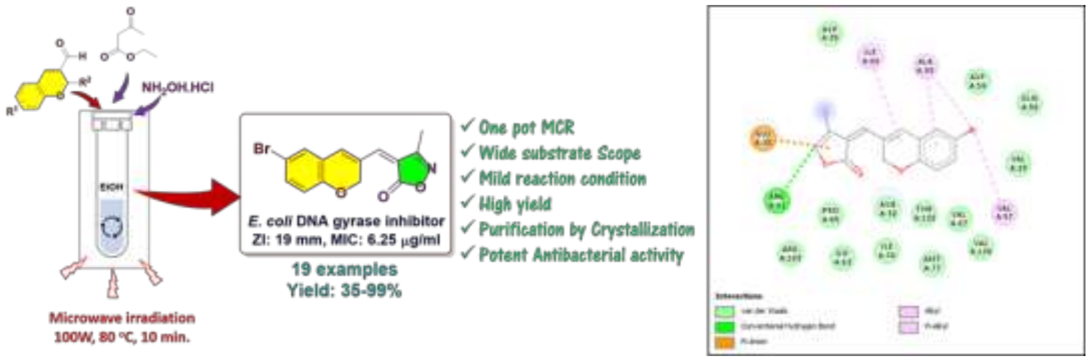

Figure 1: Synthesis of 4-((2H-chromen-3-yl)/(2-phenyl-2H-chromen-3-yl)methylene)-3-methylisoxazol-5(4H)-ones

Reference:

1. Anonymoushttps://www.who.int/news-room/fact-sheets/detail/antimicrobial-resistance.
2. W. Chem. 2015, 12, 352-358.R. Pitt, D. M. Parry, B. G. Perry, C. R. Groom, J. Med. Chem. 2009, 52, 2952-2963.
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OP-08

Green synthesis and characterization of Zinc oxide nanoparticles using Moringa oleifera leaves extract and Evaluation of Its Antibacterial and Anti-biofilm activity

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Numerous research teams are interested in the synthesis of nanoparticles (NPs) using biological systems. Although many biological agents can be employed to synthesise NPs, plant extract-mediated synthesis is gaining popularity since it is both cost- and environmentally friendly. The present work intends to synthesize zinc oxide nanoparticle (ZnONPs) using Drumstick leaves (Moringa Oleifera) which is rich in polyphenols and flavonoids. Initially, the biosynthesis of ZnONPs was confirmed by observing the absorption peak at 374 nm using UV–visible spectroscopy. The XRD data revealed that the synthesized ZnONPs have a body-centered cubic structure. Additionally, FE-SEM analysis demonstrated that biosynthesized ZnONPs was found to be spherical and rod-in shape with a size in the range of 10–50 nm. The antimicrobial activity was evaluated using minimum inhibitory concentration

(MIC) and zone of inhibition (ZOI), which demonstrated that ZnONPs are a good antimicrobial agent. The antimicrobial activity of ZnONPs against Gram-positive (S. Pyogenes) and various Gram-negative bacteria (S.flexineri, S.typhi, V.cholerae) found that the antimicrobial activity of ZnONPs increases with increasing the concentration of NPs. Additionally, the anti-biofilm activity of ZnONPs was evaluated against the biofilm-producing bacteria Staphylococcus aureus, which confirmed that ZnONPs have strong anti-biofilm activity against biofilm-forming bacteria.

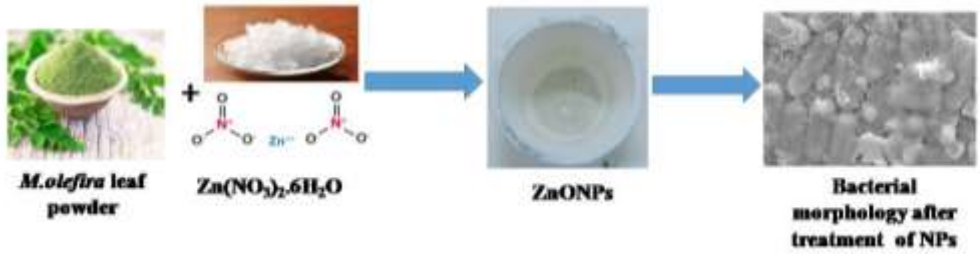

Figure 1: Representation of the green synthesis of ZnONPs and antibacterial efficacy

OP-09

An Unmediated Approach to Access Organocatalysts: A Time-Dependent, Chemoselective O-functionalization of Prolinol

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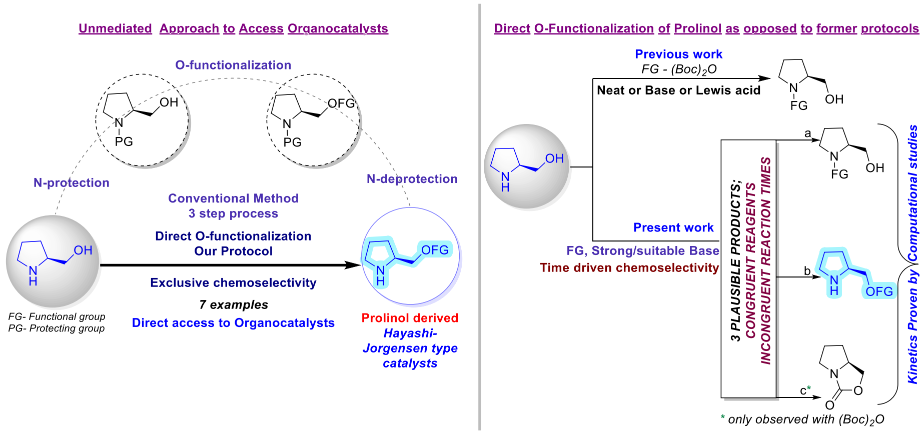
Herein, a successful chemo-selective either functionalization of the nucleophilic sites of prolinol has been reported, by exploiting the relative acidity difference and inverted nucleophilicity of the corresponding conjugate bases with a suitable base. Failing to re-enact the former protocols, a mechanistic investigation was initiated which revealed that the rudimentary steps can be controlled by: **a)** A requisite base to distinguish the differently acidic sites (NH and OH) for the formation of the conjugate base reacting to the electrophile **b**) The disparity in nucleophilicity of the completely formed conjugate basic sites. As an example, mono-Boc functionalization of prolinol for the exclusive synthesis of either NBoc/OBoc/Oxazolidinone derivatives is reported. **Never-reported-beforeO-Boc prolinol** has been synthesized in 85% yield and other known derivatives (NBoc and oxazolidinone derivatives) have been synthesized in good to excellent yields. This protocol has proven to be successful with various other substrates which might prove to be applicable as suitable organocatalysts in asymmetric reactions.



Reference:

1. Pre-print on ChemRxiv (DOI: 10.26434/chemrxiv-2022-c6htr)

OP-10

Ortho C-H bond activation by pyridine-2-aldoxime in iridium(III) metal complex

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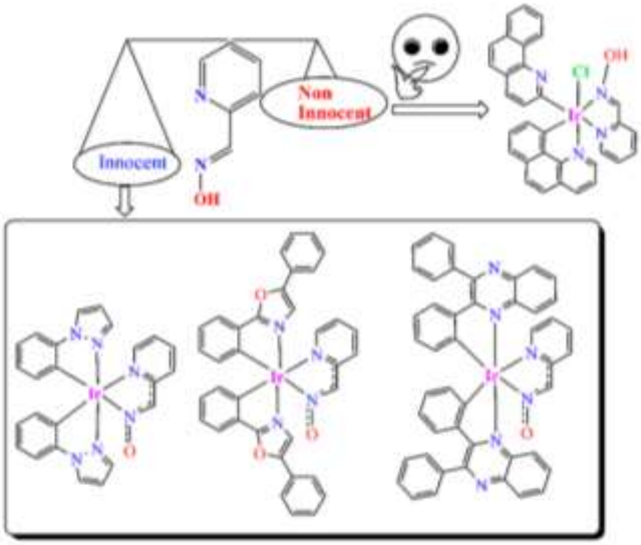
A series of Ir(III) complexes of formula [Ir(C^N)$_2$(pyrald)] were designed and synthesised from the reaction of [(C^N)$_2$Ir(μ-Cl)$_2$Ir(C^N)$_2$] and pyridine-2-aldoxime (pyrald) {C^N=1-phenylpyrazole (phpyr), 2,5-diphenylbenzoxazole (phox), 2,3,-diphenylquinoxaline (phquinox), 7,8-benzoquinoline (benzq)}. All these complexes were characterized through ^{1}H NMR, UV-Vis, emission spectroscopy, mass analysis, and cyclic voltammetric studies. The molecular structure of the iridium complex derived from the 7,8-benzoquinoline ligand, [Ir(benzq-κN, κC^{10})(benzq-κC^2)(Hpyrald)(Cl)], confirmed the first ortho C-H bond activation in iridium coordinated 7,8-benzoquinoline moiety. It was suspected that pyridine-2-aldoxime played a decisive role in causing such C-H activation. To explore such a possibility, more number of iridium complexes were prepared from three more different cyclometallating ligands and characterized. However, the complexes with other cyclometallating ligands did not display such unusual C-H activation. Thus, the role of pyridine-2-aldoxime in C-H bond activation remains inconclusive and requires more investigation.



OP-11

Dual Functionality of Ternary Mixed Co-Ni-Cu Oxide/Hydroxide for Environmental and Energy Storage Applications

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Indiscriminate discharge of effluents from various sources and excessive reliance on non-renewable energy sources are two major contributors towards increasing environmental pollution. Photocatalysis remediation of harmful contaminants from wastewaters is often preferred over other methods for several reasons. On the other hand, significant efforts are underway for the generation of green energy by resolving the intermittency nature of renewable energy sources. Among several ways, the development of devices with efficient storage and durability has received considerable attention in recent years. In this regard, supercapacitors-based storage technologies find greater attention to deal with power shortage owing to their high power density, fast charge/discharge rate, and cycling stability [1, 2]. Multinary metal oxides/hydroxides have been used as a promising