

## PP-1

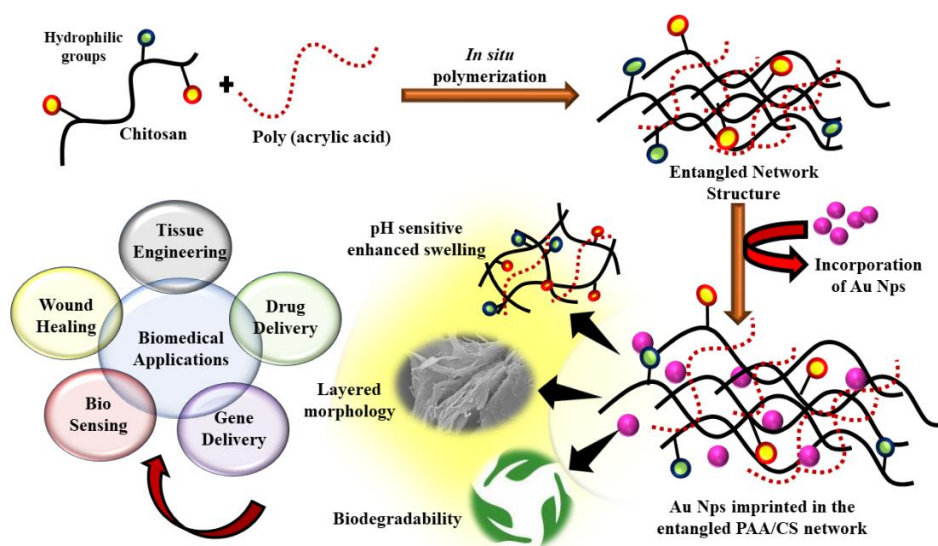
## Change in Orientation of Polyacrylic acid and Chitosan Networks by Imprintment of Gold Nanoparticles

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**Abstract:** Herein, nanogold imprinted poly (acrylic acid)/chitosan (PAA/CS) nanocomposite hydrogels are designed by green, in situ polymerization technique (Scheme 1). The interaction between Au Nps and the PAA/CS matrix are investigated by Fourier Transform Infrared spectroscopy (FTIR). The change in crystallite size and d-spacing are established from X-Ray diffraction (XRD) study. Dynamic light scattering (DLS) is used for dispersion of gold nanoparticles (Au Nps) in PAA/CS matrix. Thermal degradation of PAA, CS, PAA/CS and PAA/CS/Au nanocomposite are compared by Thermal gravimetric analysis (TGA). It is interesting to notice that the layered morphology of PAA/CS/Au nanocomposite hydrogel is achieved from Field emission scanning electron microscopy (FESEM) due to entanglement of polymeric chains by imprintment of nanogold. This orientation of polymeric chains reveals the improvement in swelling percentage at basic medium. Biodegradation of the as-synthesized material is done by sludge water treatment from which the antimicrobial activity of nanogold can be estimated. The slight compromise in biodegradation with enhancement of structural and swelling behaviour enables the synthesized material for biomedical applications.



**Scheme1:** Schematic representation of preparation of PAA/CA/Au nanocomposite hydrogel

**PP-2**

**Green synthesis of Au-C<sub>3</sub>N<sub>4</sub> plasmonic photocatalyst for enhanced catalytic reduction of nitrophenol**

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**Abstract:** Noble metal nanoparticles are currently receiving much attention due to their exceptional physicochemical properties in various fields such as optical, catalytic, biomedical, petrochemical and environmental applications. Out of which Gold nanoparticle (AuNP) is one of the most promising nanoparticles, that plays an important role in catalytic processes for the reduction of 4-nitrophenol (4NP) to 4-aminophenol (4AP). To enhance this catalytic activity, AuNPs tend to disperse over a homogeneous surface which reduce the cost of gold based nanocatalysts. Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>), an organic polymeric semiconductor mainly consisting of carbon and nitrogen having a band gap of 2.7 eV, possess high thermal and chemical stability, excellent electron transfer ability, and easy recyclability. In recent years g-C<sub>3</sub>N<sub>4</sub> has been successfully fabricated as a support to disperse and stabilize AuNPs. Currently research efforts have been developed to synthesize Au-C<sub>3</sub>N<sub>4</sub> nano-photocatalysts by using efficient, economical and green technologies. Hence, in this article we provide a room temperature assisted green synthesis of Au-C<sub>3</sub>N<sub>4</sub> photocatalyst for reduction of 4NP to 4AP by using leaf extract. Au NPs in the diameter of 5–20 nm were well anchored onto the surface of g-C<sub>3</sub>N<sub>4</sub> in 3–6 layers. The newly synthesized nanocatalysts were analyzed using standard characterization techniques such as X-ray diffraction (XRD), UV-Vis (Diffused reflectance) spectrophotometry, Fourier Transform Infrared (FTIR) spectroscopy, Field Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM). The synthesized Au-C<sub>3</sub>N<sub>4</sub> nanocomposites exhibit excellent photocatalytic activity and stability for the reduction of 4NP to 4AP in 20 minutes. It has also been observed that the enactment of Au-C<sub>3</sub>N<sub>4</sub> completely depends on the initial nitrophenol concentration, Au loading, inorganic anions, and pH of the solution. The surface plasmon resonance (SPR) effect of Au and electron-acceptor role of g-C<sub>3</sub>N<sub>4</sub> together significantly helps to enhance the photo-harvesting ability, simplify light generated charge carrier separation and more active reaction sites which ultimately leads to a surged photocatalytic activity.

**PP-3**

**Effect of phosphatidylethanolamine and oleic acid on membrane fusion: phosphatidylethanolamine circumvents classical stalk model**

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**Abstract:** Membrane fusion is one of the most important processes for the survival of eukaryotic cells, and entry of enveloped viruses to the host cells. Lipid composition plays a crucial role in the process by modulating the organization and dynamics of the membrane, as well as the structure and conformation of membrane proteins. Phosphatidylethanolamine (PE), a lipid molecule with intrinsic negative curvature, promotes membrane fusion by stabilizing the non-lamellar intermediate structures in the fusion process. Conversely, oleic acid (OA), with intrinsic positive curvature, inhibits membrane fusion. The current study aimed to investigate polyethylene glycol (PEG)-mediated lipid mixing, content mixing, content leakage, and depth-dependent membrane organization and dynamics, utilizing arrays of steady-state and time-resolved fluorescence techniques, to determine the causative role of PE and OA in membrane fusion. Results demonstrated that presence of 30 mol% PE in membrane promotes membrane fusion through a mechanism that circumvents the classical stalk model. On the contrary, membranes containing OA showed reduced rate and extent of fusion, despite following the same mechanism. Collectively, our findings in terms of membrane organization and dynamics indicated a plausible role of PE and OA in membrane fusion.

**PP-4**

### **Ground Water Contamination in Hard Rock Terrains of Keonjhar, Odisha**

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**Abstract:** Drinking water is a potential source of human exposure to toxic substances. The ground water resources in the study area, in an around Joda of Keonjhar are susceptible to be contaminated naturally as well as by anthropogenic activities because of extensive iron and manganese mining and associated activities. In this context an attempt has been made to assess the ground water quality of the study area for drinking and irrigation purpose. This can help to develop a better policy and proper planning for groundwater resource management for sustainable development. Various physico-chemical parameters such as pH, turbidity, EC, TDS, TH including cations, anions and heavy metal contents like Ca<sup>2+</sup>, Mg<sup>2+</sup>, Na<sup>+</sup>, K<sup>+</sup>, HCO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>-2</sup>, NO<sub>3</sub><sup>-</sup>, PO<sub>4</sub><sup>3-</sup>, Cl<sup>-</sup>, Zn, Ni, Cu, Mn, Fe, Co, Cd, Cr and Pb were analysed in pre-monsoon, monsoon and post-monsoon, periods in 2018-20 for 17 ground water samples. The recorded P<sup>H</sup> values ranging from 6.00-7.32 indicates that all the samples in pre-monsoon and most of the samples in post- monsoon were acidic in nature. Zn, Cu, Co, and Cd concentration were within the standard limits of BIS and WHO guidelines. Irrigation quality indices like salinity (EC and TDS) and % sodium shows excellent to good quality water for irrigation. Sodium adsorption ratio(SAR), Residual sodium carbonates(RSC),Magnesium ratio(MR) and Kellys ratio(K R) reveal that most of the samples are suitable for irrigation. Salinity diagram shows that the

water samples have low to medium salinity hazard and sodium hazard. According to WHO and FAO irrigation standard guidelines, the pH, TDS, EC, cations, anions and heavy metal contents like Zn, Ni, Cu, Fe, Co, Cd, and Pb in the studied ground water were found to be well below the standard limits throughout the study period. Mn and Cr content in a few samples exceeded both WHO and FAO Standard values. Though the overall quality of ground water in this area is suitable for irrigation but it is unsuitable for drinking purpose in some of the places like Balda, Jajang, Jururhi, Dhobakuchura and Nuabeda with respect to heavy metals. Thus, the ground water resources of the study area cannot be used for public consumption without proper treatment. Extensive mining and related activities, sponge iron and ferro manganese plants, weathering processes and domestic activities are the major causes of contamination of water bodies.

#### PP-5

##### **Lanthanide Perovskite CeCuO<sub>3</sub> nanomaterials as Efficient Visible Photocatalysts for Erichrome Black T.**

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**Abstract:** The various natural water resources are getting polluted by industrial activities, by release of Organic pollutants mainly organic dyes to water bodies. There for many technologies have been developed to clean the water bodies, among which the photocatalytic process is a greener procedure that became known as a challenging option for the destruction of various organic contaminants. Perovskite nanostructures have appeared as efficient, cost-effective, light-active substances for photocatalytic purposes. The Lanthanide perovskite, CeCuO<sub>3</sub> has been synthesized by hydrothermal method and characterized by using XRD, SEM, TEM, XPS, BET. Photocatalytic activity of synthesized nanomaterials was investigated taking hazardous EBT dye as contaminant under Visible light irradiation for 100 min.

#### PP-6

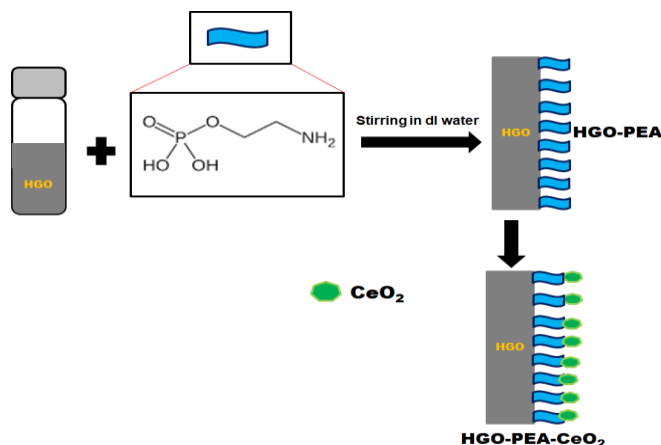
##### **Synthesis and Characterisation of HGO-PEA-CeO<sub>2</sub> for reduction of SP<sup>2</sup> hybridised carbon atom**

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**Abstract:** The present work demonstrates an efficient ternary nanocomposite HGO-PEA-CeO<sub>2</sub> has been synthesized via the popular solvothermal method. The characterization of the synthesized nanocomposite was done by using X-ray Diffraction (XRD), Raman spectrometry and Field emission Scanning electron microscopy (FESEM). The efficiency of the nanocomposite HGO-PEA-CeO<sub>2</sub> for

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the catalysis of the styrene to ethyl benzene is very remarkable. The product formation was confirmed by carrying out Nuclear magnetic resonance (NMR). The catalytic activity of ternary nanocomposite HGO-PEA-CeO<sub>2</sub> is more than HGO and HGO-PEA. The catalytic activity of the ternary nanocomposite is optimized by changing different parameters such as catalyst amount and reactant concentration.



**Figure. 1** General synthesis of HGo-PEA-CeO<sub>2</sub>

PP-7

### Flake-like Shaped ZnFe<sub>2</sub>O<sub>4</sub> Nanoparticles: Synthesis, Characterization and Applications

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**Abstract:** Flake-like shaped ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles were successfully prepared by co-precipitation method and characterized using XRD, FTIR, UV-Vis-DRS and SEM techniques. The formation, phase and crystallinity of the synthesized ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles were studied by XRD. The SEM result reveals the formation of flake shaped entities that are formed by the combination of rod shaped nanomaterial. The band gap of the prepared ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles is found as 2.14 eV using UV-Vis DRS study which can easily absorb the visible light. The ferrite nanoparticles have been successfully applied as a photocatalytic agent for degradation of dyes i.e. Malachite green dye in aqueous media. It was observed that around 99 % of degradation of this dye takes place within 150 min. for 20 ppm dye solution (Fig.1).

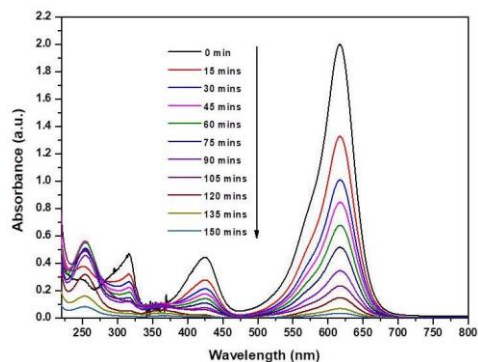


Figure 1: Photocatalytic reduction of Malachite Green dye

### PP-8

#### Green Synthesis of Metal Nanocomposites using Plant Extract and Natural Products

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**Abstract:** Research attempts have been made in recent times towards developing environment friendly and sustainable polymer composites for use in different industrial applications such as aeronautical, automotive, textile, construction, packaging, farming, and medical fields. The addition of nanoparticles to base polymers confer improved properties that make them usable in automotive, construction and medical areas. Metal nanoparticles have wide range of potential application in medicine, textile industry, food packaging, cosmetic industry, catalysis, antimicrobial activities, clean water technology, energy generation and information storage. The traditional method for synthesis of metal nanoparticles and composites involve harmful and hazardous chemicals and synthetic materials. In place of hazardous and costly chemical reagents different plant extracts can be used as green reagent for synthesis of metal nanoparticles. The present approach involves synthesis of metal nanoparticles using plant extract in combination with natural and functionalized biopolymers. In this present study Neem, Tulsi and other plants were used which are abundantly found in India and Indian subcontinents and are known for their various applications including medicinal property.

### PP-9

#### Enhanced Dielectric and Electrical Properties of Three phase PMMA-NaNbO<sub>3</sub>-Starch Percolative Composite Films

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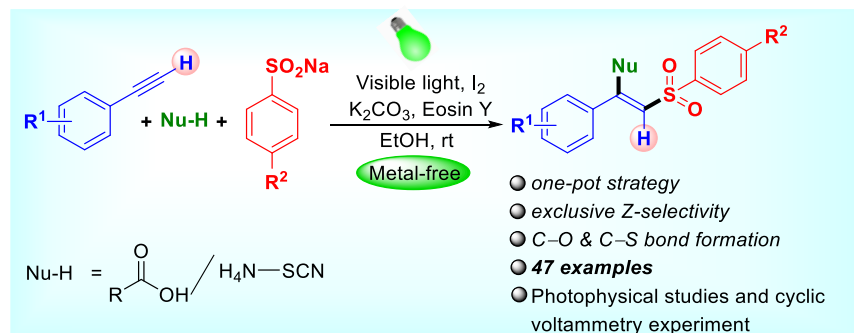
**Abstract:** The preparation of three phase PMMA-NaNbO<sub>3</sub>-starch percolative composites comprising starch and sodium niobate (NaNbO<sub>3</sub>; NN) particles embedded into poly(methylmethacrylate) (PMMA) matrix *via* solution casting technique. The experimental results showed that the three phase PMMA-NN-starch composites has a higher dielectric constant ( $\approx 395$ ) and negligible dielectric loss ( $< 0.6$ ) at 100 Hz, which is considerably superior than that of the two phase PMMA-NN composites. Moreover, the enhancement of electrical performances of the composites may be due to the synergistic effect of the NN ceramics and conductive starch particles within the polymer matrix. The uniform dispersion gives an insulating layer between neighboring conductive starch particles in the PMMA matrix, which is not only prevent the direct contact of starch but also better homogeneity of the starch particles in the composite system. In addition, the percolation theory was employed to clarify the dielectric and electrical performance of the composite. These three phase PMMA-NN-starch composite exhibited an insulator-conductor transition with 7 wt% of starch contents at percolation threshold. This work might be a novel approach to make excellent composite films with improves dielectric and electrical properties for high performance energy storage applications.

**PP-10**

### **Visible-Light-Mediated Difunctionalization of Alkynes: Synthesis of $\beta$ -Substituted Vinylsulfones Using *O*- and *S*-Centered Nucleophiles**

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**Abstract:** An inimitable illustration of a green-light-induced, regioselective difunctionalization of terminal alkyne has been disclosed using sodium arylsulfonates, and carboxylic acids in the presence of eosin Y as the photocatalyst. The present methodology is further demonstrated by employing NH<sub>4</sub>SCN as *S*-centered nucleophile instead of carboxylic acid. The mechanistic investigation reveals a radical-induced iodosulfonylation followed by a base-mediated nucleophilic substitution. The mechanism is supported by various studies *viz.*, radical-trapping experiment, fluorescence quenching and CV studies. In this protocol, *Z*- $\beta$ -substituted vinylsulfones are obtained exclusively covering a broad range of alkynes and nucleophiles which are often unaddressed. The present strategy can tolerate structurally discrete substrates with steric bulk and different electronic properties, which provides a straightforward and practical pathway for the synthesis of highly functionalized *Z*- $\beta$ -substituted vinylsulfones. Herein, C–O and C–S bonds are assembled simultaneously with the concomitant introduction of important functional groups *viz.* ester, thiocyanate, and sulfone.



## PP-11

Mg and Zn Co-Doped Sr<sub>2</sub>CeO<sub>4</sub> for White Light Emission

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**Abstract:** The rice grain shaped Zinc and magnesium co-doped Sr<sub>2</sub>CeO<sub>4</sub> was synthesized via a hydrothermal synthesis route from (Sr(NO<sub>3</sub>)<sub>2</sub>, Ce(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O, Mg(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O and Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O as precursor and (NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub> as mineraliser. XRD data showed the phase purity with orthorhombic phase Sr<sub>2</sub>CeO<sub>4</sub> and Pbam space group. Presence of characteristic vibrational stretching and bending bands in FT-IR spectra and strong Raman shifts at 299 and 401 cm<sup>-1</sup> for CeO<sub>6</sub> unit proved the formation of doped strontium cerate. FE-SEM data shows the rice grain shaped structures. To evaluate the band gap of the pure and doped Sr<sub>2</sub>CeO<sub>4</sub> UV-VIS DRS was done and band gap was deduced using Tauc plot. The photoluminescence emission spectra show a broadband emission with emission maximum at 480 nm and shows an increased broadness as well as red shift for the doped materials having CIE co-ordinate near to that ideal white light. The charge transfer based emission is redshifted due to increase in electronegativity of the dopants as well as the various defect states that are developed during doping. For the 1% Mg and 1% Zn doped Sr<sub>2</sub>CeO<sub>4</sub> a significant photoluminescence quantum yield of 40.62 % have been seen which can be a great advantage for practical application.

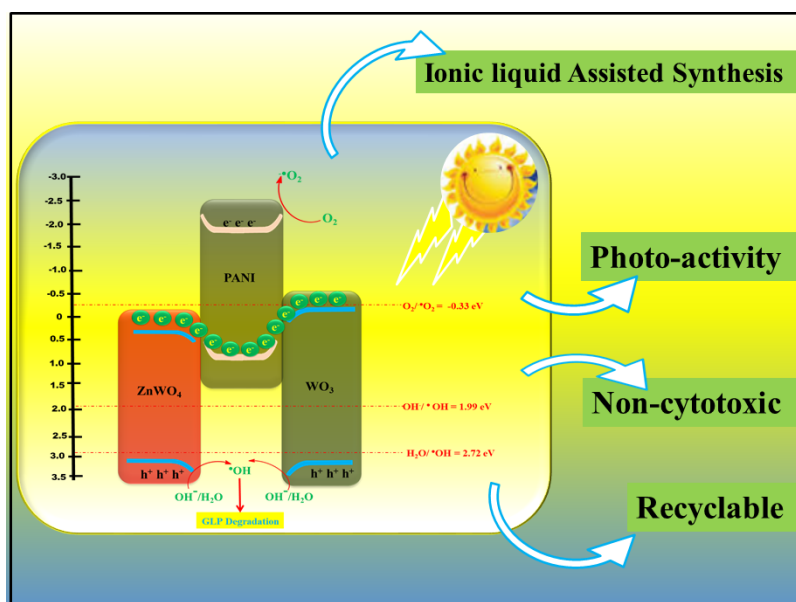
## PP-12

**Ionic Liquid-Assisted Synthesis of Novel PANI/ZnWO<sub>4</sub>/WO<sub>3</sub> Ternary Nanocomposite: A Facile Double Electron Transfer Photocatalyst for Efficient Degradation of Herbicide**

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**Abstract:** This study reports a novel, efficient, and non-toxic polyaniline-ZnWO<sub>4</sub>-WO<sub>3</sub> (PZW) ternary nanocomposite, synthesized following an ionic liquid (IL)-assisted *in situ* oxidative polymerization method. The as-prepared nanocomposites were utilized towards improved photocatalytic wastewater treatment and toxicity removal. Initially, the individual ZnWO<sub>4</sub> and WO<sub>3</sub> nanostructures were synthesized using the IL-assisted solvothermal method. Thereafter, the subsequent modification of the ZnWO<sub>4</sub> and WO<sub>3</sub> nanostructures with polyaniline (PANI) conducting polymer was done by *in situ* oxidative polymerization of PANI. Comprehensive analysis of structural and morphological properties of the nanocomposites revealed high structural integrity and close contact between the individual components. The optical and photo-electrochemical investigations suggested rapid charge carrier possibility, suitable band arrangement, and a superior lifetime of the nanocomposite. Afterward, the recyclable ternary nanocomposite demonstrated higher solar light-mediated photocatalytic degradation towards toxic glyphosate (GLP) herbicide ( $K_{app} = 0.0707 \text{ min}^{-1}$ ). Additionally, the non-toxic nature of the nanocomposite (after catalytic cycle) and treated GLP solutions were assessed *via* a standard TBE (Trypan Blue dye exclusion) assay. Furthermore, the XPS analysis, radical trapping experiment, and reactive oxygen species quantification ( $\text{HO}^\bullet$  and  $\text{O}_2^{\bullet-}$ ) study equivocally indicated a possible double electron transfer type Z-scheme mechanism, which accounts for superior solar light-assisted N-C bond cleavage of GLP herbicide.



PP-13

**Value addition to waste batteries through hydrometallurgical extraction of manganese as MnSO<sub>4</sub> – a precursor for manganese chemicals**

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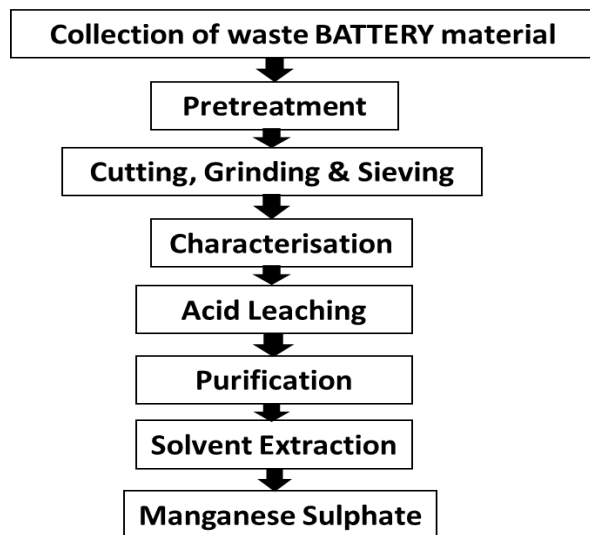
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**Abstract:** Batteries are being used in a large number of portable electronic and electrical gadgets. However, the waste batteries are generally considered as hazardous due to the harmful impurities present in them. The basic purpose of this study is to recycle the spent batteries till the end of life so that environmental pollution and use of natural resources can be reduced. This will also help in reducing greenhouse gas emissions and hence the carbon foot prints.

Present work consists of dismantling of spent batteries, their characterization followed by leaching of manganese values as MnSO<sub>4</sub> which can be a precursor material for synthesizing various manganese chemicals. Effectiveness of hydrogen peroxide as a reductant, reaction temperature, leaching time, pulp density etc. on manganese extraction have been studied. Manganese leaching efficiency of 98% have been achieved when the waste battery material was subjected to acid leaching for about 90 minutes at an optimum condition of 3M H<sub>2</sub>SO<sub>4</sub>, 5 % H<sub>2</sub>O<sub>2</sub>, pulp density 10% at 60 °C.

Solvent extraction studies were carried out with the spent batteries leach liquor bearing 0.702 g/L Fe, 0.105 g/L Cu, 0.678 g/L Al, 2.148 g/L Zn, 12.48 g/L Mn, 8.67 g/L Co, 6.28 g/L Ni, and 3.853 g/L Li. Impurities like iron, aluminium and copper are precipitated using sodium hydroxide. D2EHPA was used for selective separation of Zn and Mn, where extraction of manganese was found to be 99.9%) with 30% (v/v) saponified 40% (v/v) D2EHPA dissolved in kerosene at O:A=1:1 and temperature 25°C. Both Zn and Mn were separated by stripping with 1M H<sub>2</sub>SO<sub>4</sub> from metal loaded D2EHPA. To get pure manganese sulphate solution, solvent extraction was carried out with 30% saponified 30 % (v/v) D2EHPA. Manganese sulphate solution that is generated could be used as a precursor solution for synthesizing various manganese chemicals. A schematic process flowsheet has been appended below to highlight the unit operations involved.



**Figure1.** Schematic Flowsheet for Hydrometallurgical Extraction of Manganese

PP-14

### Green Chemistry: Utilisation of Waste to grow Plant in Pot

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**Abstract:** Study on utilisation of industrial and house waste to look forward for green farming has been carried out. Investigation has been done on the effect of fly ash, phosphogypsum, the used tea granules and coconut shell ash in green farming of Aloe Vera using sandy soil as base material. With the chemistry knowledge of coconut shell ash to increase water holding capacity, tea granules to increase water holding capacity and as organic manure, the nutritional value of sandy soil has been tried to be enhanced by addition of phosphogypsum (waste product of phosphatic plant) and coal ash (waste product of thermal and steel plant). Being alkaline fly ash has the capacity to neutralize the acidity of sandy soil, thus increasing the pH of soil. These all were taken in different proportions by volume in different pots to study the growth of Aloe Vera plant for three months. Composition of sandy soil: synthetic gypsum: fly ash: coconut shell: tea granules at the ratio 20:10:2:1:1 by volume has been found to be the best for the sustainable growth of Aloe Vera in comparison to soil only in the same environmental condition. Further studies are required for better yield.

### Triethanolamine-Mediated Magnetically Separable Palladium Nanocatalyst (Fe<sub>3</sub>O<sub>4</sub>-Pd) for Heck Coupling Reaction under Ligand-Free Conditions

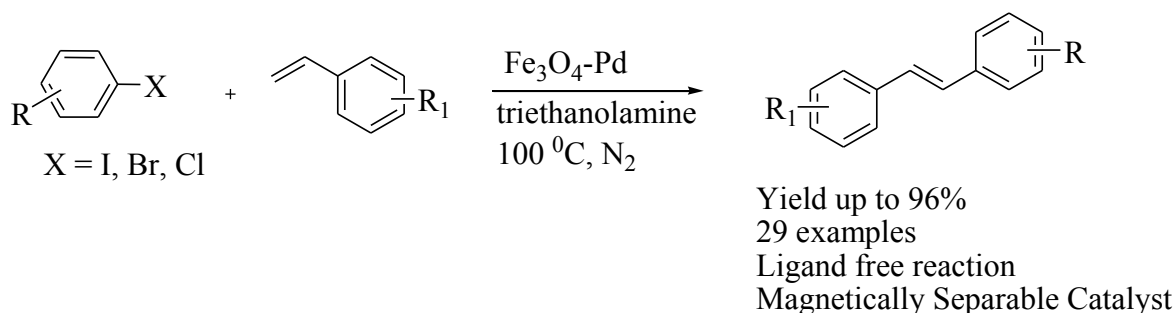
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**Abstract:** Magnetically separable Palladium nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-Pd) were successfully synthesized and its catalytic activity was explored for the Heck coupling reactions with broad substrate scope. The nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-Pd) were first prepared by one step hydrothermal method and characterized by various analytical techniques such as PXRD, HR-TEM, EDS, AAS and FT-IR. Screening experiments were conducted and Fe<sub>3</sub>O<sub>4</sub>-Pd/triethanolamine/100 °C catalytic system was found to be optimum conditions for Heck coupling reaction. Both acrylates and styrene derivatives were successfully coupled with electron-rich as well as electron-deficient aryl iodides, resulting (*E*)-alkenes in good to excellent yields. The scope of the reaction was further expanded to less reactive aryl bromides and aryl chlorides. A number of functional groups including, hydroxy, methoxy, acetyl etc. were well tolerated under the optimum conditions. More significantly the catalyst showed good recyclability and can be reused up to four consecutive cycles without any decrease in catalytic activity. Therefore, one pot and hydrothermally synthesized palladium functionalized magnetic nanoparticle (Fe<sub>3</sub>O<sub>4</sub>-Pd) has proved as an efficient, robust and recyclable catalytic system for stereoselective synthesis of (*E*)-alkenes in absence any exogenous ligand .



**Scheme 1.** Pd-nanoparticle catalyzed Heck coupling reactions

PP-16

### **Bromo aniline Derived Multifunctionalized Halogen Containing Glycolipids**

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**Abstract:** Glycolipids are one of the most important types of glycoconjugates where the sugar moiety is attached to the aglycon part through glycosidic bond. These glycolipids have found many applications in various fields of science and technology. Though the naturally occurring glycolipids have shown better bioavailability, environmental compatibility as well as lower toxicity, the tedious extraction and purification process of such glycolipids have inspired many synthetic chemists to synthesize functionalized glycolipids with structural diversity. Among the many synthetic glycolipids, the triazole functionalized has attracted significant attention due to easy synthesis, higher yield and green reaction condition and better functionalization. There are a very few reports on halogen containing glycolipids. In this work, a series of novel peptoid based glycolipids have been synthesized from bromo aniline using [3 + 2] cycloaddition reaction. The halogen containing glycolipids have the potential to be used for crystallization and purification of integral membrane protein due to heavy atom effect.

PP-17

### **Synthesis, Characterization and adsorption behaviour of Carbon Nano Onions (CNOs)@TiO<sub>2</sub> composites**

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**Abstract:** A systematic approach was employed to study the adsorption of Methylene blue (MB) by TiO<sub>2</sub> and Carbon nano-onions TiO<sub>2</sub> composite. Here (CNOs-TiO<sub>2</sub>) composites were synthesized by one pot solvothermal method. Further the composites were characterized by several methods like BET surface area analysis, X-ray diffraction (XRD), Fourier transform infrared (FTIR), Raman spectral studies, X-ray photoelectron spectroscopy (XPS) to evaluate the role of composites in promoting the adsorption. The adsorption activity of CNOs-TiO<sub>2</sub> composites were assessed for MB adsorption. The adsorption procedure was examined using various adsorption parameters, pH studies and variation of time. CNOs-TiO<sub>2</sub> composites enhance the MB adsorption as compared to TiO<sub>2</sub>.

### PP-18

#### **Gamma-oryzanol and its significances in regulating the expressions of human tumor necrosis factor alpha (TNF $\alpha$ ) using computational techniques**

**Dhananjay Kumar Tanty**<sup>1</sup>, Prachi Rani Sahu<sup>1</sup>, Lopamudra Barik<sup>1</sup>, Pabitra Mohan Behera<sup>2</sup> and Susanta Kumar Sahu<sup>1</sup>

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**Abstract:** The human TNF $\alpha$  is an important cytokine found in the vicinity of the HLA III region and involved in different cellular functions like proliferation, differentiation and apoptosis. Mutations in the promoter region of the TNF $\alpha$  gene increases its transcription which enhances the production of TNF $\alpha$  cytokine and triggers the onset of diabetes mellitus. Several TNF $\alpha$  inhibitors have been used for the neutralization of TNF $\alpha$  which increases insulin sensitivity and in turn controls diabetes mellitus. These inhibitors are also associated with the risk of adverse chemical reactions which demands the requirement of natural compounds with specific inhibition and least side effects. Gamma-oryzanol seems to be one of the natural compounds derived from the fat fraction of rice is reported in many studies to possess anti-inflammatory activities. In the current work, we report the homology models of human TNF $\alpha$  canonical and its two natural variants with suitable templates selected from PDB. Again we also report gamma-oryzanol as a probable inhibitor of human TNF $\alpha$  with the structural information of potential inhibitors reported in the literature. Our findings are quite generous and we found gamma-oryzanol suitably accommodated in the designated active sites of the designed models with docking scores (-9.0 kcal/mol) and good interactions with some conserved amino acid residues.

**PP-19**

**Formation of Fluorescent Hydrogel from 4-(3,4,5-Trimethoxyphenyl) 2,2';6',2'' terpyridine-Zn (II) Complex**

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**Abstract:** Fluorescent hydrogels obtained from small organic gelator are fascinating materials for advanced applications. A small organic gelator molecule, 4-(3,4,5-trimethoxyphenyl)-terpyridine (TMTPy) was synthesized by reacting 3,4,5-trimethoxybenzaldehyde and 2-acetyl pyridine in ethanol and characterised by different techniques. The hydrogelation of TMTPy was studied by adding the TMTPy in 0.1 N HCl with different divalent metal chlorides in 1:1 ratio. Only Cu(II) and Zn(II) were found to form hydrogel but other metal ions such as Ca(II), Mn(II), Co(II), Ni(II), Cd(II) and Hg(II) formed clear solutions. It was observed that the hydrogel formed from Zn (II) was fluorescent; whereas Cu (II) mediated hydrogel was non fluorescent. Very nice morphological features were obtained for the dried hydrogel. Cu (II) terpyridine complex was found to consist of fibrous like structure and Zn(II) terpyridine complex showed stick type of structure.

**PP-20**

**Complex catalysed fabrication and study of properties of Poly(AN-co-AM)/Crab shell powder biocomposites**

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**Abstract:** Acrylonitrile (AN) and Acrylamide (AM) monomers are copolymerized and reinforced with naturally extracted crab shell particles (CSP) as biofillers to finally obtain Poly(AN-co-AM)/CSP biocomposites with improved properties. This study explores the possibility of combining crab shell waste with monomers to create an environmentally friendly and biocompatible polymer biocomposite. The obtained data from FTIR and SEM confirmed that the composites were properly from the constituent samples. The crystal structure of the composite was maintained, as confirmed by the XRD patterns. SEM analysis revealed a homogeneous particle distribution and

CSP incorporation in the Poly(AN-co-AM) matrix. The addition of crab shell supports the favorable improvement of the prepared copolymer matrix composites aids in their development. The thermal analysis reveals that the copolymer matrix filled with CSP increases the initial decomposition temperature and the char yield of composites. Poly(AN-co-AM)/CSP composites exhibited better mechanical strength compared to Crab shell particles. The results showed that the fibrillation of crab shell was properly done. This work leads to the sustainable utilization

**PP-21**

**Thermal and optical analysis of Low Dielectric Polymer Composite: Ethylene-propylene-diene terpolymer/ Barium hexa ferrite**

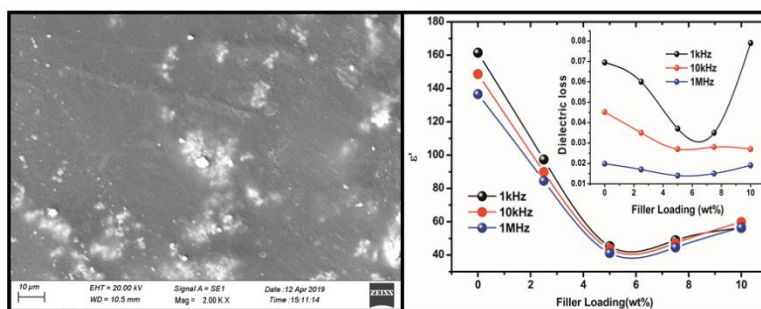
**Deeptimayee Khatua<sup>1</sup>, Rajesh K. Singh<sup>2</sup>, and P. Ganga Raju Achary\*<sup>1</sup>**

<sup>1</sup>Department of Chemistry, Siksha O Anusandhan, Deemed to be University, Khandagiri Square, Bhubaneswar

<sup>2</sup>Department of Chemistry, MSCB University, Takatpur, - 757003 (Orissa) India  
P.Ganga Raju Achary<sup>1</sup> (Email: [pgrachary@soa.ac.in](mailto:pgrachary@soa.ac.in))

The improvement of data transmission innovation towards high-frequency microwaves and profoundly incorporated and multi-utilitarian electronic gadgets has been the standard heading of the current communication technology. During signal transmission, opposition capacitance time delay, crosstalk, energy utilization increment and impedance befuddle limit the high thickness and scaling down of Printed circuit load up. To accomplish high fidelity and low delay characteristics of high-frequency signal transmission, the improvement of interlayer dielectric materials with low dielectric constant( $\epsilon_r$ ) and low dielectric loss factor( $\tan \delta$ ) has turned into the focal point of researchers. In this research, different BHF/EPDM nano composite films were synthesized by adopting solution casting method with different organic solvent. The neat EPDM polymer, BHF particles and the BHF/EPDM composites were characterized by X-ray powder diffraction, Fourier transforms infrared spectroscopy, thermo gravimetric analysis and electrical dielectric investigation in the frequency range 1 kHz to 1 MHz. The interaction between filler and the polymer matrix have been studied by stability of the material increases due to the filler loading. Properties like AC conductivity, dielectric constant and loss are increasing with filler loading.





## PP-22

### Copper Nanoparticles-Catalyzed Regioselective Synthesis of 3-Nitro-2-arylimidazo[1,2-*a*]pyridines using oxygen as oxidant

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**Abstract:** A mild, efficient and stable copper nanoparticles catalyzed regioselective synthesis of 3-nitro-2-arylimidazo[1,2-*a*]pyridines was developed. Substituted 2-amino pyridines successfully reacted with both electron-rich and electron-deficient  $\beta$ -nitro styrenes to produce the desired products in good to excellent yields. Hot filtration tests confirmed the heterogeneous nature of the Cu NPs. The nanocatalyst showed good reusability up to three consecutive cycles without any significant loss in its activity and product yield, confirmed by high resolution transmission electron microscopy (HR-TEM) analysis.

## PP-23

### Optical and Thermal Analysis of Barium Hexaferrite filled EVA Polymer Composite

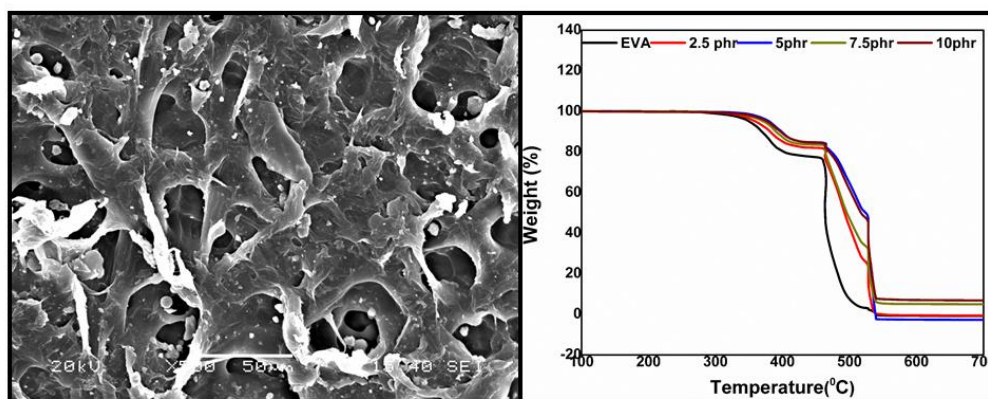
Deeptimayee Khatua<sup>1</sup>, Rajesh K. Singh<sup>2</sup>, and P. Ganga Raju Achary\*<sup>1</sup>

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**Abstract:** Now days the improvement of polymeric nano-composite has made a significant commitment to electrical industry. The quick advancement of energy storage gadgets set off the improvement of high-energy density polymer nano composite. To enhance the dielectric constant, ceramic filler with high dielectric constant have been widely introduced into a polymer matrix with high break down strength. Here we explore a two-filler polymer nano composite based on Ethylene vinyl acetate (EVA) with graphene and barium hexaferrite (BHF). BaFe<sub>12</sub>O<sub>19</sub> (BHF) powder is a popular ferroelectric -ferromagnetic multiferroic material which can used as high density recording application and magneto optical devices. BHF porous nano particle is obtained by sol gel auto combustion technique using barium nitrate, Iron nitrate, Urea, ethylene glycol etc. Different BHF/EVA nano composite films were synthesized by changing the concentration of BHF to explore the impact of each component and their potential synergetic effect on dielectric and ferroelectric properties of the composite. These polymer composites were synthesized by adopting solution casting method with different organic solvent. The neat EVA polymer, BHF particles and the BHF/EVA composites were characterized by X-ray powder diffraction, fourier transforms infrared spectroscopy, thermo gravimetric analysis and electrical dielectric investigation in the frequency range 1 kHz to 1 MHz. The interaction between filler and the polymer matrix have been studied by stability of the material increases due to the filler loading. Properties like AC conductivity, dielectric constant and loss are increasing with filler loading.



PP-24

### Membrane Cholesterol Modulates SARS Coronavirus-2 Fusion peptide(s)-induced Hemifusion Formation

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**Abstract:** Membrane fusion is an important step for the entry of the lipid-sheathed (enveloped) viruses into the host cells. The fusion process is generally being carried out by fusion proteins present in the viral envelope. The class I viruses contains a 20-25 amino acid sequence at its N-terminal of the fusion domain, which is instrumental in fusion, and is termed as ‘fusion peptide’. In spite of being a class I virus, Severe Acute Respiratory Syndrome Coronavirus (SARS) contains more than one fusion peptide sequences. We have shown that the internal fusion peptide 1 (IFP1) of SARS-CoV is far more efficient than its N-terminal counterpart (FP) to induce hemifusion between small unilamellar vesicles. Moreover, the ability of IFP1 to induce hemifusion formation increases dramatically with growing cholesterol content in the membrane. Interestingly, IFP1 is capable of inducing hemifusion, but fails to open pore.

**PP-25**

### **Preparation of Biobased Polymer nano composite and its study of Gas Permeability**

**Jayanta Kumar Nayak**, Dr. Lingaraj Behera

Department of Chemistry, MSCB University, Baripada, Mayurbhanj, Odisha

**Abstract:** Novel biobased polymer nano- composite are attracting increased attention due to their common qualities of being firm, hard or unable to bend and not easily broken, torn etc. For this properties they have been universally adopted in the field of biomedical, food packaging industry, pharmacology, transportation construction, electronics and consumer products. Biobased polymer nanocomposite demonstrative a adjustment in composition and structure over a nanomaterial length scale have been shown over the last few years to provide rare property increased relative to nontraditional composites. Organically reform ZnO can be capable of producing reinforcing agent used especially in compounding rubber to improve the physical properties (as resilience, toughness and tensile strength). Commenricial ZnO nanoparticles were modified by polyhydroxy butyrate (PHB) in aqueous system. The hydrosyl groups of nano- ZnO particle surface can interact with carboxyl groups (---C-O-) of PHB and form Poly( zinc hydroxy butyrate) complex was testified by Fourier- transform infrared spectra (FT-IR). Thermogravimetic analysis ( TGA) Indicated that PHB molecules were absorbed or anchored on the surface of nano- ZnO particle which facilitated to hinder the aggregation of nano- ZnO particles . It was found that PHB enhanced the dispersibility of nano- ZnO particles in water. The dispersion Stabilization of modified Zno nanoparticles in aqueous system was significantly improved due to the introduction of polymer on the surface of nanoparticles. The modification did partially alter the crystalline structure of the ZnO nano particles according to the X- ray diffraction patterns. The enhancement of electrical properties due to incorporation of zno nano particles in PHB was observed by The gas permeacability of the nanocomposite sample was measured by “ gas permeameter”.A considerable amount reduction in gas permeability was observed by measuring ZnO loading and through sonication ( The act of applying sound energy to agitate particles in the sample). These disruption are used for mixing of the solution

to increase the speed of dissolution of a solid into a liquid and for the removal of dissolved gases from the liquids.

PP-26

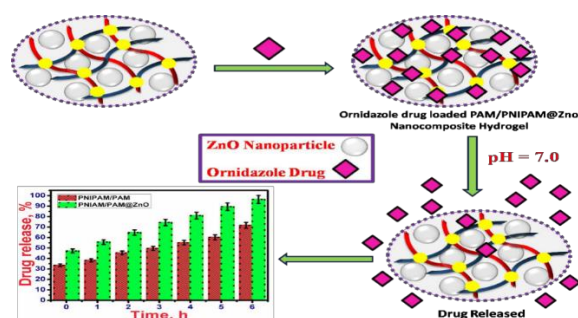
### Nano ZnO embedded poly(N-isopropylacrylamide)/polyacrylamide nanocomposite hydrogel for *in vitro* release of ornidazole

Krishna Manjari Sahu<sup>#</sup>, Priyanka Sah, Anuradha Biswal and Sarat K Swain\*

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**Abstract:** The hybrid poly N-isopropyl acrylamide/ poly acrylamide@ZnO (PNIPAM/PAM@ZnO) nanocomposite hydrogel material is synthesized by incorporating ZnO nanoparticles into the PNIPAM/PAM matrix during *in situ* preparation. The addition of ZnO nanoparticles has altered the interactions within the hydrogel matrix and these interactions and its impact on hydrogel are characterized by using different spectrometers. The detection of functional groups present within the hydrogels is carried out by FTIR spectroscopy. The influence of addition of nanoparticles on the thermal stability of pristine hydrogel is studied by TGA analysis. The stability and distribution of nanoparticles within the hydrogel matrix are determined by zeta potential measurement. The pH responsive nature is investigated by considering the swelling behavior and water retention capacity of hybrid nanocomposite hydrogel at different pH concentration levels. The fabricated system is loaded with ornidazole drug and the drug release rate at certain intervals of time is measured with the help of UV spectrometer (Scheme 1). The *in vitro* release rate of ornidazole drug from the prepared hybrid nanocomposite hydrogel is found to be 95.63% within 6 hour. The result shows the suitability of using PNIPAM/PAM@ZnO hybrid nanocomposite for *in vitro* drug administration process.



**Scheme 1:** Schematic illustration of drug release study of PNIPAM/PAM@ ZnO nanocomposite hydrogels

PP-27

**Lipid Composition dependent Binding of Apolipoprotein E Signal Peptide: Importance of Membrane Cholesterol in Protein Sorting**

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**Abstract:** Several proteins contain a short stretch of signal peptide (SP) at its N-terminal, which play a key role in targeting and sorting of protein in different organelles. Interestingly, the SP gets cleaved by membrane bound signal peptidase after the protein reaches to its destination. In order to understand the role of membrane properties in protein sorting, we have studied the affinity of Apolipoprotein E (APOE) signal peptide toward membranes with varying cholesterol composition. APOE is primarily produced by liver and macrophages, and mediates cholesterol metabolism in peripherals tissue. We have utilized batteries of steady-state and time-resolved fluorescence techniques to understand the affinity of APOE-SP toward membranes with varying cholesterol composition. The importance of cholesterol is paramount as the major sorting organelle, endoplasmic reticulum (ER), contains minimum amount of cholesterol compared to other organelles, and our study intended to evaluate the role of membrane composition for the unidirectional movement of APOE from ribosome to ER. Our results suggest that the APOE signal peptide binds tightly with the membrane having no cholesterol, and affinity reduces with increasing concentration of membrane cholesterol. However, the peptide does not have much impact on the membrane organization and dynamics, which is anticipated for a signal peptide.

PP-28

**Synthesis and Characterization of Gold Nanoparticle decorated functionalized Single-Walled Carbon Nanotube nanohybrid reinforced Polyaniline nanocomposites**

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**Abstract:** The present study deals with the synthesis of gold nanoparticles (AuNPs) reinforced functionalized single-walled carbon nanotubes (*f*-SWNTs) based polyaniline (PANI) nanocomposites, using *in situ* polymerization process to analyze the thermal and dielectric properties.

The chemical interaction and nanostructure characteristics of the synthesized nanocomposites are studied using ultraviolet-visible (UV-Vis) spectroscopy, fourier-transform infrared (FTIR) spectroscopy, raman spectroscopy, X-ray diffraction (XRD) analysis, and X-ray photoelectron spectroscopy (XPS). The morphological characterizations of the nanocomposites are carried out by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The dispersion stability and average size distribution of the nanocomposites are examined by means of dynamic light scattering (DLS) technique. The thermal and dielectric properties of the nanocomposites are investigated by employing thermogravimetry-differential scanning calorimetry (TG-DSC) and dielectric relaxation spectroscopy (DRS), respectively. The main purpose of this research work is to increase the thermal and dielectric properties of the PANI nanocomposites by modifying AuNPs on the surface of *f*-SWNT to form hybrid nanofiller and the prepared Au@*f*-SWNT hybrid nanofillers are dispersed within PANI matrix. The thermal and dielectric properties of the Au@*f*-SWNT hybrid nanofiller embedded PANI nanocomposites are significantly increased due to the strong interfacial interactions originated between hybrid nanofillers and PANI matrix.

#### PP-29

##### **Removal efficiency of sugarcane bagasse biochar modified magnetic nanoparticles as novel biosorbent materials for uptake of Cr (VI) from aqueous solution.**

**Litun Kumar Sahu**<sup>1</sup>, Amrutashree Hota<sup>1</sup>, Jitendra Kumar Sahoo<sup>1\*</sup>, Sourav Prusty<sup>1</sup>, Manoj Kumar Sahu<sup>1</sup>

<sup>1</sup>Department of Chemistry, GIET University, Gunupur-765022, Odisha, India.

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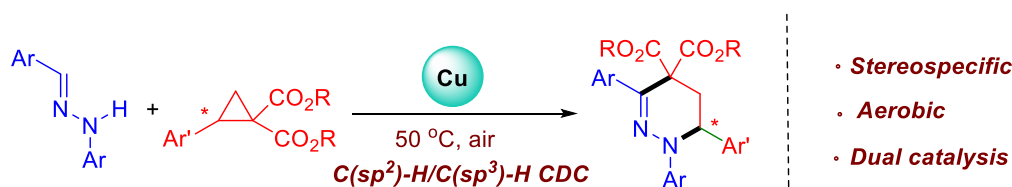
**Abstract:** In the current scenario, removal of heavy metals from contaminated water has become a major challenging task to world researchers because disposal of untreated heavy metals into aquatic environment have adverse effect towards the ecosystem. Keeping this in mind, the present study investigates to synthesize the sugarcane bagasse biochar modified magnetic nanoparticles towards the decontamination and their batch scale potential of chromium (VI) from aqueous solution. The synthesized adsorbent was characterized by FT-IR, XRD, FE-SEM, VSM and EDX. The effect of adsorbent dosages (50-400 mg/L), initial Cr (VI) concentration (5-70 mg/L), pH (3-11), and contact time (1h-25h) were evaluated Cr (VI) removal on sugarcane bagasse biochar modified magnetic nanoparticles at room temperature. The adsorption data well fit with Langmuir isotherm ( $R^2 = 0.99$ ) and pseudo second order kinetics ( $R^2 = 0.99$ ). The maximum adsorption capacity was found to be 20.47 mg/g.

## PP-30

### Stereospecific Copper(II)-Catalyzed Tandem Ring Opening/Oxidative Alkylation of Donor-Acceptor Cyclopropanes with Hydrazones: expeditious access to Tetrahydropyridazines

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Department of Chemistry, IIT Guwahati

**Abstract:** Aerobic copper(II)-catalyzed domino ring opening/oxidative alkylation of donor-acceptor cyclopropanes with bisaryl hydrazones is presented to produce tetrahydropyridazines at moderate temperature (Scheme 1).<sup>1</sup> Optically active cyclopropanes can be cross-coupled with excellent optical purities (89-98% ee). The atom economy, substrate scope, functional group tolerance and the use of air as an oxidant render the method synthetically attractive. In addition, the product can be readily subjected C-C cross-coupling processes.



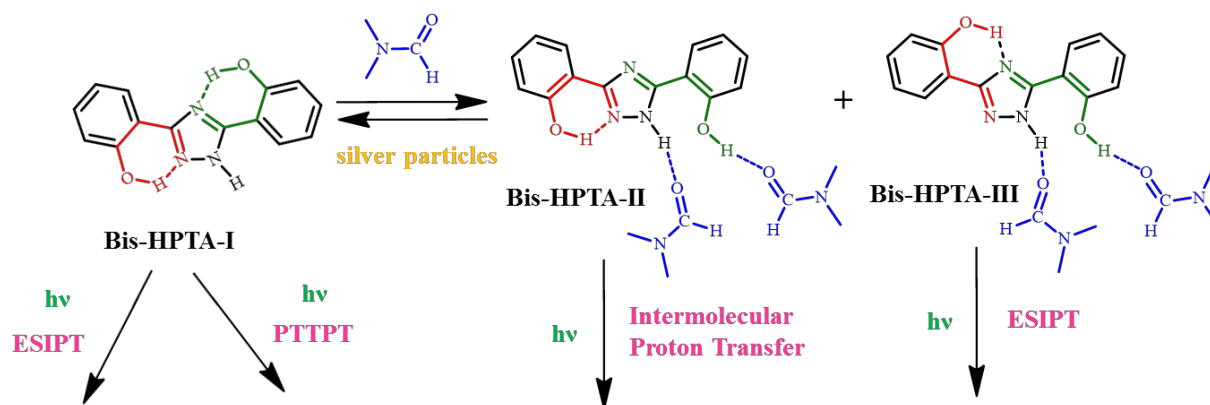
## PP-31

### Tweaking the ESIPT process of 3,5-bis(2-hydroxyphenyl)-1H-1,2,4- triazole by silver nanoparticle

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**Abstract:** The excited state intramolecular proton transfer (ESIPT) of 3,5-bis(2-hydroxyphenyl)-1H-1,2,4- triazole (bis-HPTA), a molecule possessing two intramolecular hydrogen bonded donor-acceptor pairs, has been investigated by means of absorption spectra, emission spectra and time resolved area normalized emission spectra. The molecule exists as different conformer in different solvent and hence resulting different ESIPT process. Simply by changing the solvent system, ESIPT process is tuned. In nonpolar solvents bis-HPTA undergoes not only a single ESIPT (ESIPT-I), but also a rare twin ESIPT from conformer bis-HPTA-I. The most interesting fact is that initially, only one acid-base pair is ESIPT (ESIPT-I) active and the other pair is ESIPT inactive (ESIPT-II). The first proton transfer triggers the proton transfer in the second acid-base pair and the process is labelled

as ‘proton transfer triggered proton transfer’ (PTTPT). In n,n-dimethylformamide (DMF), another two conformers bis-HPTA-II and bis-HPTA-III become the stable conformers and form H-bond with DMF solvent molecules. Bis-HPTA-II leads to intermolecular proton transfer while bis-HPTA-III leads to ESIPT-III. Regaining of ESIPT-I is achieved by removing bis-HPTA from DMF solvent cage using silver nanoparticles. Use of silver nanoparticles reverse the equilibrium and tweak the PT processes.



PP-32

### Investigation on Dielectric and Electrical Properties of Ternary Polyvinylidene fluoride-hexafluoropropylene-CuFe<sub>2</sub>O<sub>4</sub>-MWCNTs Composite Films

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<sup>a</sup>Laboratory of Polymeric and Materials Chemistry, School of Chemistry, Sambalpur University, Jyoti Vihar, Burla-768019, Odisha, India

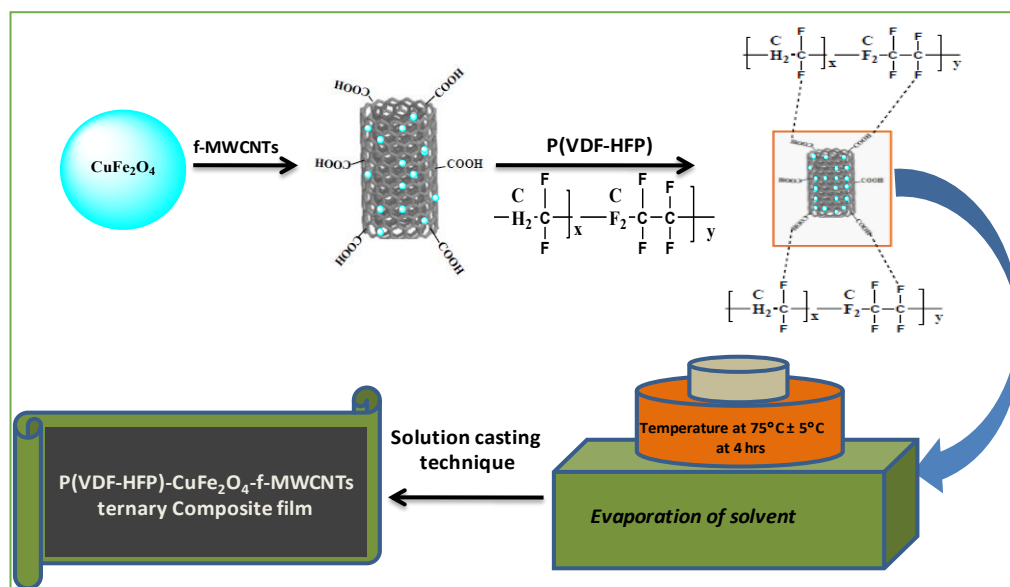
<sup>b</sup>School of Applied Sciences, Centurion University of Technology and Management, Odisha, India

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**Abstract:** The ternary composite system comprising polyvinylidene fluoride-hexafluoropropylene P(VDF-HFP), conductive carboxyl functionalized MWCNTs (f-MWCNTs) and dielectric filler copper ferrites (CuFe<sub>2</sub>O<sub>4</sub>) have exhibited improved dielectric and electrical performances. The P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-MWCNTs ternary composite films with different weight percentage of f-MWCNTs were synthesized *via* solution casting technique. Fourier transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM) techniques were employed to characterize the synthesized composite films. The dielectric [dielectric constant ( $\epsilon_r$ ), dielectric loss ( $\tan \delta$ )] and electrical [AC conductivity ( $\sigma_{ac}$ )] properties of P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-MWCNTs ternary composite films were investigated as a function of frequency. The dielectric constant of 4 wt% P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-MWCNTs is reached up to  $\approx 142$  at 100 Hz, which is much higher than that of the pristine P(VDF-HFP) matrix. Moreover, the dielectric loss of 4wt% P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-



MWCNTs composite still maintains at a low level ( $< 1$ ) at 100 Hz. We believe that the improved dielectric constant of P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-MWCNTs composite films is due to the improved micro capacitors effects and Maxwell-Wagner-Sillars effect. These P(VDF-HFP)-CuFe<sub>2</sub>O<sub>4</sub>-f-MWCNTs ternary composite gives a promising approach to fabricate novel P(VDF-HFP) based dielectric composite films for practical applications in electronics.



### PP-33

#### Photocatalytic degradation of Congo-Red by using Rgo-CeTiO<sub>2</sub> mixed oxide nanocomposites

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<sup>1</sup>PG Department Chemistry, MSCB University, Baripada

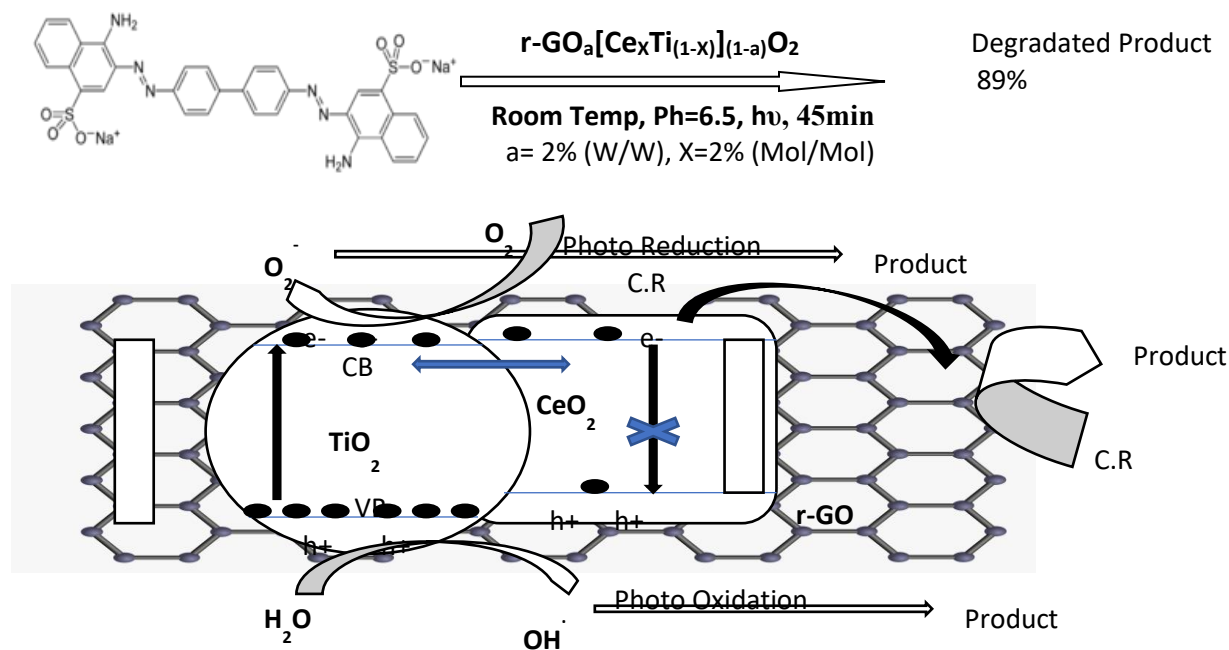
<sup>2</sup> Department of Chemistry, CV Raman Global University, Bhubaneswar

**Abstract:** Congo-Red is used since its inception from 1883 as red colouring material primarily without mordant in fabric industry. It has also remarkable effect in staining in amyloidosis in human, cell wall of plants and fungi and for the outer membrane of Gram-negative bacteria. It was initially banned for its aggressive carcinogenic effect due to having the structural moieties with Azo-linkage being synthesized as benzidine derived dyes. It is need of the hour to reduce the concentration of this pollutant in effluent generated by many industries of the community by decolourizing the resulting effluent.

Numerous study has been designed for removing the impurity through chemical treatment, adsorption and metal oxide based photocatalytic degradation methods where the photocatalytic

degradation method would have been served as the most promising methods in comparison to over all conventional method due to its stability and reusability.

In this present work of heterogeneous catalysis, we have designed in-situ synthesis of CeTiO<sub>2</sub> mixed metal oxide by sol-gel method with stoichiometric variation. Graphene Oxide (GO) has been synthesized by modified Hammer's method. Finally the composite has been fabricated with different weight ratio to form Rgo-CeTiO<sub>2</sub> as our desired photocatalyst with the principle metal oxide-graphene interface results in due synergistic effect to enhance the performance of composite significantly. Morphology, composition analysis and choosing of material suitability has been carried out by using XRD, FESEM-EDAX, FTIR, UV-Vis DRS, PL-spectral analysis, Zeta-Sizer and BET-analysis. A detail study has been carried out in the reactor with the dye Congo-Red and synthesized photocatalyst vis-a vis by varying concentration, P<sup>H</sup>, Time, reusable cycle study, presence of different anions like CO<sub>3</sub><sup>2-</sup>, SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup> etc. The percentage of degradation and kinetics are being correlated with characterized data.



Proposed Schematic Diagram showing photocatalytic degradation of Congo Red