

Oral Presentations

Oral Presentation-01

Ultrasensitive Detection of Aqueous Cu^{2+} Ions by a Coumarin-Salicylidene based AIEgen

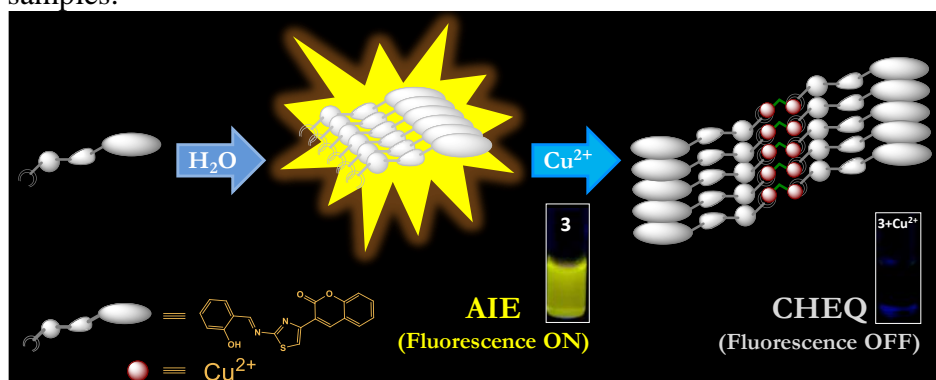
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Abstract: In this work we reports the aggregation induced emission (AIE) behaviour of a coumarin-salicylidene Schiff base (**3**) bearing a bright yellow AIE fluorescence in DMSO-water medium (f_w 80 %) buffered by 10 mM HEPES at pH 7.4. The aggregated probe (AIEgen-3) selectively discriminates Cu^{2+} ions over other interfering metal ions *via* a fluorescence “ON-OFF” strategy through a CHEQ process. DLS measurements revealed an average particle size of 372 nm for AIEgen-3 at 80% water fraction that dramatically increases to 656 nm in presence of Cu^{2+} ions indicating the formation of more structured aggregates, which was further supported by TEM and ESI-MS experiments. The binding characteristics and interference studies of AIEgen-3 with various metal ions have been carried out by fluorescence and UV-visible experiments. AIEgen-3 shows a fluorescence detection limit (LOD) of 24 nM (~1.5 ppb) for Cu^{2+} ions which is considerably far below the values of detection limits recently reported by other Cu^{2+} ion sensors in aqueous medium. Further, the analytical applications of AIEgen-3 have been demonstrated by the estimation of Cu^{2+} ions in tap water and pharmaceutical samples both in solution and solid phase which shows the potentiality of the probe for on-site detection Cu^{2+} ions in chemical, environmental and biological samples.



Oral Presentation-02

Pyrophosphate Ion Sensing by a Zn(II)-Terpyridine Complex in Aqueous Medium at Physiological pH

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Abstract: A highly fluorescent and conjugated 4'-(3,4-dimethoxyphenyl)-2,2':6',2''-terpyridine ligand **L** was synthesized by refluxing 3,4-dimethoxy benzaldehyde and 2-acetylpyridine in ethanol medium at room temperature. Then by taking this synthesized ligand, a simple Zn(II)-terpyridine complex was synthesized by the reaction with ZnCl₂ in 1:1 ratio in dichloromethane methanol mixture. Further the synthesized complex was treated as a selective fluorescent probe for pyrophosphate P₂O₇⁴⁻ (PPi) among other anions like F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, CO₃²⁻, NO₂⁻, SO₃²⁻, H₂SO₄⁻, HPO₄⁻ etc. This sensing behaviour was studied by both UV-visible and fluorescence photophysical methods. Moreover, an abnormal 1:3 binding stoichiometry was found from the job's plot analysis.

Keywords: Terpyridine, Pyrophosphate (PPi), Chemosensor

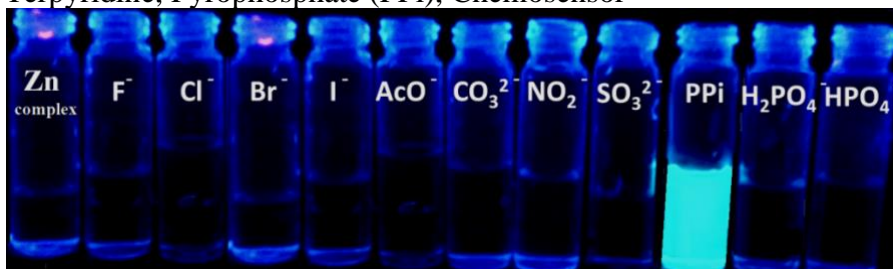


Figure 1: Image of Zinc Terpyridine Complex (50 μL), in Presence of Sodium Salts of Various Anions under UV Chamber at 365nm.

Oral Presentation-03

MnCo₂O₄ Decorated rGO/gC₃N₄-based Sensor for Highly Selective and Sensitive Detection of Chlorpyrifos

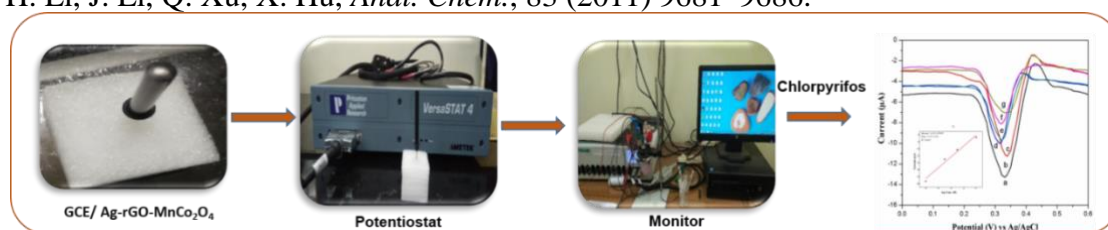
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Abstract: Chlorpyrifos, the most toxic pesticide is used mostly in the field of agriculture and significantly affects the environment [2]. Therefore, the detection of Chlorpyrifos in various food samples and drinking water became essential for the protection of living beings as well as environment. In this regard, an easy, rapid, cost-effective nonenzymatic sensor involving MnCo₂O₄ decorated (2D/2D) rGO/gC₃N₄ modified glassy carbon electrode (GCE) is designed for the first time as a sensitive and selective electrochemical pesticide sensor. The designed

nanocomposite has been synthesized via simple and rapid solution combustion route. Later on, the nanocomposite has been characterized thoroughly by various sophisticated analytical techniques such as FTIR, XRD, Raman, FESEM, TEM with EDS mapping to investigate the successful synthesis of desired nanocomposite. Later on, the electrocatalytic activity of the synthesized nanocomposite was investigated using Cyclic voltammetry and Differential Pulse Voltammetry. Then the optimized sensing conditions were obtained by varying different sensing parameters such as material loading, pH, temperature and incubation time. The designed nanomaterial was able to detect a wide range of pesticide concentrations (1 μ M-1nM) with a lower limit of detection (LOD= 0.3nM) (S/N = 3), which was further verified by Nyquist plot. Later on, the reusability and stability of the sensor were also studied for 30 days. Finally, the material was successfully applied in real sample analysis for ground water as well as fruits and vegetables.

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Graphical Abstract

Oral Presentation-04

Adsorptive Removal of Congo Red dye from Aqueous Solution using Mg-doped ZnO Nanoparticles: Kinetics, Thermodynamics and Isothermal Insights

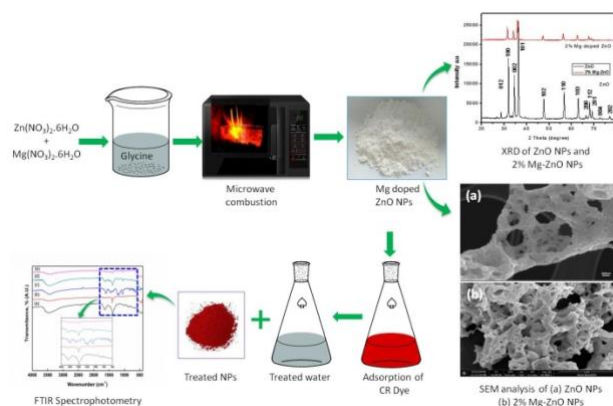
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Abstract: A facile microwave-assisted combustion method was adopted to synthesize pure ZnO and Mg-doped ZnO nanoparticles (NPs), and characterization of the NPs and the sorption behaviour with Congo Red (CR) Azo dye was extensively investigated. The structure, morphology and chemical assay of the synthesized NPs were studied with respect to the pure and 2% Mg-doped ZnO samples. The X-ray diffraction pattern confirmed the presence of crystalline, cubic phase with fluorite structure of both the NPs. The morphological differences between the pure and Mg-doped ZnO NPs were evaluated by FE-SEM, which revealed that the NPs were in the nanoscale regime with irregular crystalline morphology having a grain size of ~18–45 nm. N₂ adsorption/desorption isotherms measured at –196 °C suggested a Type II structure with limited hysteresis loops, likely due to some inter particle porosity. The BET SSA ZnO NPs obtained was found to be 32m² g⁻¹, indicating about its potential in sorption processes. Batch adsorption study for the removal of CR carried out showed that, the

Mg-doped NPs showed higher loading efficiency (125 mg.g⁻¹) than the ZnO NPs (25 mg.g⁻¹) counterpart. This was corroborated by the isotherm results in which the CR dye sorption followed a Freundlich Isotherm model for both undoped ZnO and Mg-doped ZnO NPs. The sorption of CR dye followed a pseudo-second order kinetics. The negative ΔG° (-31.91 and -109.41 kJ mol⁻¹) showed the feasibility of the adsorption process. The ΔH° was determined as +13.74 kJ mol⁻¹ and 50.7 kJ mol⁻¹ for ZnO NPs and Mg doped-ZnO NPs respectively, confirming the endothermic nature of the adsorption for removing CR dye from the solution.



Graphical Abstract

Oral Presentation-05

Preparation of High-performance Graphene Geopolymer Composites

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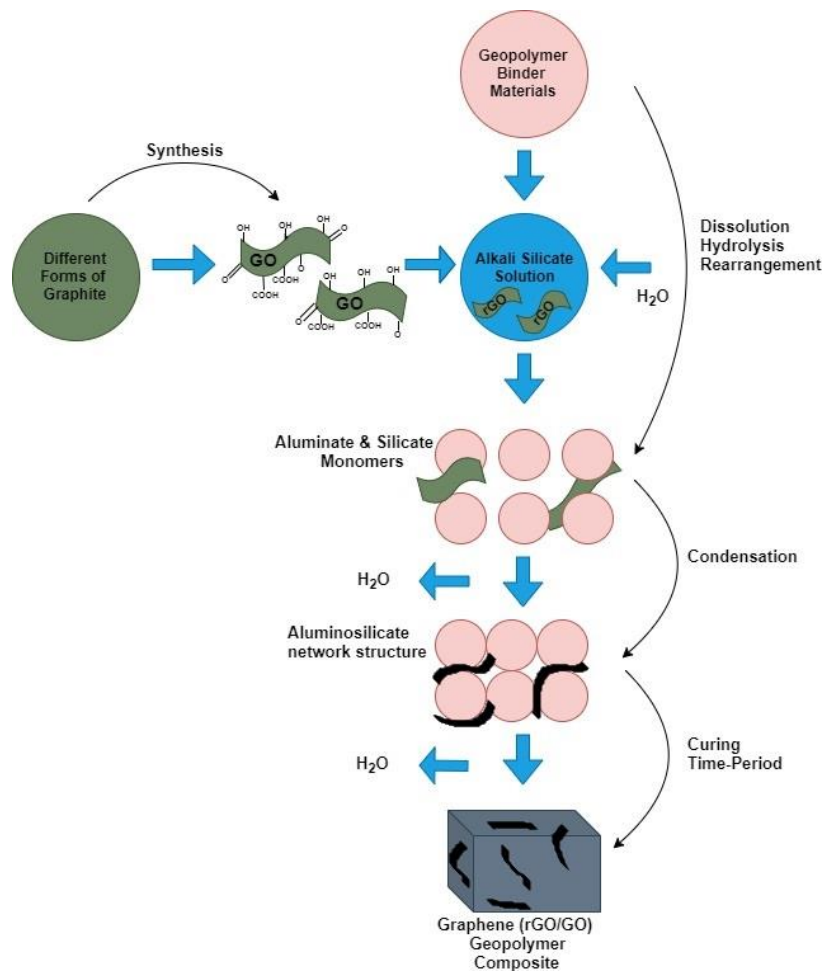
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Abstract: Graphene geopolymer composites combine both the flexibility of geopolymers along with the strength of graphene. Most of the composite is primarily composed up of geopolymers. Hence, graphene is only used as a property enhancer. Geopolymer alone stands as an eco-friendly substitute for the most commonly used Portland cement, which has its own share of demerits. They consist up of binder material and an alkali solution, which ultimately helps in getting rid of water usage and Carbon dioxide (CO₂), produced during the usage of Portland cement. The binder comprises of waste materials such as Fly-ash(FA), Ground granulated blast furnace slag (GGBFS), Ferro-chrome ash (FCA) or Rice husk ash (RHA), etc. while the alkali solution consists of Sodium Hydroxide (NaOH), Sodium Silicate (Na₂SiO₃) or Potassium Hydroxide (KOH). Throughout the years, numerous prominent scientists have explored significantly on the alkali activation reaction mechanisms of various aluminosilicate materials with different alkaline solutions. However, accurate reaction mechanism justifying the hardening and setting properties of geopolymer binders has not been comprehended by general scientific communities yet which establishes the fact geopolymerization primarily

depends on the choice of source material and alkaline solution and is a fast-complex multiphase reaction. Graphene additives play a significant role in determining the conclusive material properties of the composite. Various derivatives of graphene i.e. Graphene nanoplatelets (GNP's), Graphene Oxide (GO) or Reduced Graphene Oxide (rGO) have been experimented to determine the properties of the composite. The synthesis of graphene derivatives plays a crucial role in governing the quality of the derivatives. Among many of the adapted methods are Chemical Vapor Deposition (CVD), Chemical or Plasma Exfoliation from natural Graphite, Mechanical cleavage from natural Graphite, etc. Both of the materials prevail over each other's limitations, which results in high performance and more durable composite along with several other enhancing properties. Composites made of geopolymer and graphene can be extensively used in many sectors including construction, energy storage applications and many more. The illustrated figure follows a top-down approach by highlighting the important steps in the preparation of graphene geopolymer composites. This paper highlights the adapted methods for preparing durable and high-quality graphene reinforced geopolymer composites.



Oral Presentation-06

Effect of Phosphate on Iron Mineralization and Mobilization in Non-heme Bacterioferritin B from *Mycobacterium Tuberculosis*

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Abstract: Iron acts as a double-edged sword, both essential as well as toxic, due to its redox activities. Inside the cell, ferritin sequesters excess of free Fe(II) and detoxifies it by synthesizing hydrated ferric oxyhydroxide mineral via protein mediated mineralization reaction. Unlike mammalian ferritins, the native bacterial/plant ferritins contain significant amount of phosphate in their mineral cores. In aqueous buffer, phosphate preferentially stabilizes Fe(III) and hence alters its redox properties but its impact during the oxido-reductase (ferroxidase) reaction, occurring inside the supramolecular ferritin nanocage, is less studied. Moreover, like iron, phosphate also regulates the pathogenesis of *Mycobacterium tuberculosis* (*Mtb*), which expresses two types of ferritins: a heme-binding bacterioferritin A (BfrA) and a non-heme binding bacterioferritin B (BfrB). Therefore, the effect of phosphate on the synthesis, structure and reactivity of iron mineral core in *Mtb* BfrB was investigated. The stopped-flow rapid kinetics of ferroxidase activity of BfrB revealed the formation of a di-ferric peroxy like transient species during the initial stage of biomineralization. The presence of phosphate not only affected the kinetics of rapid iron oxidation but also decreased the size/crystallinity of the iron mineral core and inhibited the reductive iron mobilization (Fig.1). The current work demonstrates the unique ability of BfrB to rapidly sequester iron even under high phosphate concentrations indicating the role of its ferroxidase centers during *Mtb* pathogenesis.

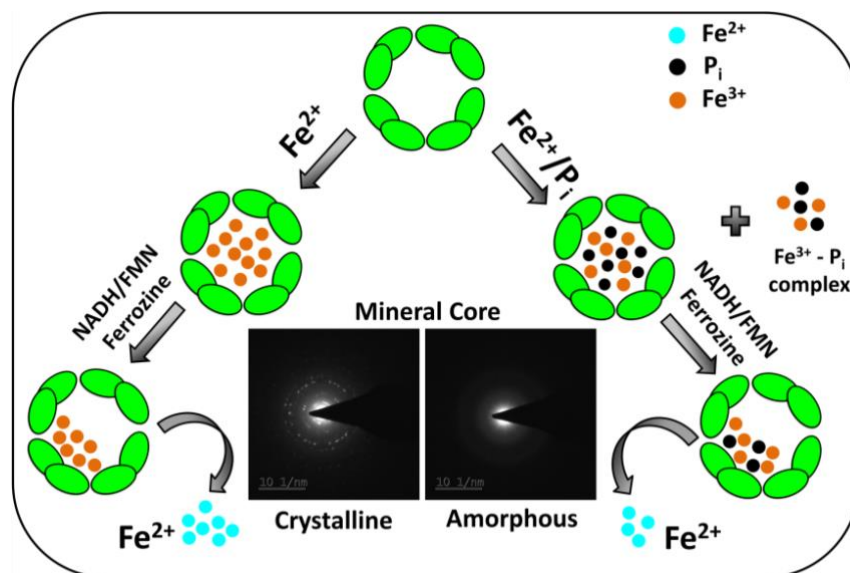


Figure 1: Inorganic Phosphate alters Iron Mineralization in BfrB, lowers the Crystallinity/Size of the Iron Mineral Core, and inhibits Reductive Iron Mobilization.

Oral Presentation-07

Incorporation of Silver Nitrate into embedded Nano Boron Nitride for the Preparation of Polyethyl Methacrylate/Polyvinyl Alcohol Nanocomposite Layered Material

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Abstract: A chemical dependable process for the EMA monomer used to synthesize polymer layered material was developed in laboratory. Purification of EMA is carried out first by monomer washing process. Then synthesis of composite material is carried by simple in situ technique maintaining temperature between 50 to 60 degree. It was properly dried for the formation of a thin film; five different nanocomposite samples were prepared by varying the concentration of BNNPs. Such as 1%, 2%, 3%, 4% and 5%. Phase analysis, microstructure, and chemical composition are examined by X-ray diffraction (XRD), Fourier transform Infrared Spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), X-ray photoelectron spectroscopy (XPS) and high resolution transmission electron microscopy (HRTEM). The surface and nano-tribological characteristics of the polymeric nanocomposite are investigated by atomic force microscopy (AFM). The thermal, antibacterial, and oxygen barrier properties of the polymeric nanocomposite are studied. The incorporation of the BNNPs enhances the barrier, thermal, and antimicrobial properties enhanced by incorporation of AgNPs into the PEMA/PVA matrix by which the material is suitable for good packaging applications.

Oral Presentation-08

Reaction of 2,4,5-trisubstituted-1-hydroxy Imidazoles with Epichlorohydrin

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Abstract: Nucleophilic substitution reactions of epichlorohydrin with various nucleophiles have been reported since a quite long time. Sivastava and coworkers have attempted the synthesis of aryloxy-propanol amines. The key step is the reaction of aryloxy ion with epichlorohydrin. This indeed tempted us to study the reaction of hydroxy imidazole derivatives with epichlorohydrin. N₁-hydroxy-2,4,5-trisubstituted imidazole derivatives were prepared as per the reported procedure. The tendency of such hydroxy imidazoles to undergo easy oxidation as well to be converted to oxide ion in alkaline medium ignited our minds to use it as a nucleophile and carry out substitution reactions to afford new derivative, which might have potential biological applications. To study we have chosen epichlorohydrin, which is very much susceptible to nucleophilic attack. Contrary to the earlier reported studies, we have obtained three different products whose structures were established with respect to ¹H, ¹³C NMR and mass spectral data. Work is in progress to find their potential applications.

Oral Presentation-09

Experimental and Theoretical Studies on the Structure of 2-chloro (o-hydroxy Benzylideneaniline)

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Abstract:The UV, FT-IR, SC-XRD studies of the Schiff's base, 2-chloro (o-hydroxy benzylideneaniline) were carried out in order to determine the optimized structural parameters of the compound and compared with the optimized data obtained theoretically following density functional theory analyses. The FT-IR and UV-VIS spectroscopic analyses were carried out at B3LYP/6-311G (d, p) level of theory. The molecular electrostatic potential surfaces were plotted to elucidate the reactivity of the molecule. The lowest spin-allowed (singlet-singlet) excited states were subjected to investigate possible electronic transitions. HOMO–LUMO energy gap of the energy levels corresponding to each of the transition were determined. A good agreement was observed between the optimized geometry obtained from Density Functional Theory and experimental single crystal X-ray diffraction (SC-XRD) structure. The occurrence of hydrogen bonding in the molecule was suggested. The FT-IR and MEP analyses also affirmed the hydrogen bonding in the compound postulated by SC-XRD results.

Oral Presentation-10

Impact of Inclusion Complexes of 2((1,3,4) Thiadiazino [6,5- b] indol-3-ylimino) methyl) Phenol and Its Derivatives with β –Cyclodextrin: Spectral, Thermal and Antimicrobial Study

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Abstract:Extensive biochemical and pharmacological studies of indole derivatives have confirmed their highly effectiveness against various strains of microorganisms as well as have various therapeutic effects. Inspired by these observations, in this research work, some substituted indoles i.e. 2((1,3,4) Thiadiazino [6,5- b] indol-3-ylimino) methyl)substituted phenols are synthesized and their inclusion complexes have been prepared with β - Cyclodextrin to enhance their stability, solubility, bio-accessibility and hence pharmacological properties. The formation of both synthesized pharmacophores and their inclusion complexes are established based on elemental, thermal and spectral (UV, FT-IR, ^1H NMR, etc.)studies. The comparative biological screening of the synthesized compounds and their inclusion complexes are made for different bacterial strains, fungi and antioxidant character. The results of the research authenticate the fact that the inclusion complexes of the synthesized compounds exhibit profound antibacterial, antifungal and radical scavenging property with respect to their bared compounds.

Oral Presentation-11

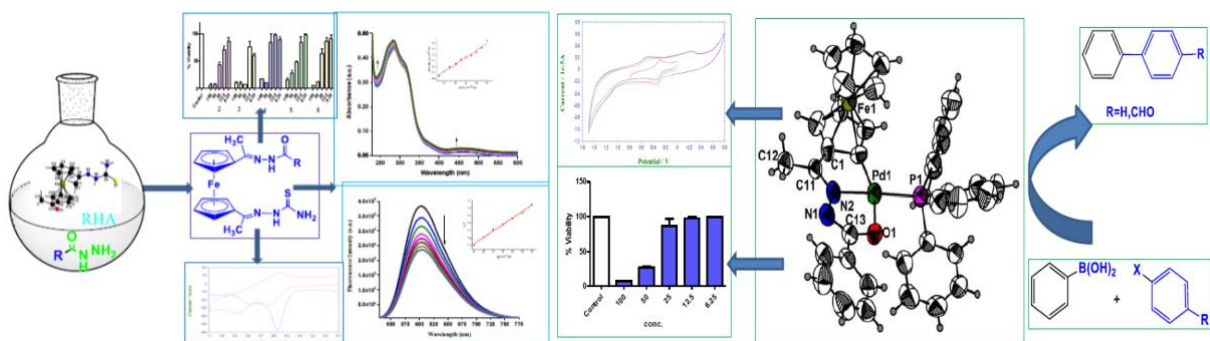
Functionalization of Ferrocene by Hydrazone and Thiosemicarbazone Fragments: Significant Cyclopalladation and Biological Properties Study

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Abstract: Ferrocene based organometallic moieties are the most versatile molecular entities in organometallic chemistry because of their distinctive structural integrity, reversible redox behavior and enormous potential in the development of material science, molecular wires, catalysis, sensing, electronic communication and bio-organometallic chemistry.[1] Recent research supports the application of ferrocenyl compounds for a diversity of therapeutic uses in which ferrocene substituted tamoxifen and ferrocenyl chloroquine derivative shows higher inhibitory activity compared to their organic analogue.[2] Our research group have currently explored the potential of several mono- and di-ferrocenyl hydrazone and chalcone based compounds which showed exciting biological and sensing properties.[3] In addition, we have also been able to synthesize unsymmetrical ferrocenyl hydrazones using a novel solvent free synthetic method by using RHA for various biological applications.[4] This encouraged us to focus on the synthesis of 1,1'- unsymmetrical ferrocenyl linked mixed hydrazones, thiosemicarbazones and study their reactivity towards metallation and CH-activation technique. A systematic stepwise / multicomponent solid supported synthetic method using precursors involving diacetyl ferrocene, thiosemicarbazide and different organic hydrazide led to the isolation of mixed ferrocenyl hydrazone-thiosemicarbazone derivatives. The intermediate was structurally confirmed by single crystal X-ray diffraction study and their electrochemical properties was studied using cyclic voltammogram. The interaction of unsymmetrical ferrocenyl compounds with calf-thymus DNA has been explored by using absorption and emission studies to observe potent cytotoxic effect on human leukemia (THP-1) cell line. Similarly, some of these ferrocenyl hydrazone and thiosemicarbazone derivatives display interesting metal binding behavior towards transition metals through imine nitrogen, enolate oxygen and enolate sulphur ligation. A unique CH-activation of the ferrocenyl ring was observed, when the complexation behavior of some hydrazones and thiosemicarbazones were carried out with tetrakis(triphenylphosphine) palladium to yield a rarely known ortho cyclopalladated complexes. The structural confirmation of the cyclopalladated ferrocenyl complexes was obtained from single crystal X-ray diffraction study. Investigation of their electrochemical properties also showed ferrocene based redox processes and distinct electronic communication behavior among the electroactive species. These types of cyclopalladated complexes have promising cytotoxic effect on human leukemia (THP-1) cell line and act as efficient reusable catalyst in Suzuki-Mayura cross coupling reactions.



References

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Oral Presentation-12

Removal of Some Cationic Dyes from Organic Medium by the Application of unmodified Silica

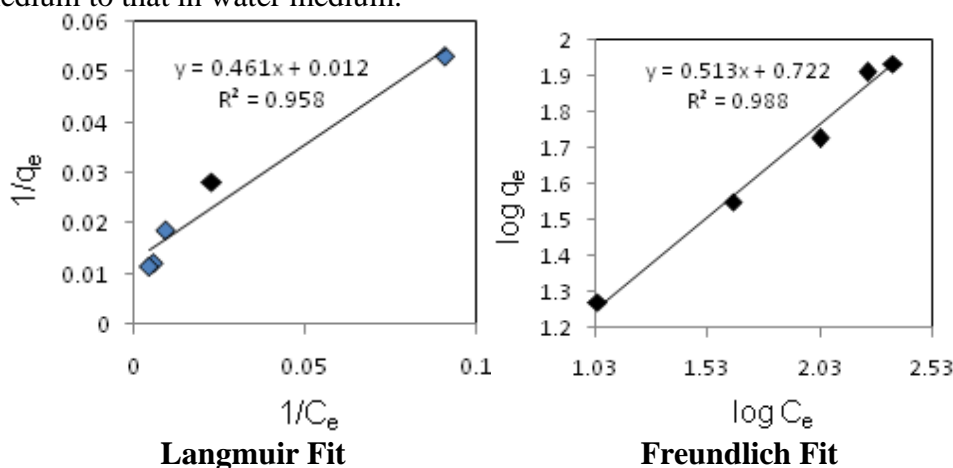
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Abstract: Removal of some cationic dyes with varying substituents and alkyl chain lengths has been carried out on unmodified silica from organic solvents. Textural property of unmodified silica was analyzed employing Scanning Electron Microscope (SEM) and X-ray Diffraction (XRD) techniques. The influences of different adsorption factors like contact time, adsorbent dosages, varying concentrations of dyes and temperature on the rate of adsorption of dyes have been studied. The mechanism of removal of dyes is in agreement with the pseudo second order kinetics. The α -styryl pyridinium dye with hydroxy substituent shows maximum adsorption as compared to that of dye with dimethylamino substituent. This can be attributed to the existence of strong Hydrogen bonding between the most electronegative element Oxygen of OH group of adsorbate and the silanol units of adsorbent. Further the dye with dodecyl alkyl chain length exhibits better adsorption rate as compared to the dyes with methyl and butyl chain length, which may be due to the excellent interaction between the hydrophobic group of adsorbate and adsorbent in non-polar medium. All the data fit well to the Freundlich

adsorption isotherm. The adsorption isotherm shows multilayer stacking of the dye molecules on the silica surface. Thermodynamic modeling has been done from three temperatures such as 20, 25 and 30°C. The thermodynamic parameters have been investigated to understand the feasibility of application of unmodified silica surfaces in the removal of dyes from organic solvent. A comparative study has been carried out between the rates of adsorption of dye in organic medium to that in water medium.



Oral Presentation-13

Partitioning Addition and Substitution Reaction: Effect of Solvent

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Abstract: Reaction of F⁻ with bromoethane leads to fluoroethane as the substituted product and ethylene as the elimination product. The present investigation reports the effect of solvents on the partition of transition state to two different pathway through potential energy surfaces (PES) and structures of the species. The PESs in gas phase have been computed at MP2 level and CCSD(T) level. The performance of several hybrid density functional, such as B3LYP, M06, M06L, BHandH, X3LYP, M05, M05-2X, M06-2X have also been investigated towards describing the elimination and nucleophilic substitution reactions. With respect to MAE values and to make the computation cost effective, we have explored the implicit continuum solvent model, CPCM in solvents like cyclohexane, methanol, acetonitrile, dimethyl sulphoxide and water. The calculated relative energies values which are negative in gas phase are found to be positive in polar solvents since the point charge in the separated reactants are more stabilized than the dispersed charge in the transient complex, which has also been analysed through NBO analysis.

Oral Presentation-14

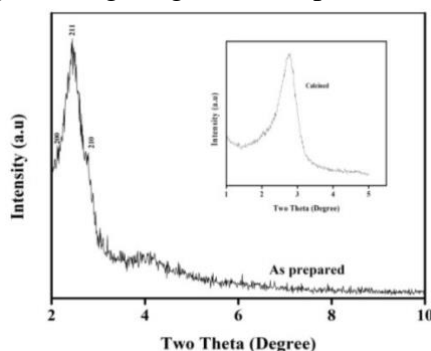
Room Temperature Synthesis of Nanoporous SBA-1

N. Parida, K. Asha, S.K. Badamali*

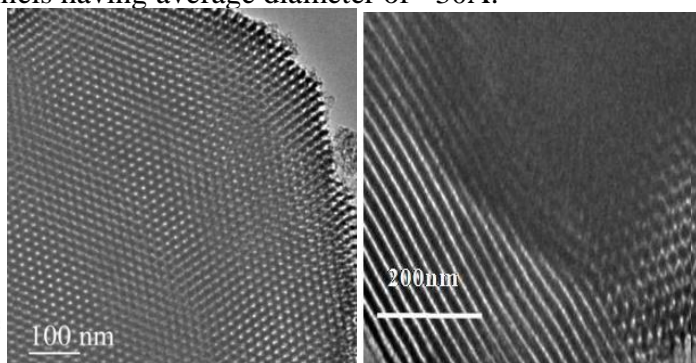
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Abstract: Nanoporous solids possessing open nanodimensional channels find widespread applications in adsorption, catalysis and host guest chemistry. Herein, we report the synthesis of a nanoporous silica (SBA-1) based material having 3-D pore architecture. The samples were prepared at RT from a gel containing TEOS, CTAB and dil. HCl and characterized by XRD, TG, FTIR, Raman and TEM studies. XRD patterns of both as-synthesized and calcined SBA-1 shows a strong reflection at $d=35.81\text{\AA}$ which is typical of ordered SBA-1 structure [1]. TGA curves of as-synthesized SBA-1 gave about 48% of total weight loss noticed in three steps indicates the porous nature of the material. FT-IR and Raman spectra of the both as-synthesized and calcined SBA-1 samples showed various bands that can be attributed to silica structure. SBA-1 possesses large number of internal surface hydroxyl groups. This observation is consistent with the TGA results of calcined SBA-1. TEM micrographs clearly showed regular long range ordered pore channels having average diameter of $\sim 30\text{\AA}$.



XRD Pattern of SBA-1



TEM Patterns of SBA-1

References

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Oral Presentation-15

Membrane Cholesterol Modulates Oligomeric Status and Peptide-membrane Interaction of Severe Acute Respiratory Syndrome Coronavirus Fusion Peptide

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Abstract: The N-terminal fusion peptide of S2 glycoprotein of the SARS Co-Virus, which is exposed upon receptor binding, is crucial for its entry into the host cell. The fusion peptide

alters the membrane organization and dynamics of the host membrane to facilitate membrane fusion. Generally, the effect of fusion peptide on the membrane is sensitive to the lipid composition of target membranes. In this present work, we have utilized steady state and time-resolved fluorescence spectroscopy in tandem with CD spectroscopy to elucidate the binding, oligomeric status, secondary structure of the fusion peptide and its impact on the depth-dependent membrane organization and dynamics. We have used depth-dependent fluorescent probes, DPH and TMA-DPH, to evaluate the effect of the peptide-binding along the bilayer normal as well as energy transfer efficiency of tryptophan between TMA-DPH and DPH to determine the relative location of tryptophan present in the membrane-bound fusion peptide. We have further evaluated the effect of membrane cholesterol on the binding and organization of the peptide on the membrane at various cholesterol concentrations. Our results clearly demonstrate that the membrane cholesterol alters the oligomeric status of the membrane-bound peptide and the effect of peptide-binding on the depth-dependent membrane organization and dynamics.

Oral Presentation-16

Synthesis and Evaluation of Dendritic Carboranyl Glycoconjugates: Promising Dual Mode Candidates for Cancer Treatment

Biswa Ranjan Swain,[†] Bismita Nayak,[§] Rashmirekha Satapathy,^{*†} and Barada Prasanna Dash^{*‡}

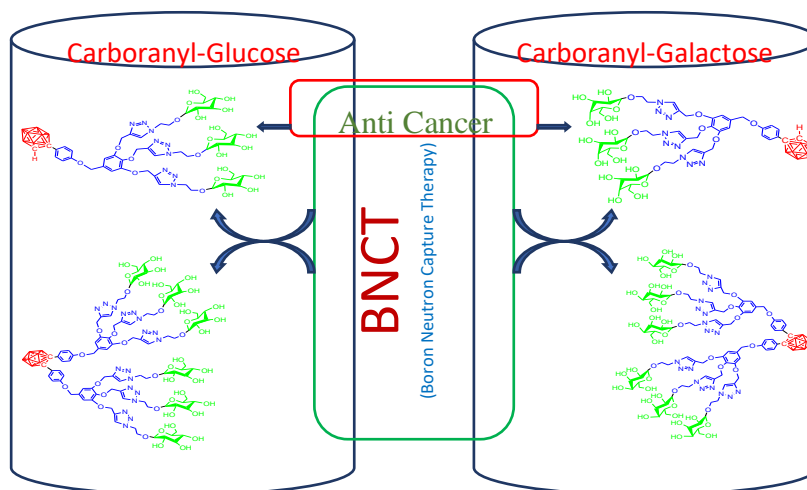
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Abstract: There are many cancer treating methods developed until today, but none of the method is fully effective because of their limitations to use. The mostly used chemotherapy method limits its effectiveness due to its toxicity to other healthy cells in the body. Several glycoconjugates of polyhedral boron clusters have been synthesized for tumor targeted delivery of boron for treatment of cancer via boron neutron capture therapy, but lacks its effectiveness. In our present work, we have synthesized four numbers of highly water soluble, active drug delivery agents which should have an ability to overcome the limitations for acting as BNCT drug, with the potential to deliver the drug to the targeted area and accumulate within tumor cells in a controlled manner, as well as the potential to show anti-cancer efficacy investigated by MTT assay. These findings could be useful for successful treatment of cancer.



Oral Presentation-17

Effect of Different Functional Groups in UiO-66 Metal Organic Frameworks for the Adsorption of Anionic Dyes: An Experimental and Molecular Docking Study

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Abstract: Water contamination from various noxious industrial wastes is a major environmental concern. These have much adverse effect on the living ecosystem. Organic dyes mostly used in textile, plastic, cosmetic and pharmaceutical industries are among the major pollutants, which affect the water quality badly. Adsorptive removal of this hazardous waste from water have been used as a successful method and exhaustive studies have been reported. However, a major challenge is to develop adsorbent materials that can selectively remove dyes from the water system. Metal Organic Frameworks (MOFs) are smart materials, which comprised of metal ions or clusters connected by organic linker molecules and form crystalline coordination polymer networks. Among these MOFs, UiO-66 MOFs stands out as a superior class of materials for their robust chemical nature, that have been successfully used for the removal of toxic dyes for e.g. methylene blue dye from aqueous solutions. Adsorption behavior of two anionic dye Congo red and reactive blue on two type of Zirconium MOF (UiO-66-NH₂ and UiO-66-NO₂) has been investigated using adsorption experiment, spectroscopic analyses, and mechanism of adsorption by theoretical calculations. Firstly, the nano-MOFs has been synthesized by hydrothermal process using a small screw cap glass tube and characterized by powder X-ray diffraction, FT-IR, UV-DRS, SEM, TEM, specific surface area by N₂ adsorption, TGA and the mechanism by molecular docking method. The adsorption process mainly controls by hydrogen bonding and π - π stacking interaction between the MOF and dye molecule. The UiO-66-NH₂ have greater adsorption capacity as compared to UiO-66-

NO₂. This is because of a greater number of binding sites presents in UiO-66-NH₂ for having the NH₂ group.

Oral Presentation-18

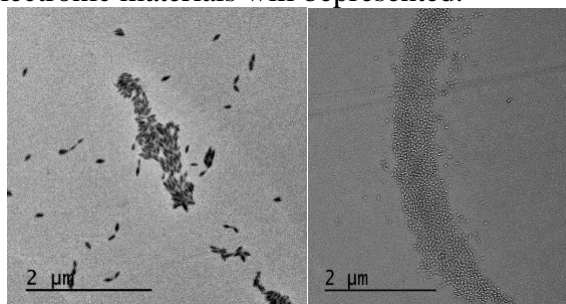
Optoelectronic Materials based on Donor-Acceptor Conjugated Systems

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Abstract: Electron-rich donor (D) and electron-poor acceptor (A) units in a conjugated material leads to reduction in the HOMO-LUMO separation. The intramolecular charge transfer between donor and acceptor units significantly reduces the band gap of such materials. Benzothiadiazole has been extensively used as an acceptor unit leading to materials with high charge carrier mobilities in OFETs, near infrared emission in OLEDs and effective light harvesting in OPVs. Incorporation of benzothiadiazole units into polyfluorene backbone results in reduction of HOMO-LUMO band gap of about 0.5 eV. Subsequent borylative fusion further reduces the HOMO-LUMO separation up to 0.6 eV. In addition, Suzuki polycondensation has been employed to synthesise a variety of benzothiadiazole-based blue, green and red emitting donor-acceptor polymers and polymer nanoparticles. The synthesis and properties of these optoelectronic materials will be presented.



140-150 nm x 40-50nm rods 40-60 nm x 15 nmrods

Oral Presentation-19

Removal of Congo Red Dye from Aqueous Solution using Zinc Oxide Nanoparticles derived from Tulsi Leaf (*Ocimum Sanctum*): A Green Approach

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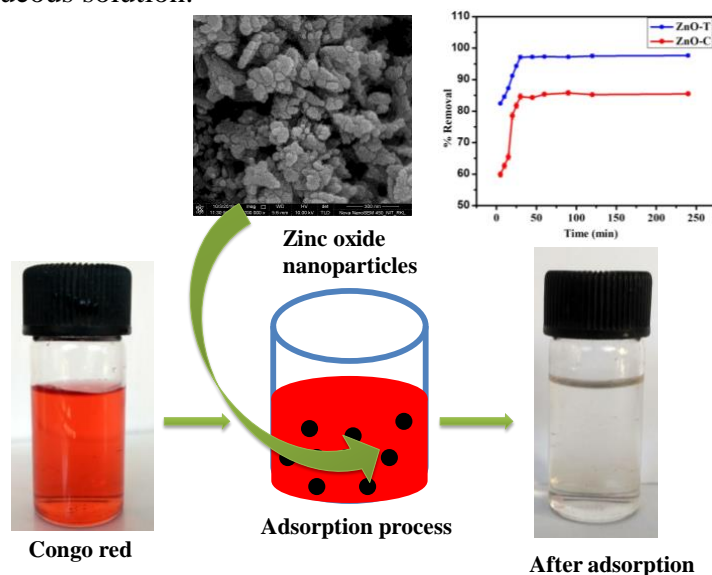
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Abstract: The main goal of the present work is to deal with the green synthesis of zinc oxide nanoparticles using aqueous leaf extract of *Ocimum tenuiflorum*. In synthesis of zinc oxide

nano particles, zinc nitrate and sodium hydroxide were used as main materials and *Ocimum tenuiflorum* leaf extract as a precursor. The resulting product was characterized by UV-visible, FT-IR, XRD, FE-SEM, EDX analysis and N₂- adsorption-desorption isotherm. The green synthesis of zinc oxide nanoparticles used as a novel and more efficient material for Congo red dye adsorption as compared to commercial available zinc oxide. The adsorption studies were carried out under various parameters such as adsorbent dosage, initial dye concentration, pH, stirring speed and time. To understand the mechanism of Congo red dye on zinc oxide nanoparticles, we have investigate two adsorption kinetics like pseudo-first order and pseudo second order. Due to high correlation coefficient value of the pseudo-second order ($R_2=0.99$) kinetics, the adsorption process follows chemisorption. The experimental data for the isotherm followed the Langmuir isotherm model. The outcome obtained from this research suggested that zinc oxide nanoparticles could be a potential adsorbent with its reusability of Congo red from aqueous solution.



Oral Presentation-20

OH/HO₂ Radical Measurements in the Troposphere

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Abstract: The removal of OH radicals to all sinks in the troposphere can be define by its total pseudo first order loss rates coefficient (k_{OH}) and which is generally termed as total OH reactivity. At MPIC, Germany, I developed and characterized an OH reactivity instrument using laser flash photolysis combined with laser induced fluorescence (LFP-LIF) technique for

wide ranges in hydrocarbon and NO_x variations during field campaigns. The Middle East has exceptional environmental qualities, with intense solar radiation, extensive deserts and water scarcity that promotes dust mobilisation. Furthermore, it is subject to high levels of air pollution due to emissions from traffic and petrochemical industry. The AQABA (Air Quality and climate in the Arabian BASin) field campaign took place in summer 2017 covering a ship track from Toulon to Kuwait through the Mediterranean and around the Arabian Peninsula and back. During the AQABA campaign, our group measured HO_x (OH+HO₂) radicals using laser-induced fluorescence (LIF) to investigate the regional influences on HO_x concentrations and budgets.

Oral Presentation-21

Synthesis and Magnetic Behaviour of Mg-Zn Nano Ferrites by Using *Aloe Vera* Extract Solution

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Abstract: Mg_xZn_{1-x}Fe₂O₄ (x = 0.25, 0.55, 0.75) ferrite nanoparticles were prepared by a modified sol-gel method using high purity metal nitrates and Aloe-Vera plant extract solution. Using of Aloe-Vera extract simplifies the process and provide an alternative process for a simple and economical synthesis of nanocrystalline ferrite. The structural characteristics of calcined sample of Mg_xZn_{1-x}Fe₂O₄ (x = 0.25, 0.55, 0.75) ferrite nanoparticles were determined by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and transmission electron microscopy (TEM). The prepared samples have spinel structure. From XRD, it was observed that particle size decreases with increasing Mg content. All the prepared samples have spinel structure with particle size of 33 nm-55 nm. Nano size of the particles was confirmed by TEM measurement. FTIR spectral analysis helps to confirm the formation of spinel structure in ferrite samples. Magnetization measurements were obtained at room temperature by using vibrating sample magnetometer (VSM), which showed that the calcined samples exhibited magnetic behaviour.

Keywords: *Aloe vera*, Electron microscopy, Magnetic properties, Sol-gel, Synthesis, Vibrating sample magnetometer

Oral Presentation-22

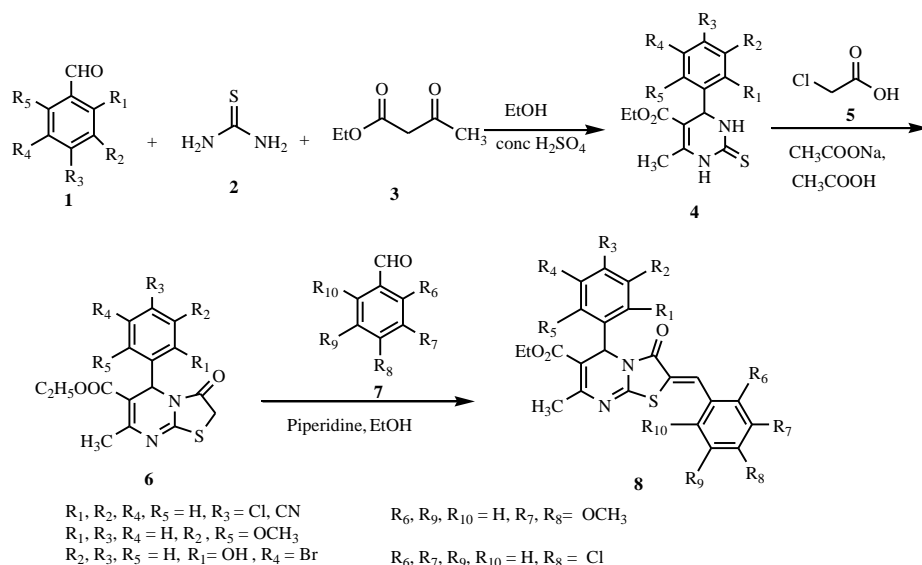
Microwave assisted Synthesis of Thiazolo-Pyrimidine Derivatives

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Abstract: Nitrogen containing heterocycles especially thiazolopyrimidines, at present era have become the focal point for medicinal chemists owing to their broad spectrum of pharmacological activities, e.g. antimicrobial¹, antitumour², anti-inflammatory³ and anti-

biofilm properties⁴. Further, the arylidene derivatives of nitrogen and sulphur containing heterocycles with α , β - unsaturated carbonyl scaffold are found to be potent anticancer agents⁵. In view of the importance of such heterocyclic molecules, a fascinating synthetic protocol was adopted for synthesis of some novel arylidene derivatives of thiazolopyrimidine using thiourea and acetoacetic ester as synthetic precursors under microwave irradiation technique.



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Oral Presentation-23

Photovoltaic Performance of Natural Dye sensitised Ni-Cd-S Photoelectrode fabricated by Dip Coating Technique

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Abstract: Colossal exploitation of fossil fuel has created noticeable pollution problems leading to climate change and health adventure, which stimulates research to develop cheap, low-cost

and clean energy technologies to the society. In this context herein, Ni-Cd-S photoelectrode has been prepared using dip coating technique on ITO glass substrate and sensitised by using chlorophyll as sensitizer. The electrode and sensitised electrode have been characterised by fabricating solar cell of configuration:

Photoelectrode+Dye// Na₂S(1M)+NaOH (1 M)+S (1 M)//C (Graphite)

The photo-electrochemical characterizations of the thin film photoelectrodes take account of the measurement of current vs voltage (I-V) in dark and light, photoresponse and power output. I-V curves show that the thin films photoelectrodes are n-type semiconductors. The power output curves show that the power conversion efficiency of electrode and dye sensitised electrode (dye- chlorophyll, deposition time- 6 hours) increases from 1.9 to 2.4 with the enhancement of short circuit current (I_{sc}) from 5.5 mA to 6.6 mA at constant open circuit voltage (V_{oc}) 0.27 V. Structural analysis has been performed by PXRD (powder x-ray diffraction) technique. The PXRD results show that the Ni-Cd-S thin films formed is nano-crystals of size ~11.12 nm. Scanning electron microscope (SEM) technique has also been performed to study the surface morphology of the fabricated films. SEM micrograms establish the polycrystalline nature of synthesised Ni-Cd-S thin films. The EDAX (energy diffraction analysis of x-ray) results demonstrate the presence of Ni, Cd and S in the thin films.

Oral Presentation-24

Kinetic and Thermodynamic Study for the Co-pyrolysis of Beeswax and Plastic Wastes

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Abstract: Continuous growth of industrialization as well as human population has increased the energy demands all over the world and this has caused in a number of energy related challenges including depletion of fossil fuels and environmental pollution. In order to overcome these problems, bio-oil is chosen as a substitute for the fossil fuel. This study reports the co-pyrolysis of beeswax and five different plastics such as high density polythene (HDPE), polypropylene (PP), polymethyl methacrylate (PMMA), polystyrene (PS) and polyethylene terephthalate (PET) with the aim to understand the effect of beeswax on the thermal degradation kinetics of the plastics using thermogravimetric analysis. TGA-DTG curve shows single stage degradation pattern of all the samples and there is change of degradation temperature of plastics due to the addition of beeswax in the co-pyrolysis experiments. Addition of beeswax to plastics is found to decrease the activation energy of the reaction, which is more pronounced in PET and PS. Thermodynamic parameters of the thermal degradation of plastics are also found decreased due to the blending of beeswax. The enthalpy value in plastic-beeswax blend is found lower than that of from respective waste plastics. For all blend samples, the maximum conversion at the peak temperatures ranged

between 661.22 and 762.11 K. The peak temperature of blend is less than that of the peak temperature of plastics. Gibbs free energies ranged between 2.011×10^5 and 1.722×10^5 J/mol for plastic and 2.041×10^5 to 1.791×10^5 J/mol for the blend. The Gibbs free energy of the plastic was close to the values of the plastic samples due to the low entropy at the maximum differential mass conversion.

Keywords- Co-pyrolysis, beeswax, plastic wastes, thermal degradation

Oral Presentation-25

Removal of Cationic Dye by using Polyaniline/Maleic Acid Composite

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Abstract: Rapid industrialization and the advent of modern technology in developing countries are the major causes of water pollution. Dyes present in the industrial effluents are stable towards light and difficult to degrade. Though several techniques are well documented for removal of dyes, adsorption is considered as a most effective technique due to its cost effectiveness and efficiency. Considerable efforts are now being made in the research and development of polymeric materials and its derivatives as basic materials for adsorption because of their simple processing, relatively easy regeneration, the possibility to shape them into most suitable form and cost effective than conventional adsorbents. In this work, a simple ecofriendly approach by using water as solvent and ammonium persulfate (APS) as an oxidant was used for the synthesis of PANI-maleic acid (PANI/MA) composites and utilized as an adsorbent for the removal of cationic dyes such as Methylene Blue (MB) from water medium. It is found that the composite selectively adsorbs cationic dye (MB) and does not adsorb anionic dye like Methyl orange (MO) (Figure-1). The prepared composites were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), Nuclear magnetic resonance (NMR) and Fourier transform infrared (FTIR) spectroscopy. The adsorption parameters like pH, temperature, adsorbent dosage, dye concentration along with kinetics and thermodynamic parameters (ΔG_0 , ΔH_0 , ΔS_0) are evaluated for the potential application in the real field.

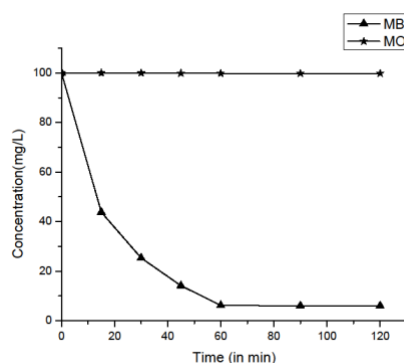


Figure 1: Concentration Profile of Cationic and Anionic Dyes in Presence of PANI-MA.