

photocatalyst for tuning the band gap energy and reduction of the recombination rate of photoexcited (e^-/h^+) pair. Also, the synergistic effect of the individual ones helps in ameliorating the capacitive performance with widened potential window [3]. Given this, the present work focuses on the study of nanostructured ternary oxide/hydroxide as a potential material for both applications. Its photocatalytic performance and as an effective electrode material for energy storage devices have been evaluated.

A facile hydrothermal approach was employed to synthesize ternary Co-Ni-Cu oxide/hydroxide followed by physical and electrochemical characterizations. The synthesized material was used as an efficient photocatalyst for the degradation of toxic and carcinogenic Congo red dye under visible light irradiation. Its electrochemical performance was also investigated and implemented as battery electrodes in hybrid energy storage devices to power electronics. The combined properties of this ternary system as effective photocatalysts and supercapacitors electrode material suggest a new dimension for applications in the environment and energy domain.

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OP-12

Synthesis and screening of some azo-dyes for application in DSSC

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Organic azo compounds find their application as a synthon in organic synthesis and various optoelectronic applications. Cis-trans isomerization of various azo compounds is reported to be as one input YES GATE way back in 1980s¹. Further development of azo derivatives finds its application in switches, push-pull chemistry, and sensors for various ions². In our objective of finding a dye to be applied in DSSC, we have synthesized ethyl orange starting from Sulfanilic acid and amines like N, N-diethyl aniline, triphenylamine, etc. The optical property of all these synthetic dyes is observed by UV-visible and photoluminescence spectroscopy. This encourages us to study elaborately the emission

spectra and attempts are being made to evaluate its application in electronic devices. Work is in progress to further authenticate its stability and suitability for DSSC.

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OP-13

Conformational Search for the Protein Fragment Structures using GGS/Force Field

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The conformations of proteins are important for the structure-function relation to undergo important mechanistic biological processes in living systems. The 20 different amino acids in different sequences form the 3-D structure of proteins. The present investigation includes research exploration using Gradient Gravitational Search Technique and Force Field Parameters. The contribution from both bonded and non-bonded terms for the considered protein fragment structures has been used for the structural optimization process. The protein fragment structure of HIV-1 has been considered due to their catalytic activity with ligand molecules inside protein to understand the inhibition mechanism. The efficiency and accuracy of such conformational searches about mean absolute error (MAE) and mean standard deviation (MSD) have also been evaluated and compared with reported other search techniques.

Keywords: Conformational Search, Gradient Gravitational Search, Proteins, Force Field, Validation.

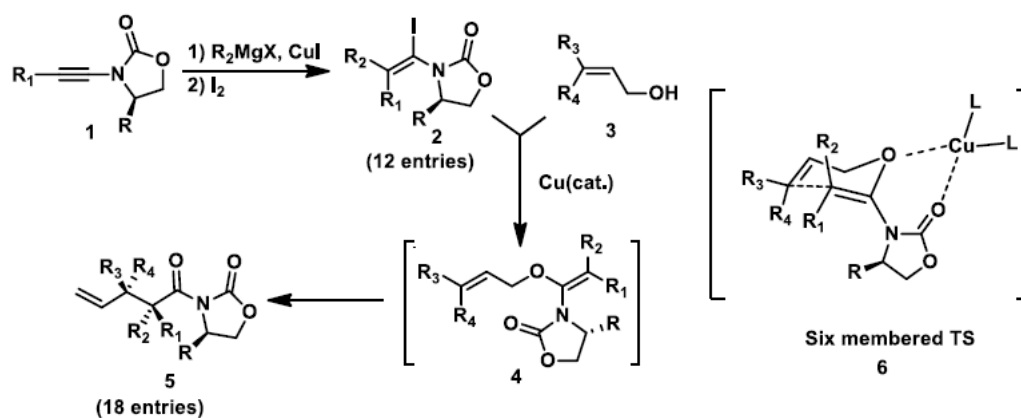
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Cu-(I) Catalyzed Stereoselective Claisen Rearrangement of AllylVinyl Ethers**Subhransu Sekhar Pati and Jaya Prakash Das***

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The Claisen rearrangement is considered one of the most efficient methods for the construction of a C-C single bond along with the formation of γ , δ -unsaturated carbonyl compounds. This reaction proceeds through a six-membered (Zimmermann-Traxler) transition state which itself provides diastereoselectivity. Furthermore, the construction of all carbon quaternary stereogenic centers along with contiguous stereo centres in acyclic systems is still a challenge to achieve. This work focuses on the design of a novel domino process that consists of a metal-catalyzed C-O bond coupling and a subsequent Claisen Rearrangement with diastereo- & enantioselectivity, which leads to the construction of two adjacent stereocenters along with the desired all-carbon quaternary stereocenter.

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Mo(VI) Potential Metallodrugs: Explaining the Transport and Cytotoxicity by Chemical Transformations

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The transport and cytotoxicity of molybdenum-based drugs have been explained with the concept of chemical transformation, an important idea in inorganic medicinal chemistry that is often overlooked in the interpretation of biological activity. Two monomeric, $[\text{MoO}_2(\text{L}^1)(\text{MeOH})]$ (**1**) and $[\text{MoO}_2(\text{L}^2)(\text{EtOH})]$ (**2**), and two mixed-ligand dimeric $\text{Mo}^{\text{VI}}\text{O}_2$ species, $[\{\text{MoO}_2(\text{L}^{1-2})\}_2(\mu\text{-}4,4'\text{-bipy})]$ (**3-4**), were synthesized and characterized.¹ The structures of the complexes were solved through SC-XRD, while their transformation in water was clarified by UV-vis, ESI-MS, and DFT. In an aqueous solution, **1-4** leads to the penta-coordinated $[\text{MoO}_2(\text{L}^{1-2})]$ active species after the release of the solvent molecule (**1** and **2**) or removal of the 4,4'-bipy (**3** and **4**). $[\text{MoO}_2(\text{L}^{1-2})]$ are stable in solution and react with neither serum bioligand nor cellular reductants. The binding affinity of **1-4** toward HSA and DNA was evaluated through analytical and computational methods and in both cases, a non-covalent interaction is expected. In vitro cytotoxicity of the complexes was also determined^{2,3} and flow cytometry analysis showed apoptotic cell death. Interestingly, $\mu\text{-}4,4'\text{-bipy}$ bridged complexes **3** and **4** were found to be more active than monomeric **1** and **2**, due to the mixture of species generated, that is $[\text{MoO}_2(\text{L}^{1-2})]$ and the cytotoxic 4,4'-bipy released after their dissociation. Since in the cytosol neither the reduction of Mo^{VI} to $\text{Mo}^{\text{V/IV}}$ takes place nor the production of ROS through Fenton-like reactions of **1-4** with H_2O_2 occurs, the mechanism of cytotoxicity should be attributable to the direct interaction with DNA that happens with a minor-groove binding which results in cell death through an apoptotic mechanism.

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OP-16

Benzothiazole-based novel probe for 1, 3-Diaminopropane through turn-on fluorometric response

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Designing sensors to obtain stimuli-generated optical responses in terms of change in colour, fluorescence intensity/ quantum yield has driven modern research for quite some time now. Recently, a paradigm shift in focus has occurred toward sensing small molecules. Small organic molecules like nerve agents, amines, volatile compounds, and thiol-containing compounds require detection in various settings due to their hazardous nature. Specific detection of aliphatic amines like 1,3-diaminopropane can help us in understanding the biological functions of other relevant polyamines. DAP tracing holds promising solutions in quality control and can help in mitigating health hazards. The probe HL containing a benzothiazole scaffold was proposed as a sensor for the exclusive detection of 1, 3- diaminopropane through turn-on fluorescence response in an aqueous medium as well as in a variety of other organic solvents. Micromolar limits of detection were achieved in all these solvents. A mechanism of detection was proposed by taking the aid of mass spectrometric and NMR studies. The results were corroborated with DFT/TD-DFT calculations. Spiking experiments performed in various real water samples demonstrated its potential to be used in day-to-day applications. Detection of DAP in gas, liquid, and solid phases was also successfully achieved. The paper strip experiments conducted, revealed the suitability of the probe for real-life applications.

OP-17

Intrinsic White Light Emitting Single-Phase Phosphor with High Color Rendering Index

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Single-phase white light-emitting nanomaterials with intrinsically balanced color components can overcome problems arising in conventional phosphors by providing high CRI and CCT. Herein, to get

the desired white light emission from a single-phase material –the Barium orthovanadate has been synthesized by a fast microwave-assisted hydrothermal method by tuning the defect states is reported. Powder X-ray diffraction (PXRD), Raman spectra, and UV-VIS absorption spectroscopy were considered to study the short, medium, and long-range defects which are confirmed by Rietveld. The hexagonal plate-like samples were investigated using FESEM and HRTEM. EDAX and XPS were used to investigate the qualitative and quantitative elemental analysis. Owing to the extensive oxygen vacancy as confirmed by XPS analysis and charge transfer bands, the nanophosphors exhibit broadband white-light emission with CIE in the range of 0.301 to 0.326, 0.362 to 0.438 with high photoluminescence quantum efficiency (PLQE) ranging from 22 to 35% by tuning the reaction time and temperature. The photoluminescence lifetime components give an obvious longer microsecond lifetime due to the forbidden triplet to singlet state relaxation. Excitation and temperature-dependent emission spectra provide a deep study of the mechanism as well as the temperature stability of materials. Such intense white light emission prompted the development of a white light emitting prototype by coating the phosphor on a 365 nm UV LED chip. It exhibits high CRI (87), CCT (5217K), and CIE (0.3394, 0.3484), meeting highly desired values for a white light emitting phosphor for different indoor-outdoor lighting, electroluminescence, and display applications.

OP-18

Bimetallic Pd-Sn Nanocatalysts for Selective Synthesis of Amines and Imines in Water

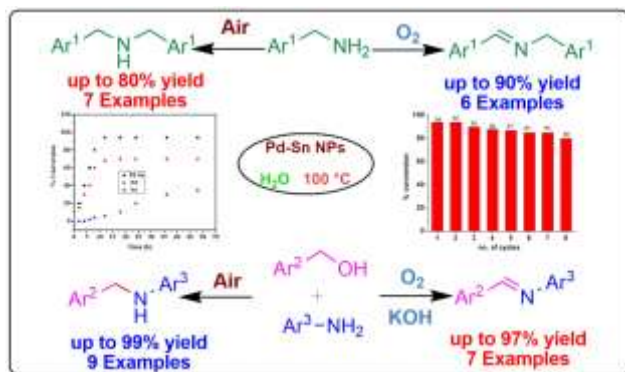
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The Pd-Sn nanocatalyst has been synthesized by a simple wet chemical reduction method and fully characterized by a library of physico-chemical techniques such as Powder X-Ray Diffraction (PXRD), High-Resolution Transmission Electron Microscopy (HRTEM), X-Ray Photo Electron Spectroscopy (XPS) and UV-Vis spectroscopy, Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-Ray (EDX) spectroscopy, and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). From HRTEM analysis the average particle size of Pd-Sn BNPs determined to be 4.2 nm and XPS analysis confirmed the dominance of Pd(0) and Sn(0) in the Pd-Sn nanocatalyst. The Pd-Sn catalyst proved to be highly efficient and recyclable for the oxidative coupling of primary

amines and tandem coupling between amine and alcohol in water. Another novel feature of the catalyst is that in presence of oxygen, both the oxidative coupling and tandem coupling stops at the imine stage. The high efficiency, recyclability, and good substrate scope of this Pd-Sn nanocatalyst are noteworthy. Preliminary mechanistic studies indicated that the reactions proceed via initial activation of the N-H bond of amine.



- Ease of preparation of the Pd-Sn NPs, and their high shelf-life;
- Low loading (0.56 mol% Pd), high TOF values; easy work-up;
- Ability to withstand up to eight cycles with minimum loss of TOF;

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OP-19

Flavone-stilbene hybrids: Synthesis and evaluation as potential antimalarial agents

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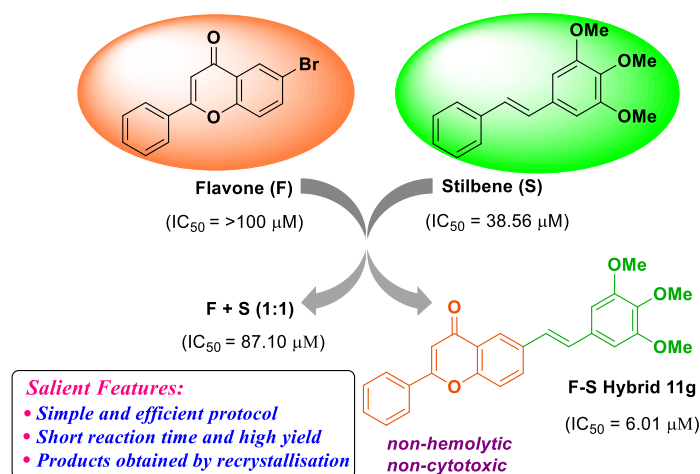
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A series of flavone-stilbene-based hybrid molecules were synthesized in good to excellent yield (65-95%) via Heck coupling as the key step under conventional as well as microwave irradiation conditions. The advantages of the developed protocol involve short reaction time, high-yield products obtained without the use of any additives, and the ability to obtain pure compounds by recrystallization obviating the need for time-consuming column chromatography. These synthesized hybrid molecules were evaluated for their in vitro anti-plasmodial activity against chloroquine-sensitive Pf3D7 and chloroquine-resistant PfINDO strains of the malaria parasite *Plasmodium falciparum* using SYBR Green I assay. With their $CC_{50S} > 200 \mu\text{M}$ the compounds were found to be non-cytotoxic toward mammalian cell line (HEK-293). The selectivity indices of >25 for the compounds suggested their specificity towards the parasite strains over mammalian cells.^[1]

Keywords: Heck coupling, *Plasmodium falciparum*, antimalarial activity, flavone-stilbene hybrid



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OP-20

Recycling of Plasticized PVC (Vinyl Flooring Sheets)

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Plastics are the widely preferred material choice in designing and developing complex, consumer products, because they are mouldable, and lightweight and are often perceived to be highly recyclable

materials many of their properties such as durability, versatility and lightweight can be significant factors in achieving sustainable development. However, recycling the heterogeneous plastics used in such durable items is challenging. A common problem with recycling plastics is that plastics are often made up of more than one kind of polymer or there may be some sort of filler added to the plastic to give added strength and other properties. Rejected or waste material usually has good characteristics for recycling. While the technology exists to recycle plastics, the feasibility to do so from high-level consumer or industrial applications is bounded by technological and economical restraints. Obstacles include the lack of a market for recyclates and the lack of cost-efficient recovery infrastructures or processes. Furthermore, there is a knowledge gap between manufacturers, consumers, and end-of-life facility operators. For these reasons, end-of-life plastics are more likely to end up down-cycled, or as shredder residue and then landfilled. This paper reviews these challenges and several alternatives to recycling plastics to broaden the mindset surrounding plastics recycling to improve their sustainability. The work focussed on the recycling of the flexible PVC (Vinyl flooring sheets) but discussion can be applied to a wide range of plastic components from similarly complex products. The main aim of this present work was to analyze the effect of phthalate plasticizers on mechanical recycling and the effect of mechanical properties of PVC material recovered from the flooring sheets.

Keywords: PVC, recycling, compression molding, FTIR, SEM.

OP-21

Oxidative Addition to the N–C Bonds Formation of Zwitterionic Intermediate in Platinum(II)–Catalyzed Intramolecular Annulation of Alkynes to form Indoles: Mechanistic Studies and Reaction Scope

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In the study, Pt (II)–catalyzed intramolecular translocation annulation of ortho-alkynyl amides to the formation of indoles is presented where a proposed intermediacy of zwitterionic intermediate has been substantiated over the oxidative addition. We focused our attention on Pt(II)–catalyzed aminoacylation of alkynes both theoretically and experimentally using low boiling solvent where the formation of the de-acylation product was suppressed simultaneously. One-step intramolecular [1,3]–acyl migration from the zwitterionic intermediate is highly unlikely which imparts a high-energy

barrier of +99.0 kcal mol⁻¹. Another possible approach involving oxidative addition to the N–C bond, migratory insertion to the alkyne, and subsequent reductive elimination are also explored through DFT studies to justify their action consequence. However, based on the computational studies it is suggested that initial zwitterion formation is highly favored over oxidative addition. We suggest the formation of an acylium intermediate, which can further react with indol-3-yl platinum species in an intramolecular manner, albeit within the same solvent cage to form 3-acylindoles.

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OP-22

Iron Mineralization in a Heme Binding Ferritin: Impact of Pores and Protein Cage

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The self-assembled ferritin nanocages, nature's solution to iron toxicity and its low solubility, scavenges free iron to synthesize hydrated ferric oxyhydroxide mineral inside their central cavity by protein-mediated ferroxidase and hydrolytic/nucleation reactions. These complex processes in ferritin commence with the rapid influx of Fe²⁺ ions *via* the inter-subunit contact points (i.e., pores/channels). The current work investigates the role of various symmetric and asymmetric pores as well as the implication of nanocompartment (self-assembly) towards Fe²⁺ uptake/oxidation and mineralization in a heme-binding bacterioferritin from *Mycobacterium tuberculosis* (*Mtb*). The work establishes the relative role of 4-fold and B-pores towards rapid Fe²⁺ uptake/oxidation and overall cage stability. Although the B-pore variants inhibited the rapid ferroxidase activity to a larger extent, they had minimal impact on their cage stability, possibly as a consequence of their differential symmetry, number of modified residues (at each pore), and heme content. Moreover, the work also highlights the importance of symmetric 3-fold pores towards self-assembly, which not only translocate Fe²⁺ from outside to the ferroxidase centers (by electrostatic guiding) but also imparts stability to the protein cage. Further, it implicates the significance of key interfacial interactions that control the protein structure, pore formation, and their functions. Therefore, these findings may help to understand the role of these pores in iron acquisition and *Mtb* proliferation under the iron-limiting condition to control its pathogenesis.

Amalgamation of natural product and synthetic drug to develop novel ‘dapson-phytochemical’ hybrid drug against *Mycobacterium leprae*

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Leprosy, caused by the slow-growing acid-fast bacilli, *Mycobacterium leprae*, continues to be a belligerent public health hazard for the causation of high disability and eventual morbidity cases with stable prevalence rates, even with treatment by the ongoing multidrug therapy (MDT). Thus, the development of potential candidates against leprosy is the call of the day. **Objective:** In the present study, the first-line antileprosy drug dapson (DDS) was chemically hybridized with phytochemicals (dapson-phytochemical conjugates or DPCs) and validated through computational and experimental methods. **Materials and Methods:** The proposed conjugates were verified through molecular docking, molecular dynamics simulation, and, other drug-ability verification program before chemical synthesis and spectral characterizations (HNMR, FTIR, UV, LC-MS, SEM). The *in vivo* antileprosy activity was monitored using the gold-standard ‘mouse-foot-pad propagation method,’ with a WHO-recommended concentration of 0.01% mg/kg for 12 weeks. Furthermore, the host-toxicity testing of the active DPC4 was seen in cultured human lymphocytes *in vitro*. **Results:** One-log bacilli cells in DDS-resistant infected mice footpads decreased by the DPC4 (dapson-thymol), and no bacilli were found in the DDS-sensitive mice hind pads. The *in vitro* host toxicity study confirmed that the DCP4 up to 5,000 mg/L level was safe for oral administration since it found a minor number of dead cells under a fluorescent microscope. **Conclusion:** The results indicated that the DPC4 could be used in place of DDS in MDT. Overall, this chemical conjugation may lead to re-active the existing clinically inactive drugs and the utilization of a higher number of phytochemicals potentially in mainstream medicine.

Keywords: *Mycobacterium leprae*, Dapson-phytochemical hybrids, Molecular docking-simulation, In vivo antileprosy activity, Cultured-human-lymphocytes.

Spectroscopic and photocatalytic behaviour studies of Nanoporous CrAPO-5

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Aluminophosphate molecular sieves commonly abbreviated as AlPO-n form a class of nanoporous crystalline materials having a pore size of $\sim 5-15 \text{ \AA}$. Among the members of this family, chromium containing AlPO-5 (CrAPO-5) has been proven to be an excellent heterogeneous oxidation catalyst in several organic transformations [1]. The present study is related to the incorporation of chromium into an AlPO-5 structure and evaluates the photocatalytic behavior of CrAPO-5 towards the degradation of methylene blue under solar radiation. The nature of the sample, the oxidation state of chromium, their location, and stability have been studied by XRD, FT-IR, DRUV-Vis, TG-DTA, EPR, N₂ adsorption-desorption, FESEM, and TEM techniques. Well-crystalline CrAPO-5 structures were obtained along with the incorporation of trivalent chromium in octahedral coordination. Upon calcination, chromium was converted into Cr(V) and Cr(VI) states. The sample possesses an ordered pore dimension ($\sim 5-8 \text{ \AA}$) and is of uniform shape. Photocatalytic behavior of the CrAPO-5 was studied by contacting with methylene blue (MB) solution under solar radiation. About 98% of MB degradation was achieved for 20 ppm and 88 % degradation by increasing the concentration to 60 ppm. A moderate to appreciable degradability was observed with CrAPO-5 residue. Photocatalytic studies indicated the extra-framework location of chromium in the CrAPO-5 catalysts [2].

Keywords: CrAPO-5; Photodegradation; Methylene blue.

Reference:

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**Advances in Electroorganic Synthesis with a case study of Industrial
Electroorganic Synthesis of Glyoxylic Acid and Glyoxal**

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Electrochemical synthesis of materials is an important subject for both research and development as well as industrial production. Although the electrochemical synthesis of inorganic material is well understood and has been widely used, electroorganic synthesis has been sparsely studied and the mechanism is yet to be properly understood. Over the period several promising methods with some limitations have emerged and been used for the synthesis of different organic compounds, the electroorganic electro organic synthesis has attracted attention from international academia and industries as an environmentally benign and cost-effective technique to develop products and use in commercial productions. It is gaining more and more importance due to the simple techniques, easy operation, precise control over parameters, and safe conversion of substrates to targeted products with precise control over by-products or side products. Glyoxylic acid and glyoxal are two important organic compounds that find many applications such as cleaning agents, precursors in organic synthesis, the production of drugs, etc. Though the art of electrochemical synthesis of glyoxylic acid from oxalic acid is known it is not used widely. These two chemicals can be synthesized electrochemically separately or combinedly by paired electroorganic synthesis with a high chemical yield of 90% and the current yield of 85% and overall power consumption 4 kWh/kg of glyoxylic acid production. The present paper will discuss the recent advances of electroorganic synthesis in both Research and Development and industrial use and also will discuss details of glyoxylic acid and glyoxal synthesis as a case study.

Keywords: Electroorganic, Synthesis, Glyoxylic Acid, Glyoxal, Electrochemical

Poster Presentations

PP-01

Effect of unsaturated free fatty acids on membrane fusion mechanism

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Membrane fusion is one of the most important processes for the survival of eukaryotic cells and the entry of enveloped viruses into the host cells. Lipid composition plays a crucial role by modulating the organization and dynamics of the membrane, as well as the structure and conformation of membrane proteins. The diversity of the lipid acyl chain in its length and degree of unsaturation originates from the variation in free fatty acids (FFAs). We have studied the effect of linoleic (LA) and linolenic (LNA) acids on the depth-dependent organization, dynamics, and fusion of DOPC/DOPE (70/30 mol%) membranes utilizing steady-state and time-resolved fluorescence spectroscopic methods. Our results suggest that membranes with 5 mol% LA stabilize the stalk-intermediate and promote lipid mixing at the early stage of the process, i.e., the fusion follows the classical stalk model. Conversely, 5 mol% LNA in the membrane induces a similar amount of lipid and content mixing at the stalk state, indicating the fusion mechanism as a nonclassical one, like DOPC/DOPE (70/30 mol%) membranes. Collectively, our results provide an in-depth understanding of the effect of unsaturation in fatty acids in membrane organization, dynamics, and fusion.

PP-02

Synthesis of novel Amphiphilic mPEG-Cholesterol Conjugates, Micellization, and Application in Curcumin Delivery

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Cancer is the deadliest illness worldwide which is still not conquered. Several approaches have been made to eradicate it by combined therapeutic modalities and the introduction of several drug carriers like liposomes, nanoparticles, micelles, etc. Among them, polymeric micelles as drug delivery carriers have gained much more attention because of their greater stability, lower CMC, solubility, small size,

and biocompatibility. In an attempt to formulate a PEG-based micelle as a hydrophobic drug carrier, we have synthesized amphiphilic mPEG-Cholesterol conjugates by condensation method. The obtained polymeric surfactants were characterized using ¹H NMR, FTIR, and HRMS spectral analysis. The micellization behavior of the surfactants was analyzed by UV-Vis and fluorescence method and the calculated CMC of the above systems were in the micro-molar range. The incorporation and delivery of hydrophobic drugs using the formulated stable micelles were studied using curcumin as a model drug. The stability of curcumin was found to be very high in the micellar medium. Drug loading efficiency was found to be 97%. From the XRD, SEM, TEM, and DSC the drug incorporation was confirmed. The drug release profile confirmed a sustained release of drugs which is vital for cancer therapy. The cell viability and anticancer activity were also studied. Overall, our formulated mPEG-Cholesterol micellar system was found to be very promising and effective as a drug delivery vehicle.

PP-03

Coordination-driven self-assembled coordination cages from Pd(II) and a non-chelating unsymmetric bidentate ligand

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Metallo supramolecular coordination cages are receiving discernible attention as an active area for researchers because of their attractive molecular cages such as triangles, squares, rhomboids, dodecahedra, adamantanoids, and nanoballs with various noteworthy applications in the field of molecular recognition, separation, drug delivery, molecular flasks, sensing and catalysis [1-3]. However, very few spherical-shaped metal-mediated coordination cages are reported [4]. Here we describe the design of spherical-shaped molecular cages from Pd(II) ion and non-chelating unsymmetrical bidentate ligand along with its host-guest behavior. Coordination-driven self-assembly is a powerful methodology used in this study for designing spherical molecular cages from Pd(II) ion and 3,5-bis(3-pyridyl)-1,2,4-oxadiazole organic linker. Quantitative assembly of Pd(II) ion with 3,5-bis(3-pyridyl)-1,2,4-oxadiazole led to the formation of the desired cage. Its host-guest interaction has also been studied and confirmed by ¹H NMR and single crystal X-ray study. This observation suggests that several three-dimensional metal-mediated supramolecular coordination cages can be constructed

using suitable metal ions and organic linkers, and their applications in different fields can also be studied.

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PP-04

Spectroscopic and calorimetric investigation of fluoride-contaminated soil of Remuna area, Balasore district, India

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The collection of fluorine-contaminated soil and its sampling was carried out in the Remuna area of the Balasore district of Odisha, India. The IR spectrum indicates the presence of fluoride in various inorganic metals such as aluminum, iron, and silicon. The ¹⁹F NMR spectrum of soil confirms the presence of fluorine in soil. The thermal analysis such as TG-DTA and DTG was used for the determination of moisture, soil organic carbon (SOC), and soil organic matter (SOM) present in the soil. The SOC content in contaminated soil varies from 0.13% to 0.38%, while SOM content is ~ 0.76%. The DSC was carried out at the heating rate of 5K min⁻¹ with the sapphire standard. The DSC study indicates that the fluorine-contaminated soil behaves exothermically in the temperature range of 296.80 K to 351.80 K. The negative specific heat capacity, C_p, decreases in magnitude with an increase in temperature and increases after 339.30 K. The minimum value of C_p is -0.30 Jg⁻¹K⁻¹ at 339.30 K and the maximum C_p is -0.62 Jg⁻¹K⁻¹ at 299.30K. The negative specific heat capacity of soil is explained using thermodynamics. All thermal analysis was carried out in presence of an N₂ atmosphere.

Organocatalytic Umpolung of Bromocations: A Stereoselective Dibromination of Unsaturated Compounds

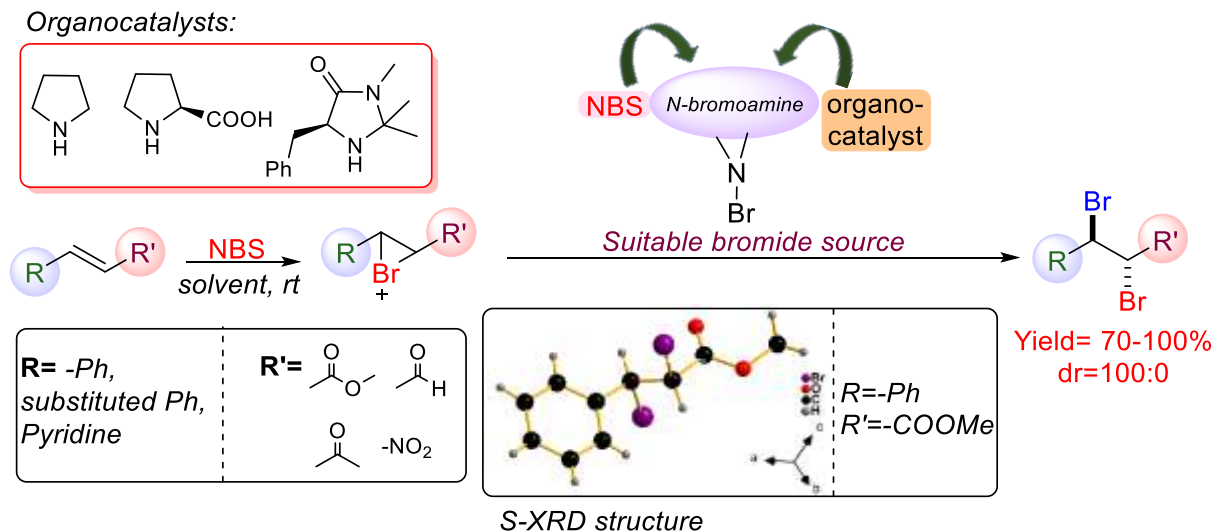
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Herein, the reversal of polarity of an N-Br bond has been achieved organocatalytically and the first-ever turn-over of polarity concept of cationic bromine using an organocatalyst is presented. The reagent NBS; a rich bromocation source was converted to a superior bromoanion reagent by H/Br exchange with a secondary amine, substantiated with spectroscopic and computational evidence. Further, the key steps of the reaction are observed through NMR kinetics, and the reaction acceleration using 10 mol% of amine accounts for its major success. The concept has further been used in a successful accelerated organocatalyzed dibromination of olefins, in a non-hazardous, commercially viable process. The protocol has been extended to a variety of substrates and the success in gram-scale synthesis proves its industrial viability.



Mononuclear Pd(II)-, Pt(II)- NHC complexes; synthesis, structural, electrochemical characterizations, and molecular docking studies**Ambarish Mondal, Joydev Dinda***

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Herein, a new family of cationic Pd(II)- and Pt(II)- complexes ligated to a novel C∩N donor N-heterocyclic carbene (NHC) ligand 3-methyl-1-(1-methyl-2-methylbenzoyl)imidazolin-2-ylidene), (**1**) have been highlighted. Compound 3-methyl-1-(1-methyl-2-methylbenzoyl)imidazolium hexafluorophosphate (**1**.HPF₆) essentially serves as a carbene precursor that delivers the NHC carbene to two novels isoelectronic and isostructural [Pd(**1**)₂][PF₆]₂ (**2**), and [Pt(**1**)₂][PF₆]₂ (**3**) complexes. All the compounds were characterized by elemental analysis, ¹H NMR, ¹³C NMR, mass spectroscopic studies, and finally single-crystal X-ray studies. X-ray crystallographic studies revealed both complexes **2** and **3** adopted square planar geometry. Electrochemical studies revealed Pt(II)/Pt(IV) reversible redox potential at 0.52 V. The catalytic activity of Pd(II)-NHC complex, **2** was tested for Suzuki coupling reactions. The structural assignments were further supported by DFT calculations. TDDFT studies have been performed to inside into the electronic properties. Molecular docking studies show a better binding affinity of **3** with Human-DNA Topoisomerase and BCL-2 protein compared to **2** and the scope of the complex **2** and **3** may be used as a drug.

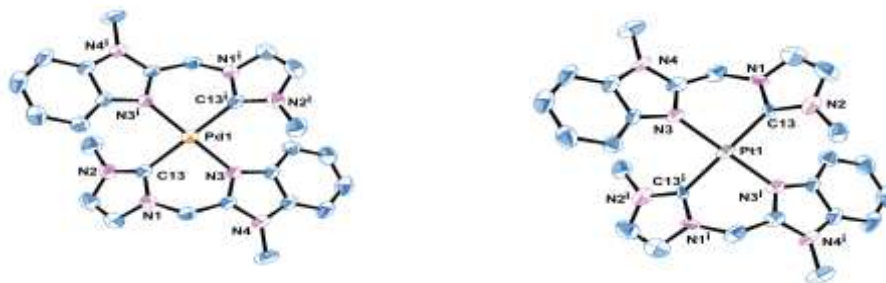


Figure 1: ORTEP view of single crystal X-ray structures of complexes **2** and **3**. The H atoms, solvent Et₂O, and the PF₆ (counter anions) were omitted for clarity.

PP-07

Assessment of ground, pond, river, and canal water quality in some municipal, residential, industrial & port areas

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The characteristics of water, air, and soil having physical, chemical, and biological are undesired changes. So, around the Globe; people are under tremendous threat. Water is highly polluted with different harmful contaminants due to manmade activity. Leaching of soils, industrial processing, residential municipal waste, etc., and weathering of rocks; natural water contaminates. Varied waterborne diseases are suffered by human beings due to the use of contaminated drinking water. So, it is necessary that at regular time interval quality of drinking water should be checked. Different physicochemical parameters are used with the calculation of WQI for testing water quality.

Keywords: Water, Physicochemical Parameters, WQI.

PP-08

A novel phase in truncated hexagonal bi-pyramid gallium ferrite nanocrystals

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Gallium ferrite or GaFeO₃ with ferrimagnetic and piezoelectric order has attracted huge attention in the last few years due to its potential applications in novel devices such as multiple-state memory elements. Gallium ferrite nanocrystals of “truncated hexagonal bi-pyramid” are explored as prospective self-cleaning material. [1] In the present work, gallium ferrite nanocrystals with polar, rhombohedral R3c symmetry are synthesized by hydrothermal route. Structural characterization using X-ray diffraction, Raman spectroscopy, and electron microscopy confirms the formation of rhombohedral R3c phase for the first time, with two different geometries and a narrow size distribution. The optical absorbance of the gallium ferrite nanocrystals was measured using UV-Vis spectroscopy. An optical band gap of 2.15 eV is obtained. Temperature-dependent impedance measurement of GFO nanocrystals over 273 K –

873 K was performed. The structural change is corroborated by a dielectric anomaly at the transition temperature.

Keywords: self-cleaning, phase transition, dielectric anomaly

Reference:

1. Mishra, M., et al., Truncated hexagonal bi-pyramidal gallium ferrite nanocrystals: integration of structural details with visible-light photo-activity and self-cleaning properties. Journal of Materials Chemistry A, 2018, 13031.

PP-09

Solvatochromic properties of naphthalene-based azo dyes: Solvent and substituent effects

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Three naphthalene-based azo dyes without substituents and with p-hydroxy and o-hydroxy substituents have been synthesized by the coupling reactions of unsubstituted and hydroxy-substituted anilines with β -Naphthol in the acidic environment at ice temperature. Solvatochromic behaviors of the dyes were studied with thirteen solvents of varying polarity. The dyes are found to sense the solvent polarities. The effect of substituents and their position on the optoelectronic properties of the probes have been analyzed. Solvatochromic behaviors of the dye molecules have been explained based on the stability of their tautomeric azo and hydrazo forms in the solvents. The correlation between solvent polarities and the hydrogen bond acceptor or donor behavior of the produced azo dyes is supported by regression analysis involving their absorbance.

Keywords: Azo dye, Solvatochromism, Tautomerism, Regression analysis.

PP-10

Conformational Polymorphs and Solvates of 1-(6-aminopyridin-2-yl)-3-phenylthiourea

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Three conformational polymorphs and two solvates of an asymmetrical N, N'-disubstituted thiourea derivative namely, 1-(6-aminopyridin-2-yl)-3-phenylthiourea (PTU) have been reported here. In all the

polymorphs and solvates, the PTU molecules self-assemble into dimers in the solid state, via two complementary N-H \cdots S bonds resulting in the formation of R₂²(8)-type of H-bond motif. The two PTU molecules in these dimers interact with each other in a head-to-tail fashion. Furthermore, the PTU molecule adopts trans, cis- conformation with an intramolecular N-H \cdots N interaction in all the crystals. However, the orientation of the aminophenyl ring concerning the phenyl ring plays a crucial role in the solid state packing of the polymorphs and solvates. Additionally, three polymorphs are distinguishable by C-H \cdots π , N-H \cdots π and $\pi\cdots\pi$ interactions. The polymorph PTU-1 crystallizes in the P-1 space group with Z'=2, whereas the polymorphs PTU-2 and PTU-3 crystallize in Pbcn and R-3 space groups respectively, with Z'=1. On the other hand, the solvate PTU-DMSO crystallizes in P2₁/c with a 1:1 host-guest ratio, and PTU-Morpholine exists in the P-1 space group with a 2:1 host-guest ratio. Hirshfeld surface analysis was carried out to compare the intermolecular interactions in the three polymorphs and two solvates of the title compound. The 2D fingerprint analysis of each of the polymorphs reveals that besides the H \cdots H interactions, C \cdots H and S \cdots H interactions contribute more to the generation of polymorphs. The contribution of C \cdots H interactions in both PTU-2 (31.6%) and PTU-3 (32.1%) are much higher than that of any molecule in PTU-1 (19.8% and 23% for Molecule A and B respectively). Additionally, a tiny amount of $\pi\cdots\pi$ interaction was observed (C \cdots C interaction, 4.5%) in polymorph PTU-1, which was absent in PTU-2 and PTU-3.

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

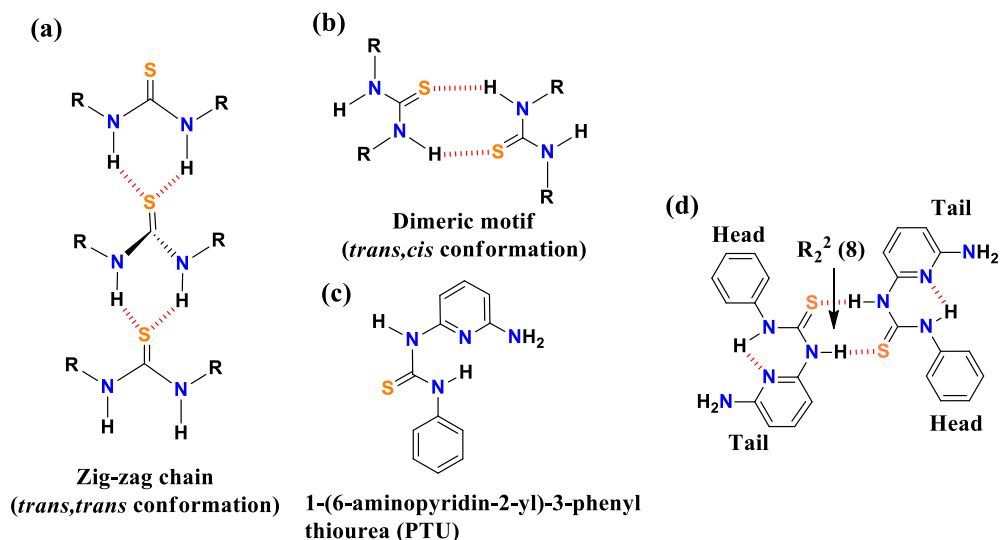


Figure 1: (a) and (b) Hydrogen-bonding motifs typically observed for disubstituted thiourea in the solid state; (c) Structure of 1-(6-aminopyridin-2-yl)-3-phenylthiourea (PTU); and (d) Formation of dimers through R₂²(8)-type of cyclic motif via two complementary N-H \cdots S interactions.

PP-11

Study on bioenergy potential of rice straw biomass belonging to different maturity duration varieties

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Pyrolysis is a major method for producing biogas, bio-oils, and charcoal. The current study used three common rice varieties with varying maturity durations to perform thermo-gravimetry and determine the influence of maturity length on kinetic parameters. Rice straw contains cellulose (32.55%), volatiles (64.7%), and 15.71 MJ/kg HHV. The average activation energy (E_a) values for medium (194.57 kJ/mol) and mid-early (180.31 kJ/mol) varieties were greater than for late duration (173.53 kJ/mol) types. For the late duration variation, A values of 10^{12} - 10^{15} , 10^{12} - 10^{15} , 10^{13} - 10^{15} , and 10^{13} - 10^{15} were reported under FWO, KAS, Starink, and Tang, respectively. Under alternative models, the A values for the other two kinds were determined to be as high as 10^{22} . D4 and D3 diffusion models were determined to be the best fit models using Coats-Redfern and master plot ($Z-\alpha$) analyses. The values of ΔH increase with the amount of conversion for Mahalaxmi and CR-D-304, suggesting the endothermic nature of rice straw combustion.

PP-12

A comprehensive study on kinetic and thermodynamic parameters of three local varieties of banana (*Musa spp*) biomass

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Biogas, bio-oils, and biochar are some of the valuable products, which are usually harnessed through the pyrolysis process. Under the current investigation, three popular banana varieties were subjected to the pyrolysis process to decipher their bioenergy potential. Thermo-gravimetric analysis was utilized to determine the kinetic parameters. The levels of E_a were roughly determined to 206 kJ/mol (Patakapura)(*Musa acuminata*), 179 kJ/mol (Champa)(*Musa Chini Champa*), and 180 kJ/mol (Bantala)

(Musa Paradisicaca). Values of A in the range of 10^{12} - 10^{15} , 10^{12} - 10^{15} , 10^{13} - 10^{15} , and 10^{13} - 10^{15} were observed under FWO, KAS, Starink, and Tang models, respectively. From the master plot analysis, it can be inferred that the reaction mechanism involved in the thermal decay of major cell wall polymers was quite complex and followed a multi-step reaction mechanism. The endothermic nature of pyrolysis was validated through the analysis of the thermodynamic parameters.

PP-13

Design, synthesis, and photophysical study of Aggregation Induced Emission (AIE) Luminophores containing tetraphenylethylene moiety and electron-donating group in phenanthroimidazole derivative

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The propeller-shaped tetraphenylethylene (TPE) avoids tight packing of the molecules in the aggregated state, which alleviates intermolecular π - π interaction. Therefore, solids of TPE derivatives can fluoresce strongly, enabling them to serve as efficient host light emitters for OLEDs. Here, AIE-based three fluorophores PI-Ph-TPE, PI-Ph-p-CH₃-TPE, and PI-Ph-TB-TPE were designed with the help of theoretical modeling and studied their excited state properties and electronic structures by the TD-DFT method. Here a popular building block for blue luminogenphenanthroimidazole (PI) was modified with the phenyl, toluidine, and tert-butyl group in the N1 position to suppress strong intermolecular interactions, and AIE active TPE unit was connected through the spacer benzene ring to alleviate the ACQ effect. PI-Ph-TPE, PI-Ph-p-CH₃-TPE, and PI-Ph-TB-TPE were successfully synthesized and confirmed by NMR and Mass Spectroscopy. The fluorophores were successfully characterized and the photophysical study reveals that all the compounds showed deep blue emission in solution with appropriate CIE coordinates but sky-blue emission in solid and thin-film states. The photophysical study with water: THF mixture shows the AIE effect with an increase in water fraction. The PLQY of three fluorophores was lesser in the solution state than that of the thin-film state. In the film state, the PLQY of PI-Ph-TPE, PI-Ph-p-CH₃-TPE, and PI-Ph-TB-TPE were measured as 73.4%, 83%, and 81% respectively.

Development of seedling pot for nursery application

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Seedling pots or sapling pots are of common interest due to their large utilization to grow a young plant in a nursery. These are previously made up of thermoplastic, cement, paper pots, etc as low-cost materials. But problems like non-degradability, stress on roots, highly expensive, brittle nature, and difficulty in transportation are drawbacks of these pots. To overcome this, some researchers applied natural fiber with thermoplastic and thermoset resin to fabricate sapling pots. But incomplete biodegradability, high weight, and high cost are the major drawbacks of these products to trade in the competitive market. In this work, completely biodegradable jute-reinforced sapling pots were developed and characterized. Physical characteristics like thickness, size, tensile properties, flexural properties, and water absorption of sapling pots were measured and reported. Jute reinforced sapling pot showed tensile strength, flexural strength and tensile modulus of 37.1 MPa, 38.4 MPa and 980 MPa, respectively. Soil burial and microbial degradation studies of sapling pots were carried out in compost soil and cultured fungal bed, respectively. It was found that after 60 days under soil burial conditions, the mechanically optimized pot lost 70% of its original weight. Weight loss, tensile loss, and FE-SEM photographs of sapling pots after biodegradation revealed that pots are completely biodegradable in nature. Hence, these sapling pots allow room for better root propagation, which can be placed directly into the soil without disturbing the tender sapling. These sapling pots can be an alternative to harmful plastic-based and other ceramic-based sapling pots.

Keywords: Seedling Pot, Jute, Soy, Biodegradation, Mechanical Properties

Impact of Heat Treatment on the Physico-Mechanical Properties of Poly Butylene Adipate-co-Terephthalate (PBAT)/Thermoplastic Starch (TPS) Films

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Research on biodegradable polymers has gained momentum to mitigate the environmental pollution issues associated with the use of conventional plastics. Several biodegradable polymers such as polylactic acid (PLA), polybutylene succinate (PBS), polybutylene adipate-co-terephthalate (PBAT), etc. have been the materials of research for the preparation of biodegradable plastics. To reduce the cost, starch has been incorporated into these systems. In the present study, PBAT/thermoplastic starch (TPS) films have been prepared by solution casting technique. After preparation, the films have been subjected to two different temperatures (80 and 110°C). The physical, mechanical, and morphological characteristics of all the types of prepared films have been evaluated. The results of the study will be discussed.

Keywords: Biodegradable polymers, Tensile strength, Water absorption, Water vapor permeability

Reference:

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2. Processes 8 (2020) 329

PP-16

Regioselective synthesis of pyrazole-based 2-aryl-3-nitro-2H-chromanes via aza-Michael addition reaction under catalyst-free condition

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Densely functionalized 2, 3, 4-trisubstituted chromane derivatives and their 4-amino skeletons are the most important structural building blocks of many bioactive natural and unnatural alkaloids possessing potent biological activities such as bactericides, antioxidant, anti-hypertensive, anti-cancer agents and in medicinally enriched drug candidates such as cromakalim, NIP-142, HMR 1556, chromanol 293B [1] etc. Amongst the procedures available in a chemist's toolbox for the construction of 2, 3, 4-trisubstituted aminochromane, the aza-Michael addition reaction has emerged as a very popular method and also plays a major role in providing ubiquitous nitrogen-oriented essential skeletons in modern organic synthesis [2]. On the other hand, pyrazole is a synthetically interesting heterocyclic molecule that shows fascinating therapeutic activities like anticancer, antitumor, anti-AIDS, antimicrobial, antimalarial, antifungal, and antitubercular properties [3]. Considering the biological activities as well as abundance in many potent drug candidates of these 2,3,4-trisubstituted aminochromanes, herein, regioselective synthesis of 1-(3-nitro-2-aryl chroman-4-yl)-1H-pyrazole derivatives have been disclosed via tandem aza-Michael addition reaction of substituted pyrazoles to 2-aryl-3-nitro-2H-

chromene derivatives at room temperature. This protocol was generated in one-pot transformation with good to high yield with excellent regioselectivity. The absolute configuration of the product was confirmed by a single crystal X-ray study. Easy accessibility, base and catalyst-free condition, wide substrate scope, high yields, and excellent regioselectivity are the major features of this protocol.

Keywords: Aza-Michael addition, regioselectivity, pyrazole, Single crystal X-ray, 2, 3, 4-trisubstituted amino chromane.

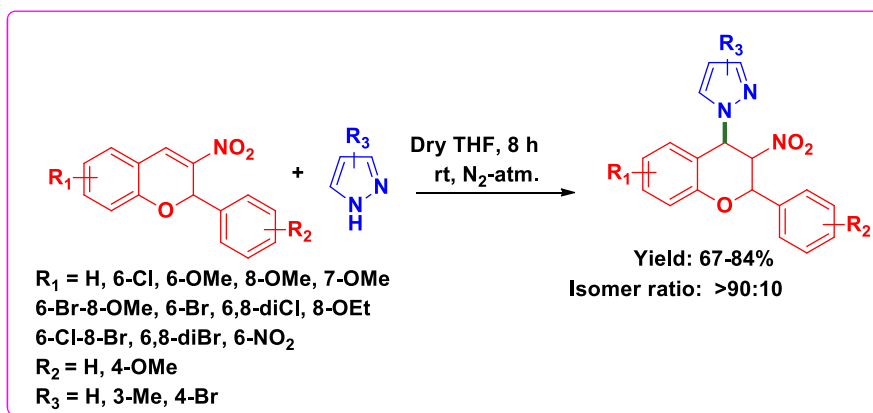


Figure: Synthesis of 2,3,4-trisubstituted amino-2H-chromane.

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PP-17

Phenanthridine-Benzilimadole Based Bipolar Blue Host Materials for Highly Deep Blue Fluorescence Organic Light Emitting Diodes and its applications

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Organic light emitting diodes (OLEDs) has shown great potential (lightweight, fast response time, flexible, and energy efficient) and emerging technology for next-generation display and lighting application. In any case, achieving efficient blue electroluminescence remains a great challenge. In this work, Seven luminophores based on tetrahydrodibenzophenanthridine (THDP) as acceptor unit and Benzi-imidazole (BI) as donor unit was designed and synthesized. Here the donor- π -acceptor approach is used to design new molecules by using benzyl imidazole(BI) as the acceptor for its good electron-

transporting mobility and phenanthridine (BT) as the donor for its good hole-transport mobility and connecting them with different linkers. In this report, we report our studies on the synthesis and characterization of 5-(4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phen-anthridine (BT-BZ) (3a-g). The thermal and electrochemical analyses, the computational studies on HOMO-LUMO energy levels, and the density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations in both the ground and excited state of the compounds for a better understanding of the electronic structures and spectroscopic properties. In that literature, all the performance parameters, and some of the new compounds described here are among the best non-doped deep-blue emitters reported recently. The blue luminophores exhibited high photoluminescence quantum yields of 66–93 % in THF solutions.

PP-18

A facile and catalyst-free microwave-assisted one-pot synthesis of (E)-(2H-chromenyl)-phenyl hydrazone derivatives and their molecular docking investigation

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Presently, the design and synthesis of heterocyclic compounds targeting specific pharmaceutical activities have become fashionable topics among synthetic and medicinal chemists. The 2H-chromene is an imperative class of oxa-heterocycle largely distributed in natural products with numerous biological activities for instance anticancer, antioxidant, anti-inflammatory, antitubercular, antiviral, antitumor, antibacterial/antimicrobial, antidiabetic, anticoagulant, antianaphylactic, diuretic, fungicidal, and anti-HIV activity.^{1,2} Meanwhile, the synthesis of hydrazone derivatives and their applications in medicinal chemistry exceedingly galvanized many research groups.³ Consequently, the chemotherapeutic potential of this class of organic compounds is enhanced significantly due to the hybridization of these two moieties. Hence, a series of novel chromene-based hydrazone derivatives were synthesized in microwave-assisted conditions. This protocol produced 2H-chromene-based hydrazone in good to excellent yield. A green synthetic approach, simple, Easy accessibility, metal-free, and high yield are the key features of this synthetic route. The synthesized compounds were subsequently evaluated for in vitro anti-bacterial assay against E. coli and topoisomerase pathogenic bacteria in comparison to the standard antibiotic Gentamicin. SAR and molecular docking revealed compounds having –Cl and –Br groups displayed improved halogen and hydrogen bond interaction

with bacterial DNA gyrase of *E. coli* (PDBID:1KZN) and topoisomerase (PDBID:1KZXN) having binding affinity of -9.1 kcal/mol and -9.9 kcal/mol respectively.

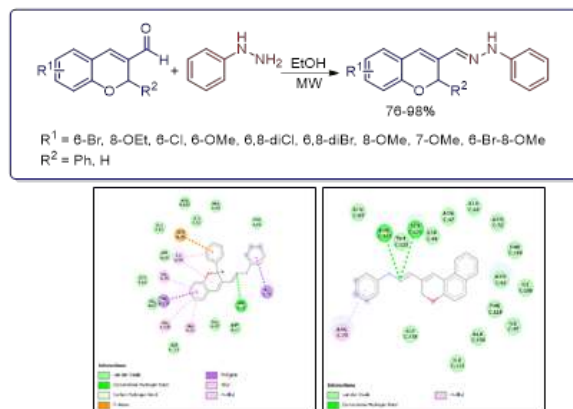


Figure 1: Synthesis of 2H-chromenyl Hydrazone.

Reference:

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3. Spectrochimica Acta Part A: Mol. and Bio. Sp., 2008, 70, 641-645.

PP-19

CuI Nanoparticles Catalyzed Regioselective Synthesis of Medicinally Relevant Nitrogen Rich Heterocycles via Domino Strategy

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Nitrogen-rich heterocycles are prevalent heterocyclic units in pharmaceuticals and bioactive natural products.¹ Among them, imidazo[1,2-*a*]pyridines are synthetically interesting heterocyclic molecules that exhibit fascinating therapeutic activities like anti-cancer, antitumor, anti-AIDS, and antimicrobial properties.² The domino strategy explores multiple bond-forming reactions under fixed reaction conditions, and thus develops a step-economy approach toward the synthesis of heterocycles. Herein we report the synthesis and catalytic applications of CuI Nanoparticles towards the regioselective synthesis of 3-nitro-2-arylimidazo[1,2-*a*]pyridines.³ The Domino strategy resulted in a library of *N*-heterocycles in good to excellent yields with high functional group compatibility. The synthesis of 3-nitro-2-arylimidazo[1,2-*a*]pyridines was achieved using CuI nanoparticles (NPs) which showed reusability up to three consecutive cycles.



Scheme

1: CuI NPs catalysed regioselective synthesis of 3-nitro-2-arylimidazo[1,2-*a*]pyridines

Reference:

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PP-20

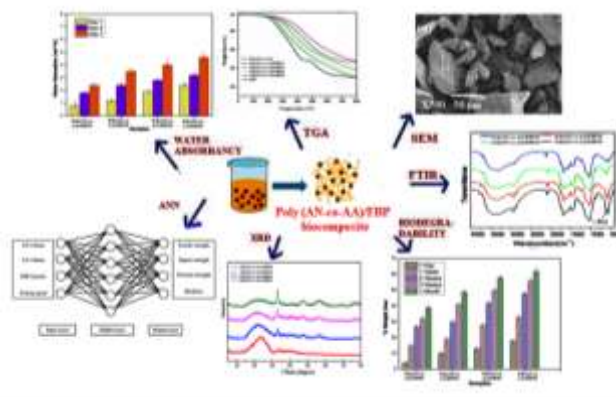
Synthesis and optimization of properties of Poly (AN-co-AA)/fish bone biocomposite by using artificial neural networks

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The purpose of the study is to synthesize a new biocomposite material by using the monomers acrylonitrile (AN) and acrylic acid (AA) with reinforcement from fish bone powder (FBP) and predict its mechanical properties using an artificial neural network (ANN) model. The Fourier transform infrared (FTIR) analysis indicates the denaturation of collagen and the presence of amide I, II, carbonate, and phosphate groups. The variation in particle size and structure has been studied by scanning electron microscopy (SEM). The X-ray fluorescence (XRF) indicates the chemical composition of raw FBP and calcinated FBP. The thermogravimetric analysis (TGA) shows the amount of weight loss of various samples at different temperatures. X-ray diffraction (XRD) indicates the homogeneous dispersion of FBP into the surface of the poly (AN-co-AA) matrix, and the crystallinity decreases due to the addition of FBP. The tensile strength, impact, and hardness of the biocomposite increase. The synthesized biocomposite shows biodegradability and water absorption capability as compared to the copolymer matrix, which is due to the interaction of fishbone powder with the copolymer matrix. The mechanical properties were measured experimentally and predicted again by using the ANN model. The training and test datasets used in this analysis have a correlation factor of more than 0.9, indicating that the predicted result for mechanical properties is in good agreement with the experimental result.

Keywords: Copolymerisation, Biocomposite, Biofiller, Fishbone powder, Mechanical strength, Water absorbency



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PP-21

Synthesis of spirooxindole pyrrolidine/piperidine fused chromane aldehyde derivatives following one pot, three component 1,3-dipolar cycloaddition reaction

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A novel and convenient methodology for the synthesis of a series of diverse 2'-oxo-6b,7,8,9-tetrahydro-6H-spiro[chromeno[3,4-a]pyrrolizine-11,3'-indoline]-6a(11aH)-carbaldehyde derivatives following 1,3-dipolar cycloaddition reaction has been demonstrated successfully. This one-pot three-component synthesis involves 2H-chromene-3-carbaldehyde, isatin, and secondary amino acid (L-proline/pipecolinic acid) in ethanol at 80 °C to produce the corresponding cycloadducts in good to excellent yields (52-91%) with a wide substrate scope under conventional and microwave irradiation. The structure and relative stereochemistry of the cycloadduct was confirmed using ¹H, ¹³C-NMR,

COSY, NOESY, and HRMS studies. The major advantages associated with this protocol include one-pot synthesis, short reaction time, wide substrate scope, and excellent yield of the products.

Keywords: 1,3-dipolar cycloaddition, 2H-chromene-3-carbaldehyde, isatin, spirooxin-dole, one-pot reaction, Microwave

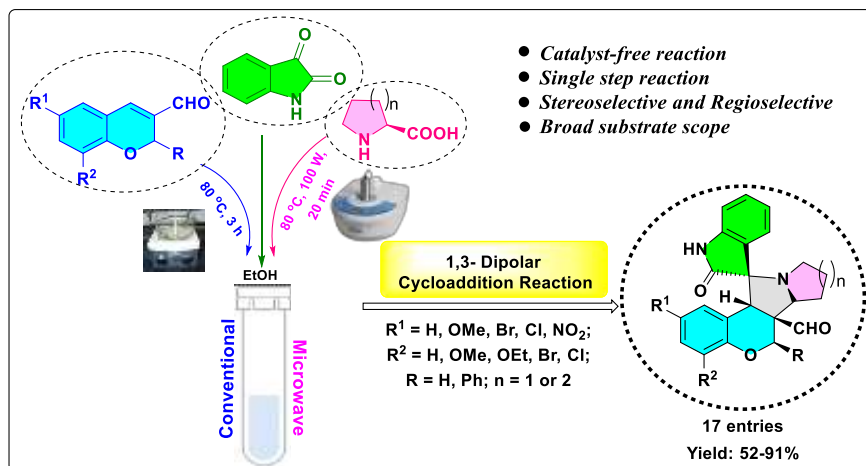


Figure 1: Synthesis of 2'-oxo-6b,7,8,9-tetrahydro-6H-spiro[chromeno[3,4-a]pyrrolizine-11,3'-indoline]-6a(11aH)-carbaldehyde derivatives

PP-22

Unveiling the Selective Photocatalytic reduction of CO₂ to Solar Fuels via Nanocrystalline Ultrathin Porous C₃N₃ Nanosheets

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Artificial photosynthesis, the light-driven CO₂ conversion into hydrocarbon fuels, is a potential approach to combat global warming and increasing energy demand simultaneously¹. The interaction of the CO₂ on the catalyst's surface and the charge transfer kinetics determined using ultrathin two-dimensional materials possess a higher degree of active sites that are distributed uniformly. The photocatalysts designed by integrating enzymes and the Nitrogen-deficient C₃N_x have shown potential for CO₂ conversion having porosity and ample room for functionalization to improve selectivity for CO₂ conversion has been undertaken in this work.²⁻⁴ The charge transport kinetics and CO₂ activation of mpg-C₃N₃ optimized MoS₂ exhibits CO₂ conversion predominantly in CO with the yield of the order of 980 μ mol g⁻¹. The characterization using XRD, TPD, FTIR, and HRTEM to elucidate their

structural and optical properties was undertaken. Further, the charge carrier dynamics, CO₂ activation on these heterostructure ultrathin photocatalysts, and underlying mechanism will be discussed in detail.

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PP-23

Effect of Barium Doping on the Photocatalytic Behaviour of Lanthanum Manganite Perovskites for the Removal of Methylene Blue in Aqueous Medium

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Nanocomposites of Lanthanum Barium Manganite (LBMO) $\text{La}_{0.75}\text{Ba}_{0.25}\text{MnO}_3$ was synthesized through a reproductive, quick, modest, and eco-friendly strategy, via citrate sol-gel technique. The sample was characterized using FT-IR, XRD, SEM, ICP-AES, and EDAX analyses. The ICP-AES data confirmed the formation of the required stoichiometric $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ Oxide. The particle size of the catalyst was calculated by the Scherer equation using data from XRD analysis. The calculations along with an analysis of SEM confirm the formation of the nanosized perovskite phase. Amazing photocatalytic property of doped (LBMO) perovskite is looked at. The behavior of this nanocatalyst for the degradation of an aqueous solution of methylene blue was investigated at wavelengths of 300-700 nm. The effects of the type and different amounts of acid, the absorbent content, pH, and temperature were studied to obtain the optimal conditions of degradation. The prepared sample shows a suitable activity for methylene blue degradation under dark conditions. The visible light catalytic degradation is faster and goes up to about 48% after 100 min of illumination, indicating a different reaction pathway with less activation energy. The linear increase in photo degradation rate was found in the sample as a

function of the time of irradiation, which was confirmed by a study of the optical properties of the resulting aqueous solutions.

Keywords: LBMO Perovskite, Nanoparticles, Sol-Gel technique, Photocatalyst behavior

PP-24

A Study on Photocatalytic Property of Sr-Doped Lanthanum Manganite Nanoparticles for Removal of Methylene Blue in Aqueous Medium

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Strontium doped lanthanum manganite $\text{La}_{0.75}\text{Sr}_{0.25}\text{MnO}_3$ having Perovskite structure shows a high degree of catalytic efficiency for the removal of Methylene blue dye from its aqueous solution. The sample powder (LSMO) was prepared through the sol-gel technique and was characterized by X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FTIR), Inductively coupled plasma-atomic emission spectroscopy (ICP-AES), Scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX) and UV-Vis spectroscopy (UV-Vis). The XRD data showed the formation of a single crystalline phase. SEM images show that the micro-sized LCMO sample has a nanocrystalline structure with an average diameter of 1-5 μm . The ICP-AES data confirmed the formation of stoichiometric $\text{La}_{0.75}\text{Sr}_{0.25}\text{MnO}_3$ Oxide. The Photocatalytic behavior of the sample was investigated on Methylene Blue as an Organic water pollutant, at specified pH and constant Irradiation dose for several hours. The result showed adequate visible light photocatalytic activity as a function of the time of irradiation and was confirmed by a study of the optical properties of the resulting aqueous solutions. It was ascertained that the photocatalytic activity increased with increased irradiation time and maximum degradability has been attained after 100 minutes of irradiation. The percentage of degradation was calculated using mathematical laws.

Keywords: Perovskite; sol-gel technique; photocatalyst; methylene blue.

PP-25

Functional Coumarins as Donor Material for Fullerene-Free Organic Solar Cells

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Organic Solar Cells (OSCs) have emerged as one of the promising sources of clean and renewable energy technologies. Nowadays tremendous growth has been seen in bulk-heterojunction (BHJOSC) using a ternary blend of complementary absorbing molecular donors and fullerene-free acceptors. Here, we demonstrate the synthesis and characterization of two wide band-gap functional coumarin derivatives possessing excellent optoelectronic and thermal properties and in combination with appropriate acceptor materials, gave high efficiencies of up to 15.28% in ternary OSCs with a low energy loss of 0.43 eV. Coumarin derivatives are considered a class of wide band-gap material that absorbs around 500 nm with a band gap >2 eV with the advantages of efficient synthesis, strong photo-response in the visible region, and tunable energy levels to match with other device components. The work also determines the importance of simple coumarin as a donor and its role in performance improvement for fullerene-free ternary OSCs by facilitating charge carrier transport with suppressed recombination.

Keywords: coumarin; fullerene-free acceptor; organic solar cells.

PP-26

An overview of Zinc Sulfide (ZnS) based catalysts for hydrogen (H₂) evolution under visible light irradiation

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Photocatalytic hydrogen production is a promising approach for a sustainable economy because it is a renewable energy source that is going to substitute fossil fuel in near future. The catalysts are vastly used for this purpose under solar light irradiation. ZnS catalyst has great potential for low-cost and

environmentally friendly solar-hydrogen production. This review article comprehensively discusses the synthetic methods of ZnS-based catalysts such as hydrothermal, solvothermal, ultrasonic irradiation method, ion exchange method, etc. This article also represents some characterization of the photocatalysts i.e. X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), UV-Vis analysis, Photoluminescence, and Raman spectroscopy. ZnS-based catalyst-assisted photocatalytic activity has been briefly summarized in this review article.

PP-27

Electrocatalytic Oxygen Reduction Activity of Surface Modified WO₃ through Different Structure Directing Groups

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Nanostructured Tungsten Oxide (WO₃) was prepared by acidification of Na₂WO₄·2H₂O. The final square-like WO₃ nanosheets were obtained by hydrothermal synthesis method after acid treatment of precursor. We observed morphological changes in the final WO₃ nanoparticles when structure-directing groups were used during synthesis. Here, we used Citric acid, 1-Vinyl pyrrolidone, D, L- Aspartic acid, Tartaric acid, Glycine, etc. as the structure-directing group for the synthesis of Tungsten Oxide. X-ray powder diffraction (XRD), field emission scanning electron microscopy (FE-SEM), and Fourier Transmission Infrared Spectroscopy (FT-IR) were used for the characterization of the synthesized nanoparticles. Changes in the size and shape of the synthesized NPs were confirmed from the SEM images. Further, the electrochemical activities for the oxygen reduction reaction of the WO₃ NPs were studied.

PP-28

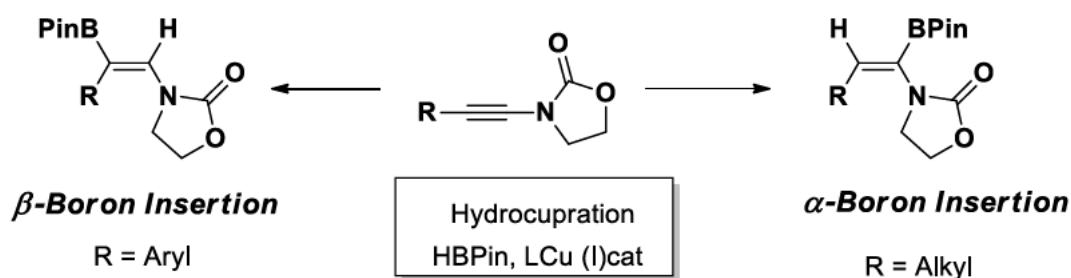
Cu(I) Catalyzed Regio- and Stereo-selective Hydroboration of Ynamides: α - and β -Borylation via Hydro-Cupration and Borylation

Subhra Roy, Archana Mishra, Subhransu Sekhar Pati, Minati Behera and Jaya Prakash Das*

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A Cu^I-catalyzed hydrocupration and borylation protocol for the region- and stereoselective borylation of ynamides utilizing pinacolborane (HBpin) as the borylating agent has been developed. The

reaction features mild conditions, good substrate scope, and functional group tolerance-representing a highly efficient and practical method for the synthesis of the region- and stereoselective tri-substituted alkenylboronates from readily available ynamides. The regioselectivity is controlled by altering substituents on the ynamides (alkyl vs aryl) and utilizing a catalytic species [LCuH] generated in situ from HBpin and [LCuX]. Suzuki coupling and other transformations highlight the synthetic utility of the method.



Scheme 1: Cu (I) – catalyzed regio- and stereoselective hydroboration of ynamides

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PP-29

Synthesis and characterization of MXene/Reduced graphene oxide hybrid nanofillers reinforced Polyvinylidene fluoride/ Polyaniline blend nanocomposite

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The current research empathizes with the development of new approaches to improve the homogeneous dispersion of the nanofillers by decorating their surface with conducting polymers. Here, MXene (Ti₃C₂T_x) nanosheets will be prepared from titanium aluminium carbide (Ti₃AlC₂) according to the modified HF etching method. MXene with the surface-endowed reduced graphene oxide (rGO) hybrid nanofiller will be fabricated by vacuum-assisted filtration. In particular, the MXene/rGO nanohybrid

effectively increases the specific surface area and accelerates the diffusion of electrolyte ions demonstrating good volume capacitance, high energy/power density, and long cycle life for application in high-performance energy storage systems. A conductive polymer blend of Polyaniline (PANI) and Poly (vinylidene fluoride) (PVDF) exhibiting relatively high dielectric permittivity (ϵ') together with a low band gap is synthesized. The synthesis and utility of MXene, rGO, PVDF, and PANI alongside their composites can be proved through the use of various sophisticated equipment like X-ray diffraction (XRD), small-angle neutron scattering (SANS), X-ray absorption spectroscopy (XAS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM), pair distribution function analysis, atomic force microscopy (AFM), nuclear magnetic resonance (NMR), Raman spectroscopy, dynamic light scattering (DLS), UV-Visible spectroscopy (UV), Fourier transform infrared spectroscopy (FTIR) and also study the thermal, dielectric and sensing properties using thermogravimetry-differential scanning calorimetry (TG-DSC), LCR meter and UV-Vis instrument.

Keywords: Mxene; Reduced graphene oxide; Poly (vinylidene fluoride), Polyaniline; Nanocomposites; energy storage devices.

PP-30

A Schiff base luminescent chemosensor for selective detection of Zn^{2+} in an aqueous medium

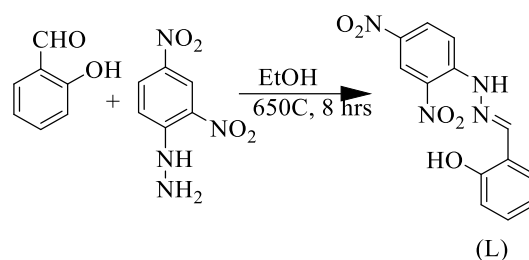
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Luminescent chemosensors based on Schiff bases have drawn tremendous research interest owing to their easy synthesis, enriched photophysical properties, and potential applications in biology and materials science. A dinitrophenyl-based Schiff base molecular probe (**L**) was synthesized and characterized to estimate its selective detection of Zn^{2+} . The probe **L** exhibits weak emission in the DMSO- H_2O solvent mixture due to excited-state intramolecular proton transfer (ESIPT). Interestingly, fluorescence is enhanced with the addition of Zn^{2+} to the DMSO- H_2O solution of **L**, whereas the emission remains unchanged with the addition of other ions. This specifies that probe **L** acts as a selective chemosensor for Zn^{2+} . The binding stoichiometry for the **L**: Zn^{2+} complex is 1:1, which was

calculated using the Benesi-Hildebrand plot from fluorescence data. Furthermore, the binding modes are also supported by density functional theory (DFT) calculation. The binding constant and detection limits are $6.35 \times 10^7 \text{ M}^{-1}$ and $1.1 \times 10^{-8} \text{ M}$, respectively. The L-Zn^{2+} complex formation is reversible upon the addition of a strong chelating EDTA ligand. In addition, **L** is also used to detect Zn^{2+} in living HeLa cells and selective sensing of Zn^{2+} in the solid phase.



Scheme 1: Synthesis of (E)-2-((2-(2,4-dinitrophenyl)hydrazineylidene) methyl) phenol (L).

Keywords: Schiff base Fluorescence Chemosensor, ESIPT, Zn^{2+} sensor, Cell Imaging

PP-31

Surface Modification of Chitosan/Gelatin composite by DBD Atmospheric Plasma

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Among several approaches utilized for surface modification of polymeric composites; cold or non-thermal plasma technology has blossomed into an effectual, facile, and economical methodology, and also it does not have any modified effect on the bulk properties except required modifications on the surface only. The treatment is more appealing for materials that are more active towards biomedical applications since it guarantees a higher degree of bio-activity, bio-selectivity, and an environmental friendly process. In this piece of work, we take bio-degradable hydrogels comprising of chitosan and gelatin (Cs/Gel) composites that have been synthesized using a nontoxic cross-linker, tetraethyl Orthosilicate (TEOS) in the presence of He and He+O₂ plasma, for enhancing various surface properties such as surface wettability, tensile strength, topographical characters, and different biological applications. The enhanced hydrophilicity was observed after plasma treatment. Also, topographical changes in the composites were found from AFM and FE-SEM studies. After plasma treatment, the surface interaction was also observed using optical emission spectroscopy (OES) and

FTIR data. Observation shows the tensile strength of the hydrogels is increased which indicates the enhancement of hardness and stability of the hydrogels in post-plasma treatment. The hydrogels displayed good antibacterial features against Enterobacter and Bacillus where better inhibition was found in the case of He + O₂. The hydrogels were found to be remarkably biodegradable and pH sensitive. It concludes that non-thermal plasma-treated Cs/Gel hydrogels can be explored for diverse biomedical applications, drug delivery and also in the food packaging industry.

PP-32

Analysis and Prediction of Ground Water Quality of Belpahar area, Odisha, India on the performance of ANN Methods

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Water is regarded as our planet's most vital resource and is used by all biotic communities, but the main issue is protecting groundwater from severe environmental contamination. The impact of contaminated water is now far-reaching, influencing every aspect of life. Hence, the proper management of groundwater resources is very effective for optimizing the quality of water. For the measurement of the water quality index (WQI), some specific parameters related to water are needed. But the conventional method of calculating the WQI is a time-consuming process, and sometimes errors are found at the time of calculation. Therefore, to overcome these difficulties, we have to use some artificial intelligence algorithms. In this study, we are using machine-learning methods to predict groundwater quality in the Belpahar area of Odisha, India. Therefore, proper management of groundwater resources is highly essential to improving the water quality index, not only in the traditional sense but also by using artificial neural networks (ANN). The major aim of this study is the collection of water samples from various important locations in the Belpahar area, analysis of the physicochemical parameters of the collected groundwater samples, calculation of the WQI using these data, and then prediction modeling of the water quality using machine learning techniques. Several statistical indices were used to evaluate the prediction models' performance.

Keywords: Water quality, WQI, contamination, Surface water, Groundwater, machine learning technique

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PP-33

Abatement of chloro containing volatile organic compounds by Non-thermal plasma treatment: A Study of degradation mechanism and computational analysis

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Increasing environmental awareness has introduced stringent regulations controlling VOC emissions and has motivated researchers to develop various kinds of strategies. The degradation of a mixture of volatile organic pollutants in a parallel plate DBD reactor using the Non-thermal plasma technique has acquired enormous applications in the fields of environment purification. These studies are analyzed with help of Paschen's curve, I-V curve, GCMS, FTIR, and optical emission spectroscopy (OES). The analyzed results are verified through a computational study using Gaussian-16W software. Volatile compounds like CB, ODCB, and DCM are taken at diff concentrations with peak-to-peak voltages of 7 to 20KV_{pp} and pulsed frequencies of 10 to 20 kHz. Effect on degradation efficiency is studied varying flow rate and specific input energy value where it is evident that greater efficiency is found at a lower flow rate. Dichloromethane is found to be the most resistant at a high flow rate but possesses higher degradation efficiency at a lower flow rate. Bi-products and fragmented products are determined by online GC-MS analysis which helped to predict the degradation pathways. CO₂, CH₄, and H₂O as the major products, alongside other polymeric products are also detected through GC and GCMS. OES spectra are used to identify the radicals which are generated in the reactor which accelerated the degradation mechanism and the possible pathways are confirmed by computational work using GAUSSIAN-16W software. The findings of these studies are indented to promote the development of energy-efficient processes for the purification of the atmosphere in both domestic and industrial utilities with the prediction of the reaction mechanism.

PP-34

Amphiphilic Donor- π -Acceptor Based Coumarin Conjugates: Design, Synthesis, and Photophysical Applications

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The development of fluorescent probes has attracted attention, due to their variety of applications like the detection of environment polarity, drug-target binding, and biophysical properties of the cell. However, they show several drawbacks they do not function in the far-red region and display limited brightness due to the small extinction coefficients of their push-pull chromophores. Therefore, currently, intensive research is focusing on the design of polarity-sensitive fluorogenic molecules of high brightness together with red-shifted emission. To address some of the above drawbacks, we focused our interest on amphiphilic Donor-Acceptor (D- π -A) based push-pull coumarin conjugates with promising photophysical properties, including emission in the far-red/near-infrared (NIR) region, large Stokes shifts, high photostability, excellent brightness and greater cell permeability required for bioimaging. 7-amino coumarin derivatives C1, C8 and C18 were efficiently synthesized. These derivatives show emission in the far-red region, large Stokes shifts, high photostability, and excellent brightness as compared to conventional coumarins. The photophysical properties of these three dyes are studied in different micellar mediums (cationic, anionic, and nonionic). A greater solubilization for coumarins C8 and C18 was demonstrated compared to the C1 probe. The presence of a hydrophobic alkyl chain helps to bind the molecule in the micellar interior. These dyes show excellent bacterial cell permeability as their fluorescence emission could be easily detected at a concentration as low as 0.5 μ M.

PP-35

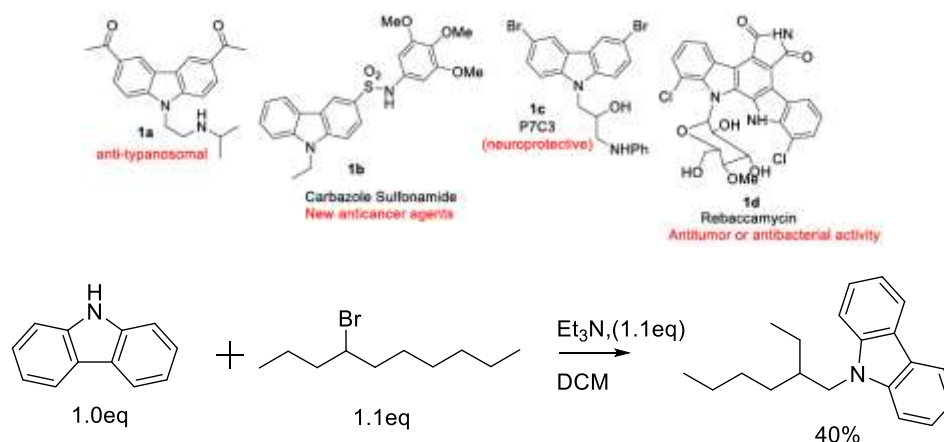
Synthesis of Easily Accessible Carbazole Derivatives

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Synthetic compounds of the carbazole Carvedilol and carprofen are used as anti-inflammatory and hypertension medications, respectively. Antimitotic medicines known as carbazole sulfonamides are

the most effective against solid tumors. a few illustrations of carbazole derivatives found naturally¹. We examined this reaction under 1.0 equivalence of carbazole, alkylating substrate, and base at room temperature. Even after stirring this reaction mixture for 6 hr, it was found that the reaction was not completed. Then, we used 1.0 equivalence of carbazole 1.1 equivalence of 4-bromodecane and 1.1 equivalence of Et₃N. We have chosen simple carbazole as the testing substrate and focussed to carry out alkylation with 4-bromodecane as reacting partner in different reaction media. The required key intermediate was prepared from commercially available, cheap starting material i.e., carbazole and 4-bromodecane using DCM as solvent and Triethylamine as the base.



Keywords: Carbazole, C-N bond formation, Biologically active molecules

Reference:

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PP-36

Computational Approach Towards Model Anti-Malarial Inhibitors of Thioredoxin Reductase (TrxR)

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Malaria is quite a well-known infectious disease around the globe. The recent report of the World Health Organization 2022 on the status of indigenous malaria cases, worldwide is alarming. In India

itself, malaria death cases are about 82% in the WHO South-East Asia region. Again, P. falciparum-resistant strains to available FDA-approved drugs encouraged the development of inhibitors for anti-malarial. The present investigation reports the exploration of selective anti-malarial inhibitors of thioredoxin reductase (TrxR) as the target protein of plasmodium falciparum based on the molecular docking approach, quantum chemical approach, and machine learning approach. The molecular docking approach is not sufficient enough to explore the inhibition mechanisms thereby quantum chemical approach has been performed for these model inhibitors about catalytic active pockets. Furthermore, the machine learning approach using SVM Gaussian, SVM, IBK, LWL, RF, and MP methods provides good correlation and a significant way to design & synthesize new inhibitors for further study.

PP-37

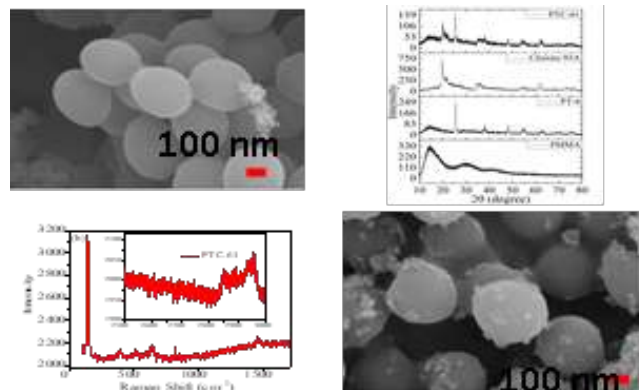
Study of Dielectric Properties of TiO₂ embedded PMMA/Clay Nanocomposite for Electronic Applications

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Many inorganic-based oxides (IOs) nanoparticles (NPs) have been synthesized and studied for dielectric behavior for many decades. It has gained popularity due to its cost-effectiveness, low toxicity, and highly durable properties. Polymer-based materials are also easily found in nature and draw many researchers' attention towards themselves for possessing good dielectric properties. This work aims to design and study of dielectric properties of Titanium dioxide nanoparticle embedded PMMA/Clay nanocomposite for electronic applications by sol-gel method. Important characterization techniques like XRD, TGA, DLS, Zeta, FESEM, Raman, UV-Vis, and FTIR have been performed for designed materials to know about the properties like crystallinity, thermal stability, size, morphology, absorbance, and chemical compositions respectively. The dielectric behavior of Titanium dioxide nanoparticle embedded PMMA/Clay nanocomposite is studied at different ranges of frequency from 10^2 Hz to 4×10^6 Hz and at room temperature. The availability of permanent dipoles, interfacial polarization, and atomic arrangements have enhanced the dielectric behavior of the nanocomposites. The prepared nanocomposite showed good dielectric behavior which provides an interesting morphology and can be applied for charge storage uses.

Keywords: Charge; Inorganic; NPs; Storage



PP-38

Layer Thickness Dependant HER activity of MoS₂ Nanostructures

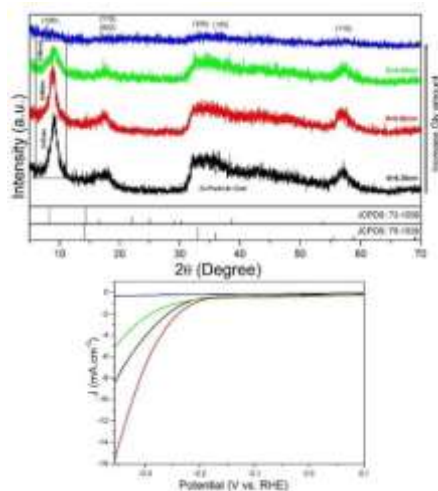
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Hydrogen is emerging as an alternative green fuel due to its highest gravimetric energy density and zero-pollutant emission to replace traditional fossil fuels and reduce environmental issues. Molybdenum disulfide (MoS₂) shows efficient HER performance comparable to that of Pt for its unique layered structure and electronic property. The edge site ‘S’ atoms in MoS₂ are found to be the catalytic active sites, on the other hand, basal plane ‘S’ atoms are inert. Herein, we report the preparation of MoS₂ nanostructures by the solvothermal method in which the solvents such as Glycerol, DMF, and water are taken in different proportions. The X-ray diffraction (XRD) studies revealed that interlayer spacing shifts to higher values with a gradual increase in Glycerol or DMF amount. The morphological analysis of the samples by Scanning Electron Microscope (SEM) shows both layered and particle nanostructures. The Energy Dispersive X-ray spectroscopy (EDX) analysis shows the presence of both Mo and S in the atomic ratio of 1:2. The catalytic activity of the samples towards Hydrogen evolution reaction (HER) was analyzed by a rotating disc electrode method in 0.5M H₂SO₄ solution. The activity of the samples was monitored in terms of onset potential and potential at

10mA/cm⁻² current density. It has been observed that an optimum layer spacing is suitable for efficient HER activity. It has also been revealed that the concentration S precursor plays a vital role in the growth of nanostructures and their HER activity.



Keywords: Hydrogen Evolution Reaction; Molybdenum disulfide; onset potential.

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PP-39

Synthesis and study of sensing behavior of 4-hydroxy-naphthaldehyde derivative of rhodamine b hydrazone for detection of mercury (ii) ions.

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The current work focuses on the synthesis of novel rhodamine B hydrazone-based 4-hydroxynaphthaldehyde Schiff base. Rhodamine b hydrazone derivatives are originally nonfluorescent in nature but once they bind with an appropriate analyte they show a strong fluorescence. This property has been investigated by using various ions such as Fe³⁺, Co²⁺, Ni²⁺, Cd²⁺, Pb²⁺, Zn²⁺, Cr³⁺, Cu²⁺, Ag⁺, Hg²⁺ Ca²⁺ and Mg²⁺. Out of all these ions used for the study of fluorescence behavior, it was found that Hg²⁺ responded positively and showed a strong absorption at 565nm. The synthesized Schiff base has

been characterized by using UV-Vis, FT-IR, and NMR spectroscopy. This ligand can be used to detect mercury in the water system.

PP-40

Multifunctional bio-based photothermal hydrogel for highly efficient seawater desalination and contaminant adsorption

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A vertically aligned porous photothermal PVA-psyllium husk hybrid hydrogel (PHH) has been prepared by introducing naturally abundant biomass psyllium husk (PH), along with nitrogen-doped carbon quantum dots-iron oxide hybrid nanocomposite (NCQD@Fe₃O₄) into polyvinyl alcohol hydrogel. Using PHH, an evaporation rate of 2.6 kg m⁻² h⁻¹ and ≈ 92% solar-to-vapor conversion efficiency have been achieved under 1 sun. After 10 cycling tests, PHH shows an evaporation rate of ~ 2.5–2.6 kg m⁻² h⁻¹ under different harsh conditions (pH 3–14 and salinity up to 250 g/kg), indicating long-lasting stability. In addition to this, the PHH evaporator shows excellent salt-resistant desalination and contaminant adsorption performance in seawater. Owing to a series of merits such as cost-effectiveness (\$5.23/m²), high vapor conversion efficiency, excellent transport, and salt mitigation properties.

Keywords: NCQD@Fe₃O₄; Psyllium husk; Interfacial evaporation; Biomass; Cost-effective.

PP-41

Synthesis, photophysical studies, and sensing applications of imidazole-based receptors

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Fluorescent materials have huge applications for technological advancements in the domain of chemosensors, bioimaging, and optoelectronic devices. Thus, different types of fluorescent materials based on nanoparticles, quantum dots, inorganic materials, bioluminescence, and organic molecules

have been developed nowadays to meet scientific demands. Amongst them, organic molecule-based fluorescent materials enjoy more advantages in terms of modular synthesis, tunable optical properties, flexibility, and bio-compatibility.¹ Therefore, we have synthesized and characterized an imidazole-based smart fluorescent organic material, diphenyl imidazole benzaldehyde (DIB), and studied its photophysical properties such as solvatochromism, solvatochromism, intramolecular charge transfer (ICT) and aggregation-induced emission (AIE) behavior. Further, the receptor shows the detection of hydroxylamine (HA) in micromolar concentration with high selectivity in 5% DMSO phosphate buffer solution at pH 7.4 via a fluorescence “turn-on” signal.²

Keywords: Imidazole, fluorescence, hydroxylamine

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PP-42

Importance of tryptophan-aspartic acid residues in designing peptide-based broad-spectrum membrane fusion inhibitors

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Membrane fusion is the initial step of the viral infection which helps the enveloped viruses to enter into the host cell and transfer its genetic material. There are efforts to develop anti-viral therapies including entry inhibitors to block the fusion between virus and host cell. The development of generic inhibitors is the need of the hour to combat emerging and re-emerging viral diseases that cause severe illness and loss of lives. We have shown earlier that a coronin-1-derived tryptophan-aspartic acid-containing peptide (TTWDSGFCVAVNPKFVALICEASG) inhibits membrane fusion. However, membrane cholesterol reduces the inhibitory efficacy of the peptide by altering lipid-peptide interaction and membrane physical properties. To overcome this challenge we have introduced another set of tryptophan-aspartic acid residues in the same peptide sequence (TTWDSGFCVAVNPKFVALICDWSG) to improve its inhibitory efficacy. Our results show that the inhibitory effect of the newly designed

peptide is less perturbed by the membrane cholesterol. This result provides a novel insight into developing broad-spectrum fusion inhibitors, whose efficacy would be independent of lipid composition.

PP-43

One pot synthesis of Poly (m-aminophenol) and its adsorption potential towards the aqueous removal of cationic and anionic dyes

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The industrial sector's rapid evolution leads to the emission of a large amount of dye wastewater into the environment, which has an apparent impact on human health along with flora-fauna species. To avoid environmental pollution, it is crucial to remove the dye by purifying it. Adsorption is one of the current research techniques. The efficacy of the adsorption technique for dye uptake from wastewater is demonstrated by several research. In this research an effective adsorbent Poly(m-aminophenol) (PmAP) was synthesized by using the chemical oxidative method and was applied for adsorptive removal of both cationic (methylene blue) and anionic (congo red),(Cr(VI)) dyes and the impact of the key adsorption capacity parameters were investigated, and the primary process is thoroughly explained. The adsorption of dyes (cationic/anionic) onto PmAP was well fitted to both Langmuir and Freundlich isotherms and it follows a second-order kinetic model with maximum monolayer adsorption capacity. Mechanistically π - π stacking interaction and electrostatic interaction played a vital role in the adsorption of dyes onto the PmAP surface. The adsorbed dyes/Cr (VI) on PmAP can be easily regenerated by using 0.1 M NaOH/0.1 M HCl. Hence from an overall aspect, PmAP is an efficient and recyclable adsorbent to remove the aqueous dyes/Cr(VI) and in the treatment of contaminated water.

Keywords: Poly(m-aminophenol); Adsorption; Methylene blue; Congo red; Chromium(VI).

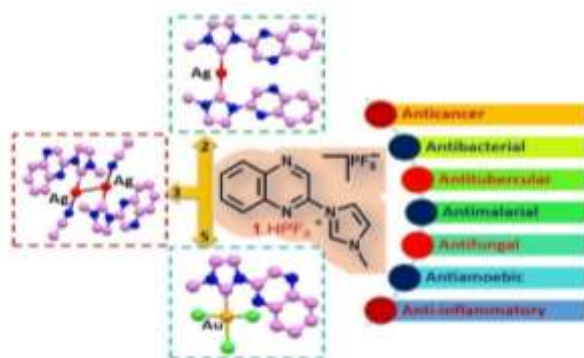
Quinoxaline-based N-heterocyclic carbene (NHC) complexes of Ag(I), Au(I), and Au(III): syntheses, structures and characterization

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N-heterocyclic carbenes (NHCs) have become universally accepted ligands in organometallic and inorganic chemistry because such ligands form strong, substitutionally inert bonds and are also electronically tunable. N-Heterocyclic carbenes (NHCs) are defined as singlet carbenes, in which the divalent carbonic center is coupled directly with at least one nitrogen atom within the heterocycle. Previous works of literature have shown the potential efficacy of metal-NHC complexes in catalysis, fluorescent materials, and biological applications. Quinoxaline derivatives not only play an important role as an organic reaction intermediate but also have a wide spectrum of biological activities. Thus, we tried to develop quinoxaline-based NHCs and their respective metal complexes by adopting a simple route of preparation. Here we present the synthetic, structural behaviors, and photophysical properties of the quinoxaline-based Ag(I)-NHC, (**2**, **3**); Au(I)-NHC, (**4**) and Au(III)-NHC (**5**). Complexes starting from proligand 1-methyl-3-(quinoxalin-2-yl)-1H-imidazol-3-ium hexafluorophosphate (**1**.HPF₆). The proligand (**1**.HPF₆) and the metal complexes have been characterized by several spectroscopic techniques. Finally, solid-state structures are determined by X-ray diffraction studies. The linear coordination geometry of Ag(I)-NHC (**2&3**) and square planer geometry of Au(III)-NHC (**5**) have been confirmed by single crystal X-ray diffraction studies.



Nickel selenide/Iron selenide for Oxygen evolution reaction

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The population escalation has resulted in energy scarcity around the globe. Our dependence on fossil fuels has resulted in numerous environmental problems and climate changes. Hence, researchers have started comprehensive research on sustainable energy production from renewable energy resources.¹ Energy production through electrochemical water splitting is one of the efficient methods to date. For this process an electrocatalyst is required which should be earth-abundant, economic, environmentally friendly, efficient, and stable.² The first-row transition metals like Ni, Fe, Co, Cu, and Mn-based materials are regarded as efficient electrocatalysts for electrocatalytic water splitting.³ In this work, we have successfully synthesized Nickel selenide/Iron selenide by facile chemical method. The structure and morphology were confirmed by various characterization techniques. The electrocatalytic activity of as-synthesized material was explored for oxygen evolution reaction. The material was further treated with hydrazine which resulted in enhanced electrocatalytic activity.

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Recycling of Polypropylene and its Effect on the Mechanical Behaviour of Injection Moulded Product

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Global demand for plastic is increasing day by day in various sectors like healthcare, automobiles, transportation, packaging, etc. However, it has been a threat to the environment as the majority of

plastic is nonbiodegradable. Recycling plastic is one of the available solutions to the aforementioned issue. However, recycling plastic affects its mechanical properties. Polypropylene (PP) is the most widely used recyclable thermoplastic polymer and hence, it is interesting to study the recyclability of PP. In the present work, injection molded PP products have been fabricated by four times recycling of PP. Mechanical properties like tensile strength, impact strength, and hardness have been determined for PP products obtained after each time of recycling. The results of the study will be discussed.

Keywords: Polypropylene; Recycling; Injection Molding; Tensile Strength; Impact Strength; Hardness

PP-47

Mxene nanomaterials and its potential use

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In recent years Nanomaterials have attracted enormous research interest owing to their unique physicochemical, optical, electrical, and mechanical properties, fascinating morphology, and structural versatility. The properties of materials at the nanoscale are distinctly different from their bulk form. The small size of nanoparticles, together with their high surface-to-volume ratio, can lead to very sensitive detection. MXene is a new and unique family of 2D Transitional metal carbides/nitrides & carbonitrides. Ever since their discovery, MXenes have received interest from scientists and academicians due to their various fascinating mechanical, magnetic, electronic, and chemical properties. MXenes are produced by exfoliation of selective MAX phases. MAX phase corresponds to the general formula



Where, n = 1,2,3

M = Early transition metal (Ti, Zr, V, Nb, Ta or Mo)

A = Group 13, 14 elements, (B, Al, Ga, C, Si)

X = Carbon or nitrogen (C or N)

In this research article, the structure of MXene and some of its properties like electrical properties, optical properties, and biocompatibility have been studied. Based on the properties there are applications of MXene in various fields such as the important use of MXene in solar panels, batteries,

sensors, etc. MXene has the potential to provide sustainable solutions to the global challenges related to protecting water, and soil, and providing cleaner air along with their use in antibacterial, bio-imaging, cancer therapy, tissue regeneration, and biosensor applications. Finally, we have discussed MXene as a promising nanomaterial for further advanced applications.

Keywords: Nanomaterials, MXene, Tunability, Metal Carbides/Nitrides.

PP-48

Waste vetiver-reinforced soy-based bio-composites as a possible replacement for non-biodegradable plastic

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The growing menace of non-biodegradable thermoplastic and our inseparable dependence on these due to their cost effectiveness and ease of use has led to a serious discussion to find alternatives to save the planet. This problem can be tackled by going back to our ancient approaches wherein we used all-natural, renewable, and very low-cost resources like grasses and leaves. The only drawback of using such grass fiber is its enhanced water absorption property and lower mechanical properties. This work engineers and characterizes composites with varying weight percentages of waste vetiver root fiber as reinforcement. The vetiver-soy composite's paramount tensile and flexural strengths were discovered to be 48.6 MPa and 50.2 MPa, respectively. Contact angle and water absorption analysis projects a minute amount yet important hydrophobic nature of the composite. Investigatory analyses such as FTIR, optical microscopy, and percentage of weight loss for post-soil burial degradation studies, suggest absolute degradation of the material. Hence, vetiver-soy composite can be crucially identified as an alternative to plastic counterparts.

Keywords: Vetiver root fiber; Soy resin; Soil burial degradation; Mechanical properties

Conversion of blended thermosetting polymer to porous carbon

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The thermosetting polymers with highly cross-linked structures make a hindrance to converting useful products and cause more pollution. The yield of major pyrolytic oil from thermosetting polymers is not significant through the pyrolysis process. The variation in thermal degradation temperature, low heat conductivity, and barriers of undesired compounds including coke, waxes, and organic acids creates a challenge for the pyrolysis of mixed plastic waste. A preferable raw material for making carbonaceous products is the thermosetting polymer. To limit the waste of both types of polymers, porous carbon can be produced from the blend of thermoplastic and thermosetting polymer utilizing physical activation, chemical activation, and the hard template approach. One of the methods listed above is Hard Template Method which uses hard templates like MgO, silica, organically modified montmorillonite, and molecular sieves like MCM-41 and SBA-15. It is a three-step process ((i) Composite production (ii) Carbonization, and (iii) Template Removal). For the production of porous carbon, some studies related to PP, PE, PS, PET, and PVC, based on the hard template method have been conducted. Further study is required to increase the yield of high surface area and porosity carbon from thermoplastic blended thermosetting polymers by the hard template method.

Keywords: Polymer; Porous carbon; Hard template method.

Water-Soluble Dioxidovanadium(V) Complexes of Aroylhydrazones: DNA/BSA Interactions, Hydrophobicity, and Cell-Selective Anticancer Potential

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Vanadium(V) complexes with aroyl hydrazones having bio-important heterocyclic moieties in the ligand backbone are very efficient for cytotoxicity studies. Another important aspect for this class of

compounds to be a good metallodrug is their solubility and stability in aqueous media which plays an important role in drug delivery to the targeted organ in its intact form. However, because of poor solubility, many well-known therapeutic drugs found to be less effective with common side effects. Therefore, incorporating such moieties for the synthesis of water-soluble complexes could be fascinating for cytotoxicity studies. Previously our group has reported the synthesis and biological study of dioxidovanadium(V)¹⁻³ systems of aroylhydrazone ligands. In continuation of that, in this presentation, we have explored the detailed study on the synthesis and biological activity of some dioxidovanadium(V), [$\{V^VO_2L^{1-2}\}A(H_2O)_n\}_\alpha$ (**1-5**), complexes with aroylhydrazone ligands having hetero cycles moiety incorporated with alkali metals as a counter cation. To study the biological behavior, complexes were tested for solution phase stability and DNA/BSA binding propensity experiments. Finally, the cytotoxicity study of **1-5** was performed against several cancer cell lines, and also for comparison a normal cell line was used.

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PP-51

Hydrothermal Synthesized Sm₂O₃ Nanoparticles as Highly Efficient Photocatalysts for Degradation of Anthraquinonic dyes

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Catalyst or template-free synthesis of Samarium Oxide (Sm₂O₃) nanoparticles were synthesized by hydrothermal method using Sm(NO₃)₃·6H₂O starting materials under basic pH conditions. The prepared sample was characterized by powder X-ray diffraction (XRD) transmission electron microscope (TEM), Fourier transforms infrared spectroscopy (FTIR), and UV–Visible diffuse reflectance spectroscopy (DRS). The powder XRD pattern confirmed the formation of cubic phase

Sm₂O₃ with a particle size of 8.46nm. The photocatalytic activity of the synthesized nanoparticles was evaluated by studying the degradation of a model dye, Alizarin red S (ARS) under visible light irradiation. The degradation of different concentrations of ARS was studied with 30 mg Sm₂O₃ and a feasible mechanism was proposed. More than 95% of ARS (50 mg/L) was degraded within 30 min.

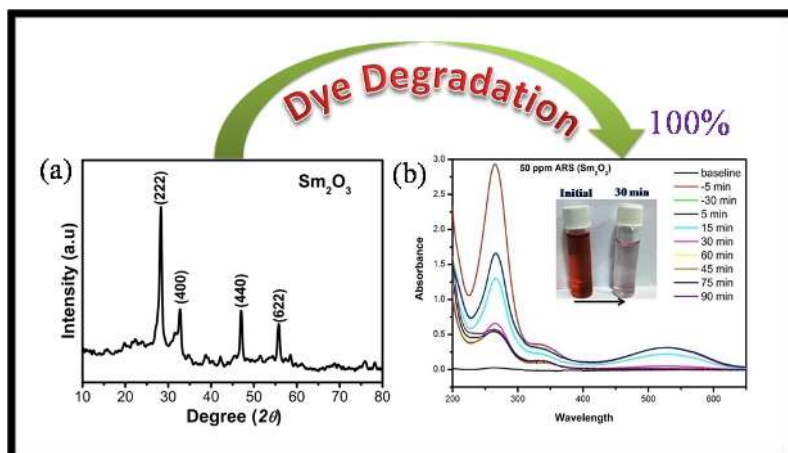


Figure 1: Sm₂O₃ as an efficient photocatalyst for degradation of ARS.

PP-52

Salophen Schiff Base Anchored with Silver Nanoparticles as Effective Sensor toward Fe²⁺ and Cu²⁺ ions

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The present work reports the synthesis and characterization of salophen Schiff base anchored with silver nanoparticles (AgNPs), and its utilization for selective detection of Fe²⁺ and Cu²⁺ metal ions in DMSO solution. Capped AgNPs were synthesized by the reduction of Ag⁺ ions with salophen Schiff base. Characterization of as-synthesized AgNPs was performed by different techniques, including UV-Visible spectroscopy, Fluorescence Spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), Transmission Electron Microscopy, Powder X-ray Diffraction (PXRD), Dynamic Light Scattering (DLS), and Zeta

Potential (ZP). In the UV–Visible absorption spectrum, the characteristic absorption band for AgNPs was observed at 408 nm. The hydrodynamic size of as-synthesized AgNPs was found to be 41.35 ± 15 nm. These AgNPs were found to be selectively interacting with Fe^{2+} and Cu^{2+} ions in DMSO solution at various concentrations. Instant color change from olive to brown as well as olive to light olive was observed while detecting Fe^{2+} and Cu^{2+} by the nano-probe, respectively. Spectroscopic investigations have been carried out to establish the sensing ability of the nano-probe.

PP-53

Influence of surfactants on the solute-solvent interactions in aqueous solutions of glycine at different temperatures

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Density (d) values of glycine have been measured at 298.15, 303.15, 308.15, and 313.15K in three different compositions (0.1, 0.2 and 0.3 wt.%) of aqueous solutions of surfactants like TX-100, cetrimide, SDS. Partial molar properties of glycine i.e. molar volume (V_m), limiting apparent molar volume (V_{ϕ}^0), apparent molar expansibility (E), and limiting apparent molar expansibility (E_{ϕ}^0) have been evaluated in these solutions from the density data. The ultrasonic velocity (U) values in these solutions have been measured at 298.15K only. Acoustical parameters such as isentropic compressibility (K_s), apparent molar compressibility, ($K_{s\phi}$), and solvation number (S) have been computed for these solutions from the values of ultrasonic velocity. The results are discussed in light of molecular interactions in the solutions. The apparent molar properties of glycine are found to be more in presence of surfactants. The higher values of apparent molar properties of glycine in the presence of surfactants indicate the presence of higher solute-solvent interaction and the solvation process takes place strongly. It has been observed that in the presence of surfactants the solute-solvent for glycine follows the order TX-100 > cetrimide > SDS. The ultrasonic velocity increases with an increase in the concentration of solute in all the surfactants which may be due to association properties. The isentropic compressibility K_s decreases as the concentration of glycine increases and also with an increase in the composition of surfactants. This may be attributed to the structure-breaking process.

Keywords: Glycine, TX-100., Cetrimide, Sodium dodecyl sulfate, ultrasonic velocity, apparent molar properties.

Reference: