

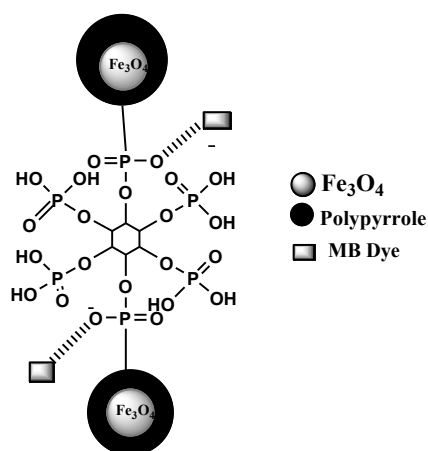
## PP-34

### Effective removal of Cationic dye using Polypyrrole based magnetic nanocomposite (PPy–Fe<sub>3</sub>O<sub>4</sub>-PA)

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**Abstract:** The presence of complex mixtures of toxic metal ions and organic dyes from industrial waste water causes harm to environment and human health. Therefore, the removal of such pollutants from water has become a challenge for researchers. Several techniques have been applied for the removal of these dyes from wastewater such as photocatalytic reduction, precipitation, membrane filtration and adsorption. However, the use of each of these methods in separation has merits and disadvantages. So considering this, the adsorption process is considered to be one of the most effective and inexpensive treatment processes to remove dyes from wastewater. Magnetic nanoparticles as an adsorbent have been widely used in different fields, due to their ease of separation using an external magnet, high specific surface area, and simple modification. A magnetic polypyrrole–magnetite-phytic acid (PPy–Fe<sub>3</sub>O<sub>4</sub>-PA) nanocomposite is prepared in a two-step method via in situ chemical polymerization of pyrrole using APS as an oxidant in the presence phytic acid (PA). The prepared nanoparticles were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), transmission electron microscopy (TEM) and Fourier transform infrared (FTIR) spectroscopy. The adsorption parameters like pH, temperature, adsorbent dosage, dye concentration along with kinetics and thermodynamic parameters ( $\Delta G^\circ$ ,  $\Delta H^\circ$  and  $\Delta S^\circ$ ) will be evaluated for the potential application in the real field.



PP-35

## A Cu(II)-Pd(II) based discrete heterobimetallic coordination compound

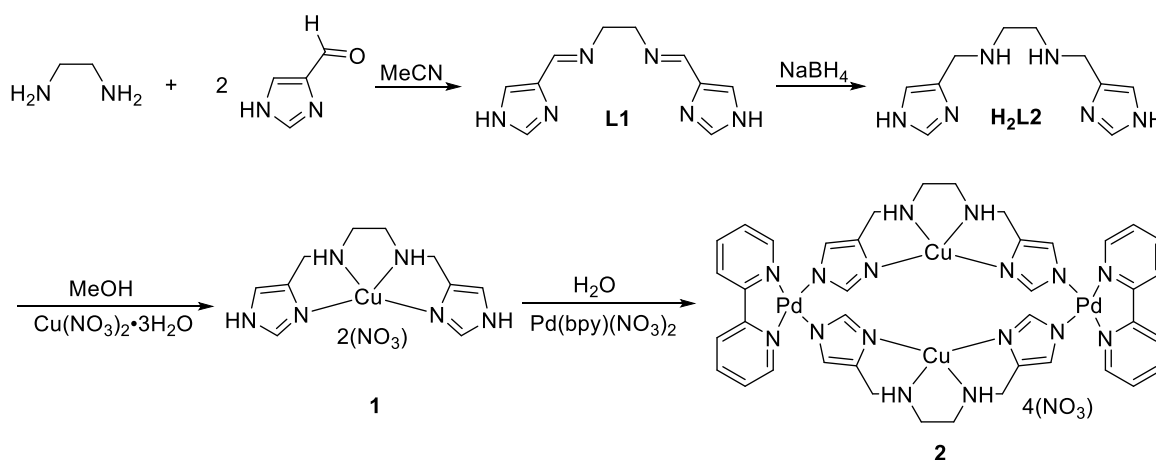
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**Abstract:** Coordination-driven self-assembly is a potential candidate for metal based supramolecular systems which can mimic biomolecules. Among various properties, enzymatic reactions in biomolecules deserve special attention. Most of the active sites in these enzymatic reactions are metals. Some metals are also involved as cofactors leading to the heterometallic system. Introducing heterometallic system in supramolecular coordination-driven self-assembled compounds is highly challenging and less explored.[1] Among various metals, Pd<sup>2+</sup> driven self-assembled structures are very interesting because of its square planar geometry, preference for soft donors towards bond formation and catalytic behaviour. There are few reports in the literature where Pd<sup>2+</sup> is used as one of the metal centres in heterometallic complexes. [2]

Flexible ligand H<sub>2</sub>L2 (Figure 1) is used for the prepare of coordination complexes with various metal centres in stepwise manner.[3] A water soluble discrete heterometallic coordination compound **2** is prepared by using Cu(II)-Pd(II) metal units (Figure 1). All the six donor sites of ligand H<sub>2</sub>L2, which were not used completely as reported in the literature are now being used suitably to coordinate with Cu(II) and Pd(II) metal unit. The heterobimetallic complex **2** has been characterised by single crystal X-ray analysis.



**Figure 1.** Stepwise synthesis of heterobimetallic complex **2**.

PP-36

### Fine chemicals from Lignin: Selective production of Veratraldehyde from lignin model compound

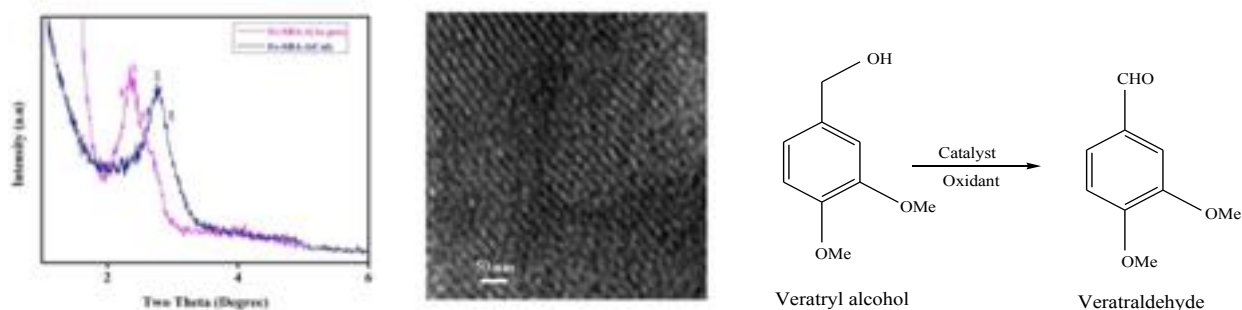
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**Abstract:** Lignin constitutes the major source of aromatics and under suitable conditions it can produce an array of fine chemicals<sup>1</sup>. It is also envisaged that lignin can produce veratryl alcohol and later it can be converted into veratraldehyde. Nanoporous solid have attracted considerable attention in recent years because of their excellent textural characteristics that made them effective catalysts in processes which allow easy diffusion of large size organic molecules, such as biomass to internal active sites<sup>2</sup>. Herein, we report the synthesis of iron substituted cubic cage type mesoporous molecular sieves (FeSBA-1) in a highly acidic media, using TEOS, CTAB, dil. HCl and iron nitrate as precursors. The XRD, TEM and thermogravimetric patterns confirmed the well ordered FeSBA-1 samples. DR UV-VIS and EPR studies revealed the oxidation and coordination states of Fe(III) in FeSBA-1. The preliminary catalytic activity studies showed selective conversion of veratryl alcohol to veratraldehyde (scheme 1) under mild conditions. The details of reaction condition, results obtained and mechanism will be discussed during presentation.



**Figure.1** XRD pattern of Fe-SBA-1 **Fig. 2.** TEM patterns of Fe-SBA-1 **Scheme 1:** Oxidation of veratryl alcohol

PP-37

### Host-guest Complexation of 3-Acetylcoumarin with $\beta$ -CD and Its Delivery to a Carrier Protein

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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  $\beta$ -CD exploiting steady-state and time-resolved fluorescence spectroscopy in tandem with molecular docking. We have further studied the transfer of 3-AC from its  $\beta$ -CD inclusion complex to BSA and determine the microviscosity of the  $\beta$ -CD cavity in presence of 3-AC. Spectroscopic and molecular docking results confirmed 1:2 inclusion complex formation of 3-AC: $\beta$ -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.

#### PP-38

#### Generation of DMSO coordinated thermally stable halogen cation pools for oxidative C-H halogenation

**Pallaba Ganjan Dalai**, Kuntal Palit, and Niranjan Panda\*

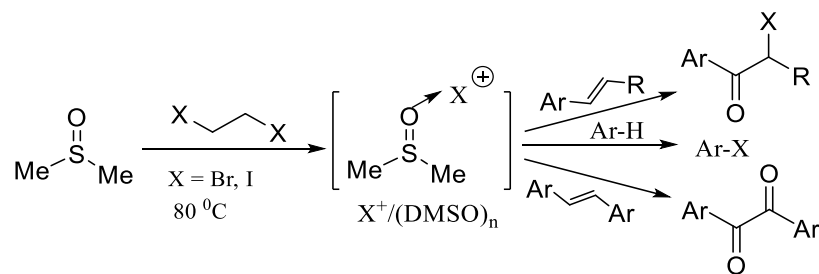
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**Abstract:** A novel method to generate halogen cation pools from the reaction of 1,2-dihaloethanes (hal = Br, I) and dimethyl sulfoxide (DMSO) for efficient oxidative halogenation of arenes and heteroarenes was reported. The initial reaction of DMSO and 1,2-dihaloethane generates the sulfur ylide, which undergoes pyrolytic elimination of ethylene by affording halonium ions. These ions were accumulated and stabilized by DMSO through coordination by forming halogen cation pools for the successful halogenation reaction. This protocol was selective for electrophilic monohalogenation of arenes at room temperature; however, polyhalogenated products were formed by raising the reaction temperature. Late-stage halogenation of heteroarenes and some commonly marketed drugs signifies the synthetic utility of this protocol in pharmaceutical chemistry. Unlike the

classical methods, the in-situ generated electrophilic bromonium ion was further exploited for the direct synthesis of  $\alpha$ -diketones from the alkenes under base-free conditions.



**Scheme 1.** Oxidative C-H halogenation

### PP-39

#### Synthesis of Chitosan based Gold nanoclusters for the detection of $\text{Hg}^{2+}$ ions

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**Abstract:** Contamination of the environment with heavy metal ions has been an important concern throughout the world for decades. Among them, mercury ( $\text{Hg}^{2+}$ ) is one of the important environmental pollutants that is widely spread in soil, water and food. Mercury can cause various diseases such as minamata, acrodynia and hydrargyria and also affects kidney, brain and nervous system that constitute a serious threat to human being. Therefore, developing a sensor that detects ppb level of mercury is a significant step for environment safety and health monitoring for researchers. Herein, a simple, facile and biocompatible fluorescent sensor using L-cysteine assisted chitosan reduced gold nanocluster (L-cys/CS-AuNC) is prepared by “one pot” synthetic protocol for ultrasensitive detection of  $\text{Hg}^{2+}$  ion which produces a strong orange fluorescence emission at 575 nm. The morphology of nanocomposites are studied by transmission electron microscopy. The detection limit (LOD) for mercury (II) is found to be 3 nM. Moreover, the L-cys/CS-AuNC can be applied to real water samples such as pond, river and tap water for detection of  $\text{Hg}^{2+}$  ion.

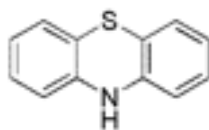
### PP-40

#### Photo induced-conformational changes of phenothiazine: Photophysics unveiled by optical spectroscopy and DFT analysis

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**Abstract:** The role of solvents with different polarity plays an important role in the excited state features of many organic molecules. We have explored the optical properties of phenothiazine (**Figure 1**) in different solvents such as dichloromethane (DCM), Dimethylsulphoxide (DMSO), n-hexane, Methanol, Tetrahydrofuran (THF) having different polarity. The UV-Vis absorption studies showed that the spectrum of each solvent contains two bands, where shorter wavelength band is due to  $\pi$ - $\pi^*$  transition and longer wavelength band is due to  $n$ - $\pi^*$ . However, the emission intensity decreases with increase in polarity of the solvents, which may be due to excited state stabilization of the molecules in polar environment. In addition, the fluorescence spectrum contains two bands. We have seen that the intensity of these bands changes in solvents of different polarity, for instance in n-hexane and DMSO. We have speculated the effect of hydrogen bonding may influence the conformational changes of the molecules in the excited state, thereby its emission pattern. The details of time resolved fluorescence measurement and DFT analysis performed to corroborate the above findings.



**Figure 1.** Chemical structure of phenothiazine

PP-41

### Fullerene-free Organic Solar Cells using Coumarin-based Donor Material

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**Abstract:** Now-a-days tremendous growth has been seen for organic solar cells based on the ternary single bulk-heterojunction using complementary absorbing fullerene-free acceptors and molecular/polymeric donors. The device achieved excellent power conversion efficiencies (PCEs) reaching up to 18%. Here, we demonstrate the synthesis and characterization of two coumarin-based organic semiconducting molecules, and its use as an electron donor in bulk-heterojunction solar cells (BHJSCs). Coumarin derivatives are considered as a class of wide band-gap material that absorbs around 500 nm with a band gap >2 eV. Coumarin-based molecules are very promising because of

their efficient synthesis, strong photo-response in the visible region and tuneable energy levels to match with other device components. The compound exhibited an absorption band ~500 nm in chloroform solution. Ternary BHJSCs fabricated by employing coumarin derivatives as a donor and fullerene-free acceptors generated enhanced PCE above 14% with high short-circuit current density, open-circuit voltage and fill factor in comparison to the binary counterparts (~11%). The increased PCE for the ternary devices may be related to the complementary absorption and well-matched energy levels, efficient exciton generation and its dissociation, resulting in an improved photocurrent and photovoltage in the device.

**PP-42**

**Adsorptive and photocatalytic properties of zinc ferrite nanoparticles derived from solid wastes**

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**Abstract:** Industrial operations such as mining, extraction, galvanizing, smelting processes lead to the generation of huge amounts of waste materials such as iron ore tailings, red mud, zinc ash, zinc dross, battery wastes, electroplating sludge etc. Due to rapid depletion of ores/minerals and stringent environment regulations, utilization of solid wastes has acquired greater relevance which relies on the basic principle of recovery, recycling and converting them to value added products. Several value added materials have been prepared from a variety of waste materials and their properties have been evaluated for different applications. In this work the preparation of zinc ferrite nanoparticles ( $ZnFe_2O_4$  NPs) using recovered iron and zinc values from iron ore tailing (IOT) and zinc ash, respectively was described. The adsorptive and photocatalytic properties of the derived material towards organic dyes were studied and reported.

Sufficiently pure zinc and iron recovered from zinc ash and IOT, respectively following the reported methods and used in the preparation of  $ZnFe_2O_4$  NPs by sol-gel method. The synthesized material was characterized by several spectroscopic (PXRD, FT-IR, UV-Vis-DRS, PL, Raman), microscopic (FE-SEM, TEM) as well as magnetic measurements. XRD data revealed the formation of spinel mono-phase in the range of nanometric crystallite size which was also confirmed from TEM. The material showed a band gap energy of 2.42 eV indicating its photocatalytic activity under visible light. Adsorption behaviour of  $ZnFe_2O_4$  NPs was assessed by adsorption of an anionic dye (Congo red) under varying conditions. The photocatalytic efficiency was tested for the degradation of Congo red and reduction of Cr(VI) to Cr(III) under visible light irradiation in single as well as binary systems. Based on the analyses of data, suitable adsorption and photocatalytic mechanisms were proposed.

PP-43

**Enhanced Dielectric and Electrical Properties of Polyvinylpyrrolidone (PVP) Treated Graphene Oxide (GO)-Poly(vinylidene fluoride hexa-fluoropropylene) [P(VDF-HFP)] Composite Films**

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**Abstract:** Polyvinylpyrrolidone treated graphene oxide-poly(vinylidene fluoride-co-hexafluoropropylene) composite films with good flexibility and higher dielectric constant were synthesized via solution casting method. Different compositions of treated graphene oxide utilized as filler were embedded in to poly (vinylidene fluoride hexafluoropropylene) (PVDF-HFP) polymer matrix. Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) techniques were employed to characterize the synthesized composite films. In this study, the PVP treated GO, together with the P(VDF-HFP) matrix forming the three component composite films with enhanced dielectric and electrical performance. The composite films filled with 1wt% treated GO particles showed a high dielectric constant and the maximum value of the dielectric constant reaching  $\approx 115$  while the dielectric loss was only  $< 0.5$  at 100 Hz. However, the excellent performance of the composites is attributed to the improved uniform dispersion and superior interfacial compatibility between the treated particles and polymer matrix, suggesting three component composites may be a better option over their two components in synthesizing high performance dielectric composites. Moreover, the AC conductivity increases from lower to higher frequency with the increment of frequency for entire composite films. This study offers new possibilities for the fabrication of three component P(VDF-HFP) composite films and provides a valuable approach for improving dielectric performance for energy storage applications.

PP-44

**Fluorescent sensing of water in DMSO by 2,4-dinitrophenyl hydrazine derived Schiff base**

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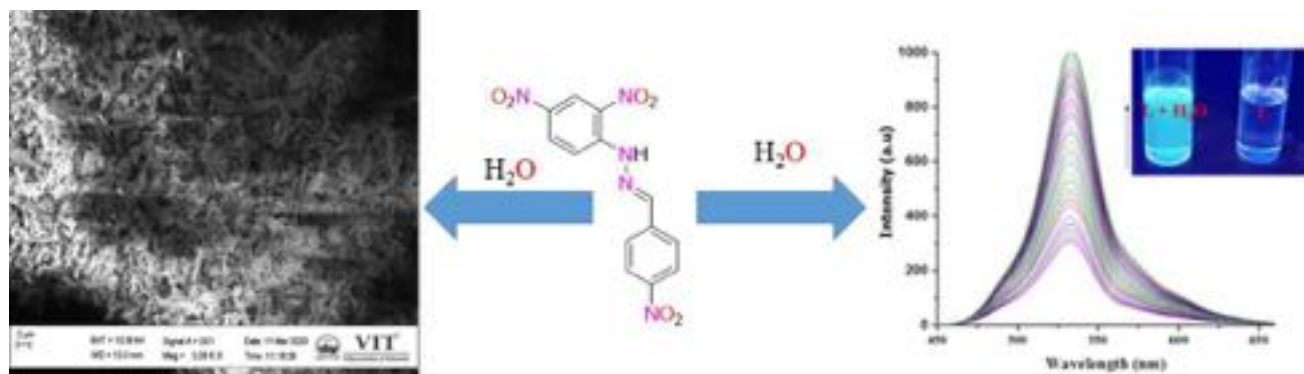
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**Abstract:** The quantitative analysis of trace water in organic solvents remains a hotspot in current research because of the importance in both industrial and laboratory scale chemistry. This study

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introduced a fluorescence chemosensor (**L3**) for the detection of trace water in dimethyl sulfoxide (DMSO). Addition of water into the DMSO solution of **L3** resulted a significant fluorescence enhancement at 533 nm with a detection limit of 0.002 wt %. The fluorescence turn-on response is occurred due to the formation of aggregates of **L3**. Also, other possible mechanism for trace water detection by **L3** in DMSO is attributed to the specific water-**L3** interaction and partially to the increase in polarity of the solvent caused by an increase in water concentration. Dynamic light scattering (DLS), <sup>1</sup>H NMR, scanning electron microscope (SEM), transmission electron microscope (TEM) and quantum mechanical studies were performed to support the water sensing by **L3** in DMSO.



#### PP-45

#### Inorganic Oxide with Carbon based nanocomposites for Dielectric studies

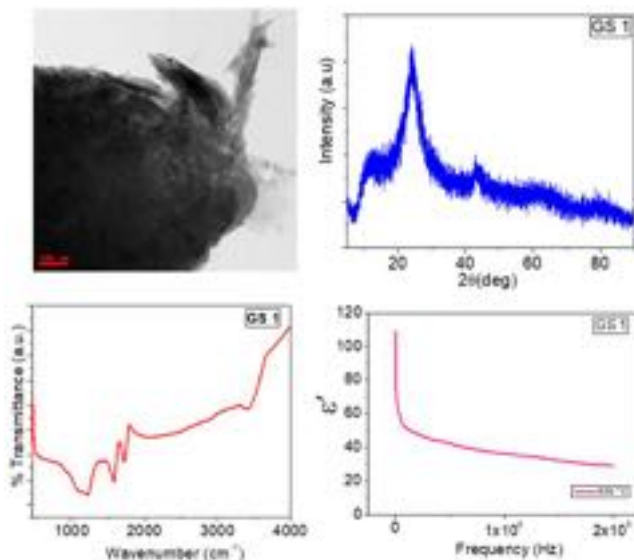
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**Abstract:** Many inorganic based oxides (IOs) nanoparticles (NPs) have been synthesized and studied for dielectric behaviour for many decades. It has gained popularity due to its cost-effectiveness, low toxicity and highly durable properties. Carbon-based materials are also easily found in nature and drag many researchers attention towards themselves for possessing high dielectric properties. This work aims to design several metal oxides (MOs), hetero metal oxides (HMOs) and nonmetallic oxides (NMOs) NPs with the carbon-based NPs by modified sol-gel and chemical reduction method. Important characterization techniques like XRD, TGA, DSC, DLS, Zeta, TEM, UV-Vis and FTIR has been performed for designed materials to know studying crystallinity, thermal stability, size, morphology, absorbance and chemical compositions respectively. The dielectric behaviour of carbon-

based inorganic oxide is studied at different ranges of frequency  $10^2$  Hz to  $2 \times 10^6$  Hz and temperature of  $25^\circ\text{C}$ - $600^\circ\text{C}$  respectively. The availability of permanent dipoles, interfacial polarization and atomic arrangements have enhanced the dielectric behaviour of the nanocomposites. The prepared nanocomposite showed a good dielectric behaviour provides an interesting morphology and can be applied for charge storage uses .



PP-46

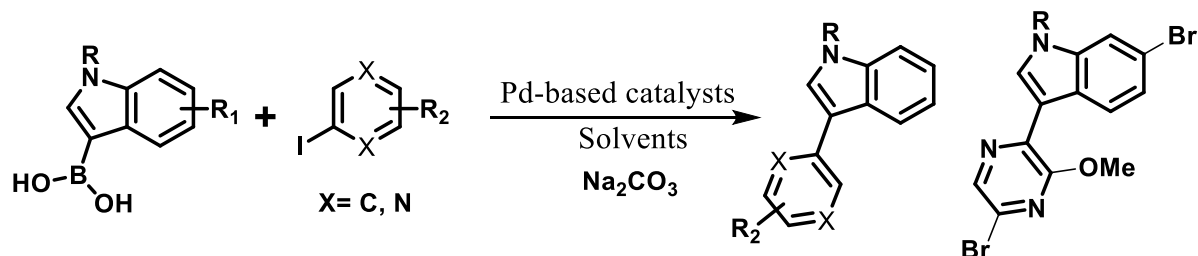
### Palladium catalyzed cross-coupling reactions

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**Abstract:** Among the broad range of transition metal catalyzed reaction, the Heck and Suzuki reaction are excellent methodologies which are frequently used for synthesis of natural and biologically active products. Palladium catalyzed cross coupling reactions of two or more fragments directly create complex molecules under mild conditions from readily available starting materials. Suzuki, Heck reaction are Pd(0) catalyzed cross-coupling of boronic acid-aryl halide and aryl or vinyl halide with an alkene. It is also used for constructing tertiary stereocenters named vernolepin, capellenols and quaternary stereocenters named terpenoids, peptinoids, kaurene, abietic acid by carbon-carbon bond formation. Catalytic activity of Pd-catalyzed coupling reactions have been investigated and optimized based in solvent like water which is a green media without any additional reagent.



## PP-47

**Solvothermal Synthesis and Characterization of TiO<sub>2</sub>-reduced graphene composite catalysts**

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**Abstract:** TiO<sub>2</sub>-xRGO composite catalysts were synthesized using solvothermal method. We report here one step solvothermal synthesis using a mild reducing agent, Dimethylformamide (DMF). The unique solvothermal condition facilitates several transformations to occur simultaneously. The reduction of graphene oxide to reduced graphene oxide (RGO), controlled nucleation of TiO<sub>2</sub> particles on RGO and development of intimate chemical bonding between precursors, occur synergistically. Under the non-equilibrium condition in the solvothermal process, even a mild reducing agent such as dimethylformamide (DMF) showed enhanced reducing ability, which eliminated the use of any strong reducing agent or structure directing chemicals. The composites were characterized by HR-TEM, XRD, FTIR, RAMAN etc. TiO<sub>2</sub> particles in the size range of 4 – 9 nm were formed on the reduced graphene sheets. A reduction in the size of TiO<sub>2</sub> nanoparticles is attributed to the presence of graphene sheets which did not allow aggregation TiO<sub>2</sub> particles in the composite. The TEM figures also show that TiO<sub>2</sub> nanoparticles are well dispersed on the RGO sheets. From the HR-TEM, we observed that TiO<sub>2</sub> nanoparticles are linked via graphene sheets. The composite catalysts have large fluorescence quenching, indicating an efficient separation of photogenerated electrons and holes.

PP-48

**Photocatalytic Performance of Hydrothermally Synthesized Surface Functionalized TiO<sub>2</sub> Nanocrystals towards *Allamanda Cathartica* Dye Degradation**

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**Abstract:** A direct and environmental friendly synthesis method was developed to produce acetylacetone functionalized TiO<sub>2</sub> semiconducting nanoparticle by hydrothermal synthesis. Photo induced interaction between surface functionalized TiO<sub>2</sub> semiconducting nanoparticles and *Allamanda Cathartica* dye was investigated. The charge transfer interaction between dye and semiconducting nanoparticles was studied by UV-VIS spectroscopic study. Present work demonstrates the efficiency of the developed nanocrystals towards photocatalytic degradation of *Allamanda Cathartica* dye. It was observed that complete degradation dye occurs within half an hour. Further, to validate the properties of the synthesized TiO<sub>2</sub> nanoparticles different characterization techniques such as X-Ray Diffraction (XRD), UV-Vis spectroscopy, Scanning Electron Microscopy (SEM) were performed. UV-VIS spectroscopy showed significant hypochromic shift of absorption maxima. The bandgap of the TiO<sub>2</sub> nanoparticles was calculated from the absorbance spectra. UV-VIS as well as SEM analysis confirmed that the synthesized particles were at nano scale. The crystalline nature of TiO<sub>2</sub> nanoparticles was confirmed from different X-ray diffraction peaks.

PP-49

**Red mud modified with Al(OH)<sub>3</sub> for the removal of Zn(II) ions from aqueous solution**

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**Abstract:** The unwanted industrial waste red mud (RM) embedded with Al(OH)<sub>3</sub> was prepared and applied to remove excessive Zn(II) ions from aqueous solution. This prepared adsorbent has high affinity toward zinc, which offers distinctive advantages including high adsorption capacity, easy preparation, easy isolation from sample solutions. Several characterization techniques such as FT-IR, XRD, SEM and EDX were employed for the adsorption process. From the results of kinetics and isotherm data, it has been inferred that the experiment was well-established to Pseudo Second Order kinetics with R<sup>2</sup> value 0.9945 and followed Langmuir adsorption isotherm (R<sup>2</sup> = 0.9938) with maximum adsorption capacity 26.87 mg/g at Ph 5. The results suggested that the Al(OH)<sub>3</sub>/RM

adsorbent material have strong affinity to zinc and could be used as an excellent adsorbent for zinc contaminated water treatment.

### PP-50

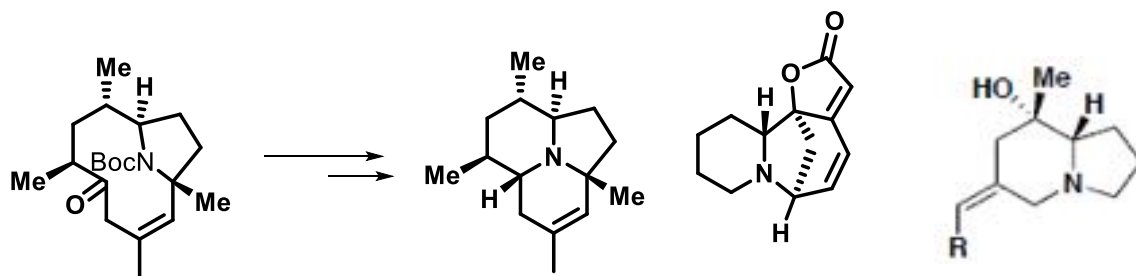
#### Synthesis of biologically active Heterocyclic scaffolds

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**Abstract:** Natural products have great importance in human life as the effectiveness of regimen for Chemotherapy concerned. Diverse bioactive Heterocyclic Scaffolds are used as FDA-approved potential drugs. Synthetic Indolizidine analogues include various pharmacological properties such as anti-oxidant, central nervous system depressant, anti-psychiatric, analgesic, anti-biotics, anti-cancer, larvicidal, and anti-retroviral are reported. Though varieties of synthetic methods have been established to access a large number of relevant heterocyclic scaffolds, still need for sustainable synthesis of it is essential. Thus, the synthesis of diverse heterocyclic compounds like indolizidine derivatives of medicinal relevance is important and a prerequisite. Indolizidine, a class of N-Heterocyclic compounds that contain one-six membered rings fused to a five-membered ring bridging through a nitrogen atom has a wide range of biological activities. The selected synthetic methods involve the use of recyclable catalysts and eco-friendly approaches. The structure-Activity-Relationship (SAR) studies led to derivatives of Indolizidines, which could be tested against the oncocyte linages for the development of different drugs, used in chemotherapy for malignancy.



### PP-51

#### Dearomative Organo-transformation by Quaternary Ammonium Tribromides

Saumyaranjan Panda, Dr. Debayan Sarkar

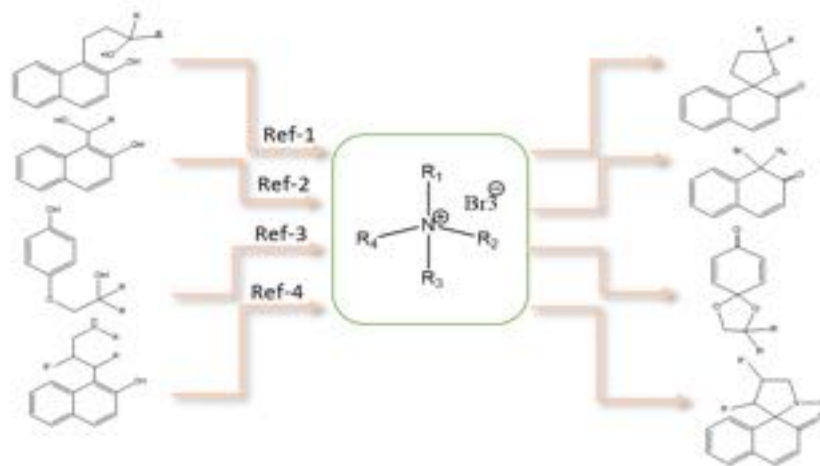
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**Abstract:** Dearomatization of abundant arenes are the most powerful approach for the versatile transformation of a wide range of molecular architectures from simple starting materials. The main

advantage being the possibility of converting an aromatic ring into a three-dimensional molecule generating multiple chiral centres in one shot, creating an aromatic C-H activation at the expense of aromatic energy. Among the reported dearomatization methods, tribromide mediated dearomatization exhibits economical, metal and ligand free one pot accomplishment of these significant transformations.

Quaternary Ammonium Tribromides are effective reagent for spiro-etherification as well as brominative dearomatization of naphthol with varied substitution diastereoselective [1]. It is an effective reagent for oxidative C(sp<sup>2</sup>)-C(sp<sup>3</sup>) bond cleavage of 1-Hydroxy alkyl-2-naphthol via oxidative dearomatization [2]. Tribromides have been employed for intramolecular Spiro cyclisation for synthesis of para-quinone monoketals and their derivatives [3]. It has been also implemented for the synthesis of N-substituted spiro-azacyclo compounds [4].

A series of Ammonium Tribromides have been screened for exploring the role of ammonium counterpart attached to tribromide on generation of stereo selective spiro-furans via oxidative dearomatization of naphthol and successfully achieved on a large-scale [5]. Recently we are working on asymmetric version of tribromides with proline, cinchonine, DHQ-PHAL and Maruoka unit for enantioselective dearomatization.



## PP-52

### Spectroscopic, cytotoxicity and molecular docking studies on interaction between 2,4-dinitrophenyl hydrazine derived Schiff bases with bovine serum albumin

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**Abstract:** Three new 2,4-dinitrophenyl hydrazine derived Schiff bases €-1-(2,4-dinitrophenyl)-2-(n-nitrobenzylidene)hydrazine (where, n = 2, L1; n = 3, L2 and n = 4, L3) were synthesized and characterized by FTIR, <sup>1</sup>H NMR and mass spectra. The interaction of the ligands (L1-L3) with the protein BSA was investigated by fluorescence spectroscopy and molecular docking methods. The fluorescence titration experiments of BSA resulted fluorescence quenching with the incremental addition of the ligands (L1-L3). The fluorescence quenching is static in nature and the estimated Stern-Volmer constants of the ligands with BSA followed the order of L1 > L3 > L2. The modes of binding of the ligands with BSA were explored by molecular docking analysis. In addition, the cytotoxicity of the ligands was examined in live HeLa and HT-29 cells. The IC<sub>50</sub> values were found in the range 13 Mm-243 Mm.

### PP-53

#### Thermal Properties of Halloysite Nanotubes Filled Ethylene-Vinyl Acetate Copolymer Nanocomposites

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**Abstract:** Halloysite nanotubes filled EVA/HNTs nanocomposites were synthesized by solution mixing method. Thermal properties of these EVA/HNTs nanocomposites were investigated by the TGA, DTG, DTA and DSC along with SEM images of cryogenically fractured EVA/HNTs nanocomposites. The thermal degradation of these composites was found to follow a two step decomposition process. SEM images show that the roughness of the fracture surface increased with the increase in HNTs loading. The thermal stability and the percent of crystallinity increases with 0-10phr halloysite loading. The kinetics of thermal degradation of these EVA/HNTs nanocomposites were studied by Flynn method, Coats-Redfern method, Freeman-Carroll and Freeman-Anderson method. The thermal conductivities of the samples were found to be in the range of 0.188 W/Mk to 0.202 W/Mk.

### PP-54

#### Thermal analysis of phosphate containing mixture enable for energy storage materials

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**Abstract:** In order to mitigate the energy related problems without disturbing the environment is the main challenge of the world community. The energy demand of the human community is mitigated using various carbonaceous fuels since last few centuries. The use of carbonaceous fuels affects the environment a lot due to generation of green house gases. In last few decades the use of renewable energy such as solar energy, wind energy, etc. continuously increases. In last few years the use of solar energy sours drastically in the world community. In this respect we synthesize phosphate containing energy saving materials. This energy saving materials can be used as coating materials in various households for all weather season. This mixture is characterized with thermal analysis (TG-DTA and DSC) as well as UV-Vis-NIR spectroscopy. The Calcium carbonate with adhesive is a good reflect coating materials. The addition of phosphate changes this behaviour of CaCO<sub>3</sub> with adhesive in the visible region. The DSC was measured from 271 K to 342 K using sapphire standard for various phosphate mixtures in N<sub>2</sub> atmosphere. The calculated dielectric constant and band gap of this mixture is 6.66 and ~ 2.15 eV. The maximum specific heat capacity is observed for mixture containing 2.50 % Co<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> in adhesive added CaCO<sub>3</sub>.

**PP-55**

### **Protein Nanoparticles: Future Perspectives and Challenges**

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**Abstract:** Nanoparticles have several advantages, including tiny size, high surface area, and functional group modification for increased capacity or selectivity. Nanoparticles containing proteins are particularly noteworthy because they can be utilised to target specific sites. Particulate systems, such as nanoparticles, have been employed to alter and improve the pharmacokinetic and pharmacodynamic aspects of numerous pharmacological compounds using a physical method [1]. Chemicals and biomolecular medications, including as anticancer agents and therapeutic proteins, have been delivered using it extensively [2]. Because of their safety, natural biomolecules such as proteins are an appealing alternative to synthetic polymers frequently utilised in nanoparticle creation. Protein nanoparticles provide a number of advantages, including biocompatibility and biodegradability. Nanoparticles' drug release and polymer biodegradability are important criteria for optimal drug delivery [3]. Despite the use of protein nanoparticles has shown some promising outcomes and has a bright future ahead of it, comparative data on the performance and treatment



effectiveness of protein nanoparticles vs other existing delivery technologies is still lacking. As a result, more research is needed.

**PP-56**

**Chitosan based Gold nanoclusters as Switch-off Fluorescent Probe for Hg<sup>2+</sup>Sensing**

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**Abstract:** Herein, we have synthesized gold nanocluster (Au NC) using chitosan as reducing agent. The nanoclusters are synthesized using “one pot” protocol and after that the as-synthesized nanoclusters are characterized by different techniques. Fluorescence spectra of gold nanoclusters give the maximum intensity at 538 nm which confirms the formation of nanoclusters. The surface functionality, structural analysis and morphology of nanocomposites are studied by FTIR, XRD and TEM respectively. The nanocluster is stable to long time at freeze condition and also stable at wide range of pH (4 to 10). The detection of Hg<sup>2+</sup> ion in aqueous medium using nanoclusters is based on decrease in intensity of fluorescence spectra of AuNC. With increase in concentration of Hg<sup>2+</sup>, the intensity of AuNC decreases as well as blue shifting occurs. The limit of detection and limit of quantification for Hg<sup>2+</sup> ion is 3 nM and 15 nM respectively. The as-synthesized nanocluster is applicable to real water samples through a cost-efficient, one-step assay protocol as it does not require additional functionalization with specific ligand molecules.

**PP-57**

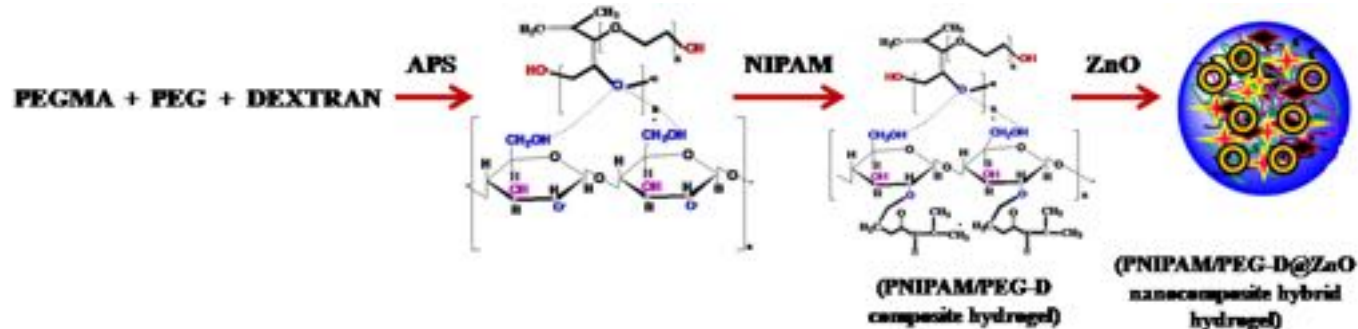
**Dextran Hybrid Poly (N-Isopropylacrylamide)/Polyethylene glycol Composite Hydrogels for In Vitro Release of Ciprofloxacin**

**Swapnita Patra<sup>#</sup>**, Kalyani Prusty, and Sarat K. Swain\*  
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**Abstract:** The development of efficient drug nanocarriers has remained as a major challenge in advanced drug delivery in human body. We investigated a novel drug delivery system for the *in vitro* release of ciprofloxacin (CFX) antibiotic drug, using thermally-sensitive nano ZnO imprinted poly (N-isopropylacrylamide)/polyethylene glycol-dextran (PNIPAM/PEG-D@ZnO) nanocomposite hybrid hydrogels which are prepared via *in situ* technique (Scheme 1). The formations of

nanocomposite hybrid hydrogels are evidenced by FTIR, XRD, FESEM, EDX, XPS, and TGA. Zeta potential measurement revealed the distribution of particles in the nanocomposite hybrid hydrogels. Furthermore, swelling behavior, water retention, thermo responsive and mechanical properties are systematically examined. The rheological studies bespoke the gelling strength and gelation time of synthesized materials. From antibacterial study, it is found that, *E. coli* (EC) is the most resisting bacteria, while *B. cereus* (BC) is the least resisting one among all gram positive (*B. cereus* and *L. Inuaba*) and gram-negative bacteria (*E. coli* and *S. Flexneri*). The drugs are allowed to release in aqueous medium through the soaking technique. Ciprofloxacin (CFX) is used as an antibiotic model drug to estimate the drug delivery applications of the nanocomposite hybrid hydrogels. The maximum drug release rate is 98.2 % in duration of six hours in basic medium. This slow release behavior shows the controlled delivery of drugs by the synthesized vehicle. The cytotoxicity investigations corroborated the non-toxicity of nanocomposite hybrid hydrogels, which stands as a clear evidence for their biocompatibility attracting special attentions towards their possible use as drug delivery vehicles. The results indicated that the PNIPAM/PEG-D@ZnO nanocomposite hybrid hydrogels exhibit pH-sensitivity and have the potential to be applied efficiently as biodegradable carriers for *in vitro* release of ciprofloxacin (CFX) model drug.



**Scheme 1:** Schematic representation of preparation of nanocomposite hybrid hydrogels  
PP-58

### Toxicity study of ternary metal complex of Vanadium on Albino mice

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**Abstract:** Toxicological studies subjected to make a decision about whether a new drug should be accepted for clinical use or not. Toxicity study gives information on toxic doses and therapeutic indices of drugs and xenobiotic. Acute toxicity studies are designed to study adverse effects after

administration of a single dose or multiple doses of a test sample given during a period not exceeding 24 hours. Acute toxicity studies in animals are necessary for early stage preclinical stage to evaluate the perspectives of their further development. The information obtained from such studies are also useful in choosing doses for efficacy studies, providing preliminary identification of the target organs for drug-specific toxicity and in some cases revealing delayed toxicity. It is a scientific, ethical and regulatory requirement that before any potential new medicine administered to humans, its safety must be investigated in animals to define safe human doses.

A novel ternary metal complex of vanadium with metformin and glycine derivatives was synthesized via a one-pot condensation reaction in refluxing ethanol. The structure of the newly designed drug-metal complex was confirmed and characterised by UV, IR, <sup>1</sup>H NMR and GCMS studies. Both in vitro and in vivo studies were made in order to evaluate the antidiabetic activity effect of the newly synthesized drug complex. The potential toxicity of the gum acacia of ternary metformin complex were investigated through the method of acute and sub-chronic oral administration in mice and rats. In acute toxicity experiment, female and male mice (n=6/group/sex) were orally administered with the extract at single doses of 50, 300, 1000, 1500 and 2000 mg/kg in gum acacia and observed for 21 days. In the sub-acute study, the extract was orally administered daily at doses of 50 and 500mg/kg to male rats (n=8) for 6 weeks.

During the acute toxicity test, there were no deaths or any signs of toxicity observed after administration of ternary complex at 300mg/kg, and no adverse effect was observed. The extract at a dose of 2000 mg/kg led to the death of one female and one male mouse (LD<sub>50</sub>>2000 mg/kg). In sub-acute toxicity experiment, the extract induced no mortality or significant changes in body weight, general behaviors, hematological parameters, serum biochemical factors and histopathology of the heart, liver, kidney, and brain up to the highest dose tested of 500mg/kg. To optimize the dose levels, 1/16th(125 mg/kg body weight), 1/8th(250 mg/kg body weight) and 1/4th(500 mg/kg body weight) of the maximum dose(2000mg/kg body weight), given for the acute toxicity study as per OECD 423, were selected for the evaluation. The short-term use of ternary metal complex does not appear to produce significant toxicity up to a dose of 500mg/kg.

Moreover, toxicity studies play a significant role in drug development procedure providing information on toxic doses and therapeutic indices of potential drugs. In this study, we report the acute and sub acute toxicity studies of EASPA of the IC in female Wistar albino rats.

#### **PP-59**

### **Highly Effective Zn/Ti/Rgo Nano-composites for Steering Dual Functional Photocatalysis Activity**

**Tapan Kumar Behera**<sup>1</sup>, Pramod Kumar Satapathy<sup>1\*</sup>, Priyabrat Mohapatra<sup>2\*</sup>

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**Abstract:** Photo catalysis technology is an efficient, unique and cost-effective method to solve the environmental and energy issues in the near future. The development of active, cheap, efficient and visible-light-driven water splitting and dye degradation (Methylene blue) by catalysts is currently the center of intense research efforts. Amongst the most promising avenues, the design of Ti and Zn nanoparticle hybrids is particularly appealing more research interest. Again nanoparticles supported with graphene exhibits excellent charge carrier mobility with fast electron transfer pathway to suppress charge recombination and enhance the interfacial charge transfer processes. The photocatalytic activities of the Zn/ Ti/Rgo nanoparticles were synthesized by Co-PPt method and studied their characterized properties. From UV-DRS and Photoluminescence spectroscopy (PL) studies, it was confirmed that Zn/ Ti/Rgo matrix leads to the inhibition of recombination of charge carriers thereby, enhancing photochemical quantum efficiency and this leads to both dye degradation of methylene blue and water splitting reactions. The prepared nanoparticles demonstrated excellent photocatalytic response because of their small size, excellent crystalline structure, increase in threshold wavelength response and maximum separation of photo generated charge carriers.

**PP-60**

### **Mono/Bi-metal Complexes Catalyzed ROP of Lactide**

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**Abstract:** Nowadays, it has been constant challenge for modern scientists to search and synthesize new polymeric materials with modified architectures having controlled molecular weights and favorable properties. Ring Opening Polymerization (ROP) is the method, where a wide variety of cyclic compounds have been browbeaten, to secure the polymers of disired architecture, which was first discovered by Szwarc. The ROP of cyclic ester lactide has received renewed attentions in recent years. Polymer scientists have synthesized polylactic acid (PLA) by using transition metal complexes as catalysts/initiators by different bi-dentate, tri-dentate and tetra-dentate Schiff base ligands. The PLA is extensively used in biomedical and pharmaceutical applications, especially in tissue engineering and drug delivery. PLA has attracted immense interest because of its favourable properties such as good biocompatibility, biodegradability, and mechanical strength. PLA has been used to build three-dimensional scaffold for the regeneration of tissue engineered organs and has gained the approval of U.S. Food and Drug Administration (FDA) for a variety of human clinical applications. Out of the various methods that have been employed, metal containing initiators have become increasing industrially importance. Nowadays, metal alkoxides have been proven to be efficient catalysts for the ROP of lactide, mainly due to their great success in initiating living ring-

opening polymerization, producing polymers with well-controlled molecular weight and narrow molecular weight distribution.

Our main efforts comprise for controlled ROP and in understanding the role of ligands present as a catalyst component towards polymerization behavior. Our investigations have been mainly restricted to the synthesis of mono/bi-metal complexes for the ROP of lactide using salen ligands. Through this presentation, we will describe the understanding of the polymerisation process key to the development of suitable technologies through suitable case studies.

**PP-61**

**Green synthesis of graphene derivative and its composites with transition metal oxide nano particles for energy storage application**

**Yashabanta Narayan Singhabu**

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**Abstract:** In this study, sustainable, waste natural carbon source, *Aeschynomeneaspera* (AA) plant is used towards green and scalable synthesis of carbon two-dimensional materials and its composites with NiO are fabricated as an anode in high-performance lithium-ion batteries. XRD, Raman, XPS, and TEM data revealed that both graphene oxide (GO) and reduced graphene oxide (RGO) can be synthesized from AA plant by simply tuning heating temperatures in inert atmosphere. It is elucidated that the synthesis condition at which the carbon material exhibits better Li-ion storage properties does not show better performance when used as a composite material. This implies that an optimum balance between the oxygen functional groups and conductivity is important to exhibit excellent performance. The RGO-NiO composite fabricated with AA plant heated at 1000 °C shows initial discharge capacity of 1312 mAh g<sup>-1</sup> at a current density of 50 mA g<sup>-1</sup>. Even after 100 cycle at 100 mA g<sup>-1</sup>, a reversible specific discharge capacity of 847 mAh g<sup>-1</sup> is retained with a columbic efficiency of 93.6%, along with capacity retention of nearly 100%. In addition, ex-situ XRD and XPS measurements reveal reversible nature of the conversion reaction occurring in the composite electrodes. This study will profoundly impact not only in terms of choosing other sustainable, cheap, waste natural carbon sources but also on optimizing its synthesis conditions towards the fabrication of composites with transition metal oxides towards high-performance lithium-ion batteries that are cost-effective and industrially viable.

**PP-62**

**Conformational Search of Small Peptides Based on Gradient Gravitational Search (GGS) Algorithms**

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**Abstract:** The conformational search is a highly complex optimization problem which cannot be solved by simple mathematical models. A complete conformational search based on *ab initio* methods is computationally very demanding. Searching the best conformation of a larger molecule or finding the lowest possible energy of a larger protein may take days for computing the final output. In this regard, adaptation of novel techniques such as evolutionary algorithms could be more effective to solve the relevant problems specific to conformational search and even extended to global optimization. The rate of convergence and global optimality of an evolutionary algorithm rely on the combination of intensification and diversification. The aim of the present work is to explore conformational search of small peptides based on Gradient Gravitational Search (GGS) algorithm. Gradient Gravitational Search (GGS) algorithm<sup>1</sup> includes minimum and maximum gradient of the gravitational field and it is better in locating the next local minima. The present work includes the conformational search techniques by using the CHARMM force field parameters<sup>2</sup>. Moreover, all described energy terms have been computed by using respective connectivity through bonds, angles and dihedral angles.

**PP-63**

**Graphene Quantum dot decorated magnetic graphene oxide filled polyvinyl alcohol hybrid hydrogel for removal of dye pollutants**

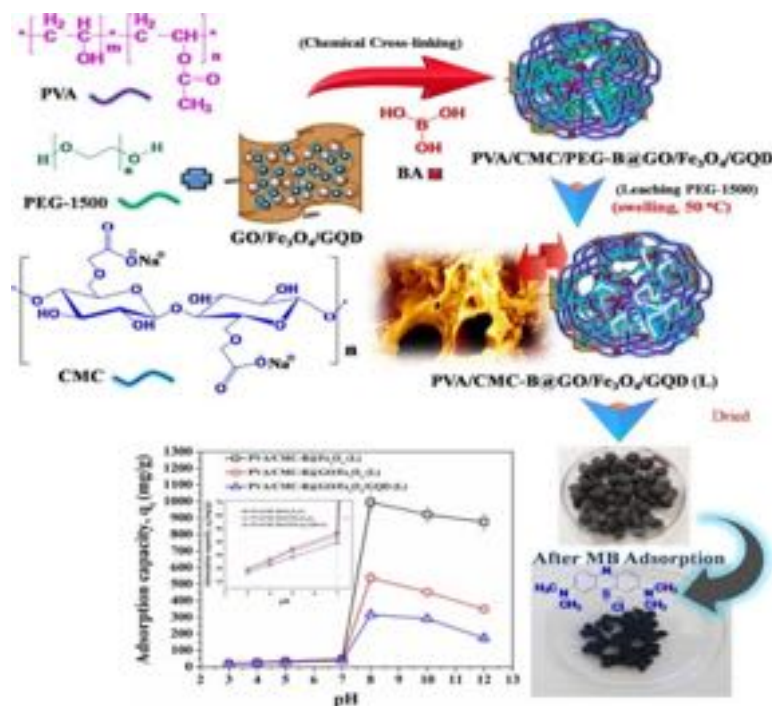
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**Abstract:** Herein, the graphene quantum dots (GQDs) integrated magnetic graphene oxide (GO/Fe<sub>3</sub>O<sub>4</sub>/GQD) can be easily prepared by using ethanol-HCl as destabilizing agent (Scheme 1). For performing the dye removal application with more environmental sensitive and eco-friendly the ultra-high surface area of GQDs with layered graphene like structure is highly responsible. The as-prepared nanohybrid filler is then in situ incorporated within PEG-1500 induced macroporous polyvinyl alcohol/carboxymethyl cellulose hydrogel beads. For the characterization of the prepared PVA/CMC-B@GO/Fe<sub>3</sub>O<sub>4</sub>/GQD (L) nanocomposite hydrogel SEM, TEM, XRD and FTIR is taken. Apart from this surface topography and roughness of the nanocomposite hydrogel is evaluated through AFM microscopy, while pore distribution in the nanocomposite hydrogel is explored through

BET adsorption isotherm and mercury porosimetry. Moreover, pH responsive swelling behaviour of the nanocomposite hydrogel is well studied along with detail investigation towards removal of cationic pollutants (MB/RhB) with respect to contact time and solution temperature.



**Scheme 1:** Synthetic Scheme of PVA/CMC-B@GO/Fe<sub>3</sub>O<sub>4</sub>/GQD nanocomposite hydrogel

PP-64

### Utilising Egg Shell effectively in preparation of Potash Fertiliser from Feldspar

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**Abstract:** To recover potassium from feldspar a bio-waste i.e. eggshell was used. The chief composition of eggshells is calcite. As it is a rich source of Ca, hence it is used with HCl to produce calcium chloride. Feldspar is an alumino-silicate mineral which bears potassium in the interstitial sites. To unlock the potassium from the interstitial sites it was roasted with calcium chloride prepared



by mixing eggshell and hydrochloric acid. At roasting temperature  $\text{CaCl}_2$  melts and penetrates into the alumino-silicate matrix to replace K with Ca. Potassium ion released from the silicate matrix combines with chloride ions to form potassium chloride which solubilised in water during the leaching process of the roasted feldspar. For the elucidation of mechanism of the roasting process, shrinking core model was applied to the roast-leach data and diffusion through product layer was inferred as the rate determining step. Order of the roasting process was found to be 2.158 and activation energy calculated to be 155.3 kJ/mole. Apart from potassium, sodium and excess calcium also got co-leached. To recover potassium from the leach liquor selectively, sodium perchlorate was added to precipitate potassium as  $\text{KClO}_4$ . Further potassium perchlorate was thermally decomposed to give potassium chloride which is of fertiliser grade being 99.81% pure.

### PP-65

#### **Isothermal kinetic analysis of thermal degradation low-rank Indian coal**

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**Abstract:** The isothermal kinetics of thermal degradation of low-grade Indian coal was examined by thermo-gravimetric analysis under the isothermal condition at a wide range of temperatures (375°C, 400°C, 425°C, 450°C, 475°C, 500°C) in a nitrogen ( $\text{N}_2$ ) atmosphere for 2 hours. The data obtained was inspected, and the degree of conversion ( $\alpha$ ) was calculated, which was then introduced into the isothermal kinetic equation to determine the activation energy ( $E_a$ ) and pre-exponential factor (A) of the coal sample during the thermal degradation process. The TG data shows that the degree of conversion of the sample is the function of time. The isothermal kinetics equation was utilized in describing the decomposition kinetics throughout isothermal pyrolysis of coal sample. The value of activation energy was found as 46.25 kJ/mol and the pre-exponential factor with an average of  $500 \times 10^3 \text{ s}^{-1}$ . The mechanism by using the rate law on TGA data was found to be first order reaction mechanism. Utilizing the kinetic equation various reaction models were tested for the degradation of the coal sample but the random nucleation-(F1) mechanism was found to be best suited for the thermal degradation of the sample.





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Leveraging our core competencies in chemistry with years of "real world" on-field experience, we continually strive to assist in new product design and development or enhance prevailing materials and formulations. Our innovative and highly experienced team works on work culture **S-A-C-H** which can be defined as **Sustainable solutions, Accountability, Customer centric and High performance and efficiency.**

Our trademark product ranges, **CLEARTECH** and **CLEARFINN** take us one step closer to promote eco-friendly habitat and be sustainable.

Our endeavor is to differentiate ourselves from the crowd through transparency in our dealings, quick response times, competitive pricing, with better performance, consistent quality and excellent pre and post sales support.

