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PP-54

Improved photodegradation and antimicrobial activity of hydrothermally synthesized 0.2Ce-TiO₂/RGO under visible light

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Highly water-dispersible cerium-doped titania nanoparticles deposited with reduced graphene oxide (Ce-TiO₂/RGO) have been prepared by a hydrothermal technique. The uniform deposition of Ce-TiO₂ on RGO increases the absorption of titania from ultraviolet to the visible region. From the photocurrent study, it was found that the optimum deposition of 0.2% cerium-doped titania with 10 wt% RGO significantly increases the photocurrent density under visible light. During the photocatalytic process, the generated active species can be detected by trapping reactive species in presence of different scavengers. It was observed that h⁺ and [•]O²⁻ are responsible for the photocatalytic action of the composite. The developed heterogeneous photocatalyst has more degradation efficiency for a cationic dye methylene blue, and two pesticides quinalphos and imidacloprid as compared to conventional TiO₂ catalysts under visible light.

Keywords: Ce doped TiO₂; Reduced graphene oxide; Heterojunction catalyst; Photocatalytic degradation; Antibacterial activity

3D Assembly of CoAl₂O₄ Spinel Nanosheets for High-Performance Energy Storage Application

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We demonstrate the formation of a 3D assembly of thin Co-Al spinel sheets and Carbon composite through a facile two steps process: hydrothermal synthesis of CoAl Layered double hydroxide (LDH) followed by heating of this LDH at high temperature to form CoAl₂O₄/C. This composite with a high specific surface area of 102.7 m² g⁻¹ is capable of delivering a specific capacitance of 1394 F g⁻¹ under 1 A g⁻¹ current with 87% capacitance retention after 5k cycles. The device CoAl₂O₄/C//AC exhibits a high energy density of 76.34 W h kg⁻¹ at a power density of 750.045 W kg⁻¹ with good cyclic durability of 79 %. The improved electrochemical activity may be due to the 3D assembly of thin 2D Co-Al spinel nanosheets that allows easy electron and mass transport, high surface area, synergistic interaction among different components, etc. for which Co-Al spinel/C composite will find application in energy storage.

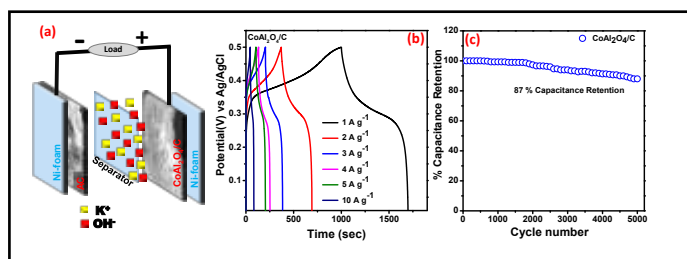


Figure 1: (a) Schematic representation of the device, (b) GCD profile, and (c) cyclic durability of CoAl₂O₄/C at 10 A g⁻¹ currents.

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Carbon-Supported Ag Nanostructures for electrocatalytic Hydrogenation of 5-(Hydroxymethyl)furfural to 2,5-Hexanedione in Acidic Conditions

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A growing interest in the electrochemical conversion of biomass-derived compounds is attributed to the extremely high sustainability of this process, which has the potential to generate value-added products and renewable electricity from biowastes. Design and synthesis of a high surface area interconnected porous network of metal nanomaterials are desirable for their application in the field of catalysis. In this work, the synthesis of carbon-supported Ag nanostructures (Ag-NSs/C) for electrocatalytic hydrogenation of 5-(hydroxymethyl)furfural (HMF) is studied. The conversion of HMF to 2,5-hexanedione (HD) via ring opening using ambient pressure and temperature is demonstrated. High faradic efficiency of 78% and selectivity of 77 % are observed for the conversion of HMF to HD on Ag-NSs/C at -1.1 V vs. Ag/AgCl in 0.5 M H₂SO₄. This direct 6-electron reduction of HMF to HD can provide a new route to produce valuable intermediates from biomass.



Figure1: Schematic representation of the electrocatalytic hydrogenation of HMF to HD

Keywords: biomass, aerogel; electrocatalytic hydrogenation; 5-(hydroxymethyl)furfural; 2,5-hexanedione; Faradic efficiency

Reference:

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Sol-gel Synthesized SrSnO₃ nanoparticles as NIR-Triggered for Triple Negative Breast Cancer Therapy

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Chemotherapy is the main systemic treatment option for rare cancer called triple-negative breast cancer (TNBC)¹. With the increase in multidisciplinary work on nanotechnology, photodynamic therapy (PDT) a new technique has been developed which is an alternative to chemotherapy. Photodynamic therapy uses nano-photocatalyst which absorb the energy of an appropriate wavelength and then the energy is transferred to the surrounding oxygen molecules to generate reactive oxygen species (ROS). This ROS helps in killing the cancer cell and tumor ablation. Here, we have synthesized nano-photocatalyst Strontium Stannate (SrSnO₃) by simple sol-gel method. The prepared catalyst was characterized by XRD, SEM, EDX, and XPS techniques². The nano photocatalyst (SrSnO₃) has been used against Triple-negative Breast Cancer (TNBC) treatment using appropriate wavelengths such as near-infrared (NIR). The results show, SrSnO₃ regulated NIR-photocatalytic generation of holes oxidizing glutathione and efficiently destroyed TNBC cells by elevated levels of intracellular ROS. Thus, the nanocatalyst-based drug-free approach offers effectiveness and biosafety of cancer therapy through drug-free therapy.

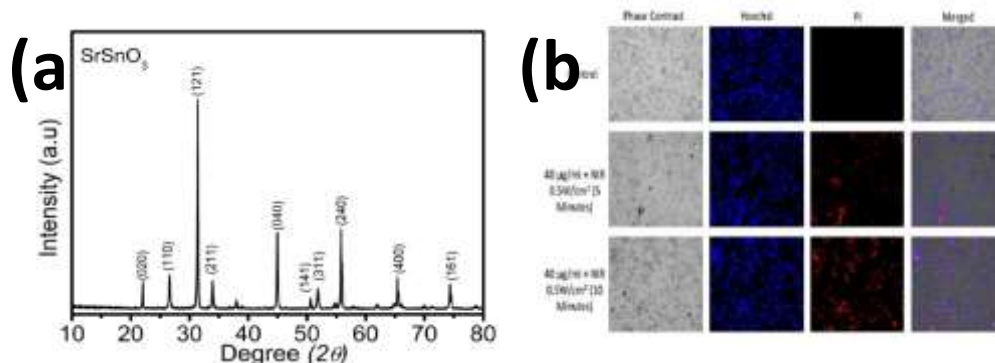


Figure1: (a) XRD graph of Synthesized SrSnO₃ and (b) Representative bright-field (Phase Contrast) and LIVE/DEAD fluorescent images of MDA403MB-231 cells

Keywords: SrSnO₃, Triple-negative Breast Cancer, photodynamic therapy, reactive oxygen species

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PP-58

Biocompatible Composite Films for Device Application

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The PVA-GO-Starch composite films were prepared via solution-casting techniques. These composite films consist of graphene oxide (GO) and conductive starch particles that have been incorporated into a PVA matrix. Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscopy (SEM) were utilized to investigate the structural characteristics and surface morphology of the PVA-GO-Starch composite films. The results of the experiments showed that the PVA-GO-starch composite films have a superior dielectric constant (≈ 92) and suppressed dielectric loss (<1.2) at 100 Hz, which is noticeably higher than that of the PVA-GO composites. The UV-VIS spectroscopy shows that the absorbance of the composite rises as the starch content increases. Furthermore, the synergistic action of GO and conductive starch particles inside the polymer matrix may enhance the electrical performances of the composites. The higher homogeneity of the starch particles in the composite system is a direct result of the uniform dispersion, which acts as an insulating barrier between surrounding conductive starch particles in the PVA matrix. The preparation of biocompatible composite films by adding starch can improve the dielectric performance, expand the applications in the area of electronic industries and enhance the research of biodegradable composite films that can be used in practical applications.

Keywords: Poly (vinyl alcohol), Graphene Oxide, Starch, Biocompatible Composite films, Dielectric properties, Device application

PP-59

Transition Metal Oxide Modified Onion-Like Carbon for Electrocatalytic Nitrogen Reduction at Ambient Condition

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Effective and simultaneous adsorption and activation of N₂ molecules on the surface of the electrocatalyst are required for electrochemical N₂ fixation. Transition metals are promising catalyst materials for NRR due to their N≡N activation capacity and π -back donation process. OLC has strong covalent bonding with a concentric hollow structure which shows nitrogen adsorption and suppresses the side effect of hydrogen evolution. To drive the N₂ reduction to NH₃, Fe₂O₃-modified OLC has been synthesized via the solvothermal method. Fe₂O₃/OLC the diffraction peaks appeared to correspond to diffraction planes of the rhombohedral structure of α -Fe₂O₃ (hematite), implying the formation of single-phase hematite.[3] The characteristic peak at 24.5° (002) of graphene was shadowed by the (012) peak of α -Fe₂O₃ at a similar diffraction angle. The modification of Fe₂O₃ nanoparticles on OLC was confirmed from the SEM image. Electrocatalytic NRR was conducted using electrode H-cell, 0.1 M Na₂SO₄ as electrolyte at ambient conditions. α -Fe₂O₃ nanoparticle modified OLC shows an ammonia yield of 18.66 $\mu\text{g h}^{-1} \text{mg}^{-1}$ at -0.1 V vs. RHE and faradic efficiency of 17% at 0 V vs. RHE in 0.1 M Na₂SO₄, which is higher than that of bare OLC. It is due to the synergistic effect of efficient iron oxide absorption at carbon porous structure.

PP-60

Recent progress in Cadmium Sulfide (CdS) based catalysts towards photocatalytic dye degradation

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Water pollution abatement is a challenging issue. The semiconductor-based photocatalysis is vastly employed for the purification of water. The Advanced Oxidation Process (AOP) is applied for the

photocatalytic degradation of dyes. This short review discusses the utilization of different CdS-based photocatalysts for the degradation of several dyes for water pollution abatement. These photocatalysts were synthesized by common methods like the hydrothermal method, solvothermal method, sol-gel method, solid-state method, ion exchange method etc. The as-synthesized catalysts were characterized by different techniques such as X-ray diffraction (XRD), Transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM), UV-visible spectroscopy, etc.

PP-61

Surface modification of Ar-plasma treated PVA-pectin crosslinked polymer thin film and its applications

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Plasma surface treatments show distinct advantages because they can modify the surface properties of inert materials with environment-friendly devices. During cold plasma treatment, on polymer surfaces, three main effects can be observed depending on the plasma treatment conditions, 1) the cleaning effect 2) the increase of micro-roughness (etching) 3) and the production of radicals to modify hydrophilic/hydrophobic surfaces. The most desirable advantage of plasma treatments is that the modifications turn out to be restricted in the uppermost layers of the substrate, thus not affecting the overall desirable bulk properties. Gas plasma treatments are set to revolutionize surface engineering technology. Much less energy is consumed than in equivalent conventional treatments and other properties, that can be improved by gas plasma treatment are adhesion, biocompatibility, resistance to wear and tear, rate and depth of dyeing, etc. Polyvinyl alcohol (PVA) is one hydrophilic, bio-friendly, water-soluble synthetic polymer and pectin is a Galacturonic-acid rich natural, non-toxic, inexpensive, amorphous, bio-compatible, bio-degradable and eco-friendly polysaccharide. The PVA-PECTIN composite solution can be electrospun from an aqueous solution to form PVA-PECTIN thin film. This composite has a strong interaction since PVA has hydrophilic nature and pectin has hydroxyl groups in its chain backbone. Additional cross-linking of PVA-PECTIN films with crosslinkers (glutaraldehyde, citric acid, TEOS, acrylic acid, etc) resulted in reinforcement of their structure. PVA, PECTIN, and their blends with different component ratios were exposed to low-temperature Ar plasma for surface modification. The physicochemical changes in the surface properties have been studied by FTIR, and contact angle measurements. The few seconds of Ar plasma treatment caused more effective surface modification such as an increase in hydrophilicity, surface roughness, and water permeability. The Ar-

plasma-treated PVA-PECTIN polymeric thin films have shown a wide range of applications, i.e. drug delivery, tissue engineering, food packaging, pharmaceuticals, nutraceuticals, biological-cell proliferation, wound healing, skin regeneration, mesenchymal stem cell attachment, textile industries, etc. Thus, plasma treatment of polymeric materials can lead to greener sustainable technology.

PP-62

Evaluation of the antiulcer activity of herbal remedies in experimental animals

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The plant is traditionally confirmed for the use of healing different disease conditions like pain, psoriasis, mouth ulcer, anemia, constipation, and diabetes. As it is good with healing properties, the present study is intended to evaluate the toxicity profile and antiulcer properties of the plant extract in experimental animals. Male and female Wistar rats were studied for acute and subchronic toxicity. Animal body weight, food intake, selected organ weights, and water consumption was among the major toxicological endpoints investigated. Different blood elements were observed like hemoglobin concentration, total leukocyte count, erythrocyte count, MCH, MCHC, and platelets. Additionally, biochemical parameters such as urea, sugar, alanine, alkaline phosphatase, total proteins, aspartate, and creatinine were also observed. Antiulcer properties of the extract were evaluated using indomethacin-induced peptic ulcer where ulcer indices were significantly decreased. For the separation and identification of compounds, TLC method was also intended in this study. A solvent fractionation process was used to obtain the fractions. The result confirmed that the *O. psittacorum* has no sign of toxicity and it is safer to use with good antiulcer properties.

PP-63

Study of extraction behavior of Li(I) using various conventional and ionic liquid extractants

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The recovery of precious metals, such as Li, Co, and Ni, from spent lithium-ion batteries (LIBs), has drawn a lot of attention due to the rising demand for environmental preservation and energy conservation. However, the majority of standard recycling techniques fall short when it comes to recycling lithium, despite being highly effective at recovering Co and Ni. The extraction of lithium is presently too inefficient to be economically or commercially viable. In this work, the effectiveness of several extractants on lithium extraction was analyzed. The various extractants engaged for the extraction of Li were TOPO, TOA, Cyanex 272, D2EHPA, Aliquat 336, [A336][Cy272], [A336][D2EHPA], and [CyphosIL 101][D2EHPA]. Experiments are performed with the variation of operating parameters such as the pH of the aqueous solution and concentration of extractants, etc. With all extractants and kerosene as the diluent, maximum lithium extraction was obtained at pH 6. About 27% and 30% of lithium were extracted using 0.1 mol/L Cyanex 272 and 0.1 mol/L TOPO respectively. Similarly, using 0.1 mol/L Aliquat 336 and 0.1 mol/L TOA as an extractant, below 20% lithium was extracted. About 53% of lithium was extracted by using the functionalized ionic liquid [Cyphos IL101][D2EHPA]. However, by adding lactic acid to the aqueous phase, 0.1 mol/L D2EHPA showed enhanced lithium extraction. When the O/A ratio was maintained at 2:1, about 70% of lithium was extracted at pH 6. Also, the extraction of lithium was studied in the presence of several alkali and alkaline-earth metals such as Na⁺, K⁺, Mg²⁺, and Ca²⁺.

PP-64

Ag/r-GO nanocomposites and Rhodamine B-based fluorescent sensor for highly selective detection of Hg²⁺ in aqueous medium

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The daily consumption of toxic mercury (Hg²⁺, Hg⁺, Hg) and its slow accumulation in living organisms from soils or water bodies cause various disorders like brain damage, kidney failure, lung problems,

and other severe diseases like acrodynia, Hunter-Russell, and minamata. The higher concentration of mercury (II) in blood vessels and the brain has also been accused for the development of Alzheimer's disease. Therefore, the maximum permissible range of mercury has been restricted to ~ 2 ppb in drinking water by the U.S. Environmental Protection Agency. Herein, we have synthesized rhodamine B-based Ag/r-GO nanocomposites for Hg²⁺ sensors, that are non-fluorescent. When these interact with Hg²⁺, rhodamine B is separated from Ag/r-GO and gives a high fluorescence emission. The surface plasmon resonance peak of the silver nanoparticle is observed at 410 nm from UV-Visible spectroscopy of nanocomposites. Transmission electron microscope (TEM) analysis of nanocomposites is carried out to find the surface morphology. The surface functionalities and structural analysis of Ag/r-GO nanocomposites are studied by Fourier transform infrared (FTIR) and X-ray diffraction (XRD) respectively. The lower limit of detection (LOD) and limit of quantification (LOQ) of the Ag/r-GO@RhB nanocomposites are found to be 1 ppb and 3 ppb respectively.

Keywords: Silver nanoparticle, Reduced Graphene Oxide, Rhodamine B, Mercury

PP-65

Synthesis, Characterization, and Environmental Application of Bio-capped Zinc Sulfide Nanoparticles

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Fascination with and the need for evermore applications of nanoparticles in numerous fields of science and technology have been the cornerstones for developing new materials and methods for their creation. Researchers across the Globe have been constantly putting their effort to find out novel materials through diverse routes. For example, metal sulphide nanoparticles are fabricated using a variety of methods which include physical, chemical, and biological means. However, the nanoparticles generated by biological methods are non-toxic, cost-effective, and benign to the environment as compared to physical and chemical methods. In the present investigation, we have produced zinc sulfide nanoparticles (ZnS NPs) by employing potent herb Mimosa pudica root extract as reducing as well as a stabilizing agent. We also varied the amount of extract to study the effect of

the stabilizing agent on the preparation of ZnS nanoparticles. The ZnS NPs have been characterized by UV-Visible, FT-IR, XRD, and Raman analysis. The UV absorption spectra confirm the formation of ZnS NPs while the biomolecules present on the surface of the nanoparticles are identified by FT-IR analysis. The XRD spectra indicate the formation of crystalline and pure cubic ZnS NPs. The Raman analysis was also carried out to study the presence of various vibrational modes that arise due to the bio-stabilized ZnS NPs. Furthermore, the bio-capped ZnS NPs have been used for the degradation of hazardous environmental contaminants and obtained excellent activity against the contaminants.

PP-66

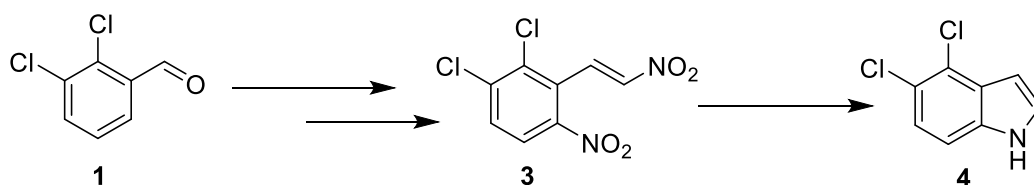
Novel, Practical, and Efficient Process for the Preparation of 4,5- Dichloroindole

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A novel, practical, and efficient three-step process for the preparation of 4,5-dichloroindole **4**, an important starting material for a wide range of fine chemicals and pharmaceuticals have been developed. The process comprises nitration of commercially available 2,3-dichlorobenzaldehyde **1**, a telescopic process for the Henry reaction, and subsequently reductive cyclization of resulting α,β -dinitrostyrene intermediate **3** into 4,5-dichloroindole **4** using iron powder in methanol and acetic acid by the Nenitzescu reaction. The large-scale applicability of this novel and the improved process have been successfully demonstrated on a multikilogram scale by carrying multiple batches to produce **5** in 67–70% yields and 96–98% purity without column chromatography. The reactions are facile, safe, and easy to scale up.



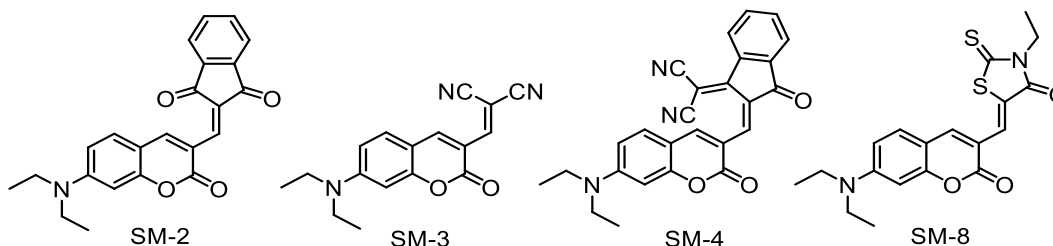
Synthesis and Characterization of functionalized Coumarin derivatives for Solar Cell Applications

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Utilizing renewable solar energy to meet the continuous demand for electricity by human civilization is a continuing research project which is driven by environmental pollution, the energy crisis, and so on. Recently organic solar cells are attracting a lot of attention due to their flexibility in molecular design and device fabrications, low cost, lightweight, and large-area applications. Currently, the power conversion efficiencies (PCE) have reached up to 19%. In this work, we have synthesized three coumarin derivatives (SM-2, SM-3, SM-4, SM-8), which were characterized by NMR, and Mass spectroscopy. The molecular orbital energy levels were determined from the electrochemical measurements. These coumarin derivatives show strong photoresponse in the visible region with higher molar extinction coefficients, sensitivity to solvent polarity, strong fluorescent properties, and tunable energy levels. The optical and electrochemical properties of these three coumarin derivatives fulfill the criteria for their use in organic solar cells.



Keywords: Power conversion efficiency; Coumarin Derivatives; Organic solar cells.

Leaching of energy-critical elements from spent lithium-ion batteries using a mineral acid

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Because of the rapid rise of lithium-ion batteries (LIBs) for portable electronic gadgets and electric vehicles, the number of used LIBs has increased. Spent LIBs contain not only hazardous heavy metals

but also poisonous compounds that endanger ecosystems and human health. As a result, considerable effort has gone into developing an efficient procedure for recycling wasted LIBs for both economic and environmental reasons. To meet the market's need for critical metals like lithium, cobalt, etc the recycling of post-consumer lithium-ion batteries has become essential. The efficient recycling of valuable metals from discharged lithium-ion batteries (LIBs) promotes resource efficiency and environmental preservation. This research work focused on the establishment of an effective process for recycling spent LIBs by leaching cathode active material from spent lithium-ion batteries using hydrochloric acid as a leachant. The process parameters like acid concentration, time, temperature, and pulp density were optimized. On increasing acid concentration, the leaching percentage of the metal ions increased. From the leach liquor, maximum recovery of 84.5% Mn and 92% Li was found using 3 mol/L HCl at room temperature, for 1 h and maintaining pulp density at 10 g/L.

Keywords: Leaching; lithium-ion battery; hydrochloric acid; manganese

PP-69

Semi-synthesis of flavor and pharmaceutical grade (-)-menthol from citronellal-rich essential oils using novel composites

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(-)-Menthol is a terpene alcohol with a strong minty odor, cooling effect, and taste. Menthol is the third most popular flavor after chocolate and orange flavor. It is produced from the *Mentha arvensis* essential oil. It is well recognized for its flavor and also finds application in pharmaceutical industries. (-)-Menthol has a long history of use as a topical analgesic. Clinical studies have proved that topical use of (-)-menthol is safe and effective in treating a variety of painful conditions, including musculoskeletal pain, injuries, neuropathic pain, and migraine. The Global demand for (-)-menthol crystal is more than 12,000 tons. Thus there is a need for a greener process for the production of (-)-menthol from low-value essential oils. Recently, our group has developed a two-step catalytic process for selective semi-synthesis of flavor grade (-)-menthol from citronellal-rich essential oils such as *Cymbopogon*

winterianus and Corymbiacitriodora by using novel bi-acidic composite. The bi-acidic Sn-B-NaYZE composite was developed to cyclize 99% of citronellal directly from the essential oils to isopulegol isomers with 99% selectivity via a liquid CO₂ medium in 45 min. Further, these isopulegol isomers were reduced to 98% of menthol using 1%Pd/AC at moderate reaction conditions such as 40 PSI H₂ pressure and 60 min reaction time in ethanol. The reaction mixture was slowly frozen to -40 °C for trouble-free isolation of the crude menthol. Further, pharmaceutical and flavor grade (-)-menthol was purified from the crude menthol through the esterification process. This isolated (-)-menthol was found to be 100% biobased on ¹⁴C radiocarbon dating to authenticate as nature-identical. This catalytic process is based on greener solvents such as liquid CO₂ and ethanol as the reaction medium. The liquid CO₂ condition is easily attained in normal cylinder pressure. The overall process is considered to be greener and economically suitable for the production of nature-identical (-)-menthol for flavor and pharmaceutical applications.

PP-70

Green Synthesis of Cubic Ag/RGO Nanocomposite for Photoreduction of Cr(VI) and Antibacterial Activity

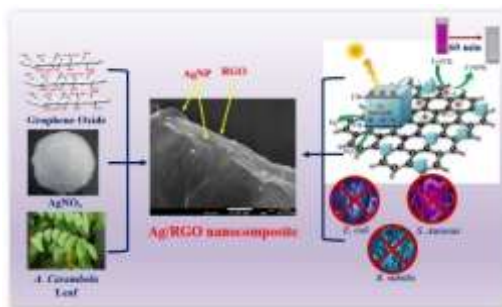
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We report a unique, environmentally friendly, and one-pot synthesis of cubic Ag nanoparticles (AgNPs) fabricated on reduced graphene oxide sheets (RGO) in presence of Averrhoacarambola leaf extract as a green reducing and stabilizing agent without using any toxic and expensive chemicals. Here, A.carambola leaf extract played a major role to reduce both Ag⁺ to Ag⁰ and GO to RGO to obtain cubic-like Ag nanoparticles over RGO sheets. The biomolecules present in the leaf extract controlled the structural, optical, and electronic properties of cubic-like Ag nanoparticles. Further, the phase purity, uniform distribution of nanoparticles and reduction of GO to RGO is well characterized through XRD/XPS, FESEM/TEM/HADDF-STEM/EDS-mapping, and Raman/FTIR analysis. Additionally, RGO sheets play a key role in successful transfer and separation of photo-excited charge carriers resulting in better catalytic activity compared to neat Ag nanoparticles. Several batch experiments were performed to investigate the photocatalytic activity of Ag/RGOnanocomposites, in comparison to both chemically and green synthesized AgNPs under visible light irradiation. Among the designed composites, 5 wt% cubic AgNPs loaded on RGO i.e. 5Ag/RGO showed superior

photocatalytic performance towards the reduction of Cr(VI) in comparison to both chemically and green synthesized AgNPs under visible light irradiation. In presence of ethanol as a hole scavenger, 5 wt% cubic AgNPs loaded on RGO showed 99.7% Cr(VI) reduction. It is observed that the presence of ethanol as a hole scavenger and pH value act an imperative role in the photocatalytic reduction of toxic Cr(VI). 5Ag/RGO photocatalyst can be reused up to 4 cycles without any remarkable loss. The observed high photocatalytic performance of 5Ag/RGO is attributed to synergetic chemistry operating between RGO and Ag components that causes effective separation and channelization of excitons to active sites. The separation efficiency is well supported by PL analysis. For all the nanocomposites along with AgNPs, the reaction kinetics was best described by the zero-order rate equation. In addition, the as-prepared nanocomposites showed remarkable antibacterial activity against various human pathogens. 5Ag/RGO exhibited the highest activity against *S. aureus* than the other two pathogens such as *Escherichia coli* and *Bacillus subtilis* as compared to GO.



Room temperature assisted eco-friendly in-situ fabrication of cubic Ag nanoparticles over RGO sheets for photoreduction of Cr (VI) under visible light irradiation and its antibacterial activity.

PP-71

Spectral Behaviour of Synthesized Azo Dyes in Micellar Medium

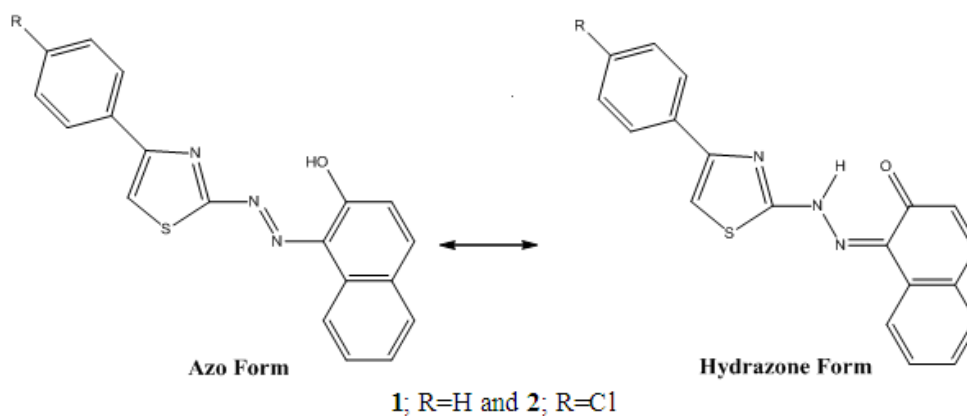
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Spectral behavior of synthesized azo dyes (**1**; 2-[β - hydroxynaphthyl azo]-4-phenylthiozle) and (**2**; 2-[β -hydroxynaphthyl azo]-4-chlorophenylthiozle) has been investigated in solvents and water-methanol mixture by UV-visible spectroscopy. Also, its behavior has been studied in anionic (sodium dodecyl sulfate; SDS), cationic (cetyl trimethylammonium bromide; CTAB), and nonionic (Triton X-100; TX-100) surfactant systems. In organic solvent, the absorption maxima (λ_{\max}) of azo dye **1** and **2** shows a

sharp band around 500 nm whereas in aqueous solution bathochromic shift (≈ 75 nm) with a broad spectrum is observed for azo dyes **1** and hypsochromic shift (≈ 40 nm) is observed for dye **2**. Similarly in surfactant solution, a broad spectrum for dye **1** was observed below CMC whereas above cmc the spectrum became sharp with the hypsochromic shift. For dye **2** the spectral behavior does not change in all the surfactant solutions. Spectral behavior of the dyes **1** and **2** have been rationalized in terms of azo-hydrazone tautomerism as well as formation of H-aggregation.



PP-72

Host-guest interaction between Ofloxacin- β -Cyclodextrin complexes in acidic and neutral pH: A fluorescence quenching study

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Ofloxacin (OFX) which is a poorly soluble fluoroquinolone drug exists in the cationic form in acidic pH and zwitterionic form in neutral pH. The behavior of host-guest interaction of Ofloxacin (OFX) with β -Cyclodextrin (β -CD) has been investigated by fluorescence quenching method in the acidic and neutral mediums using copper as a quencher at various temperatures. Using the Benesi-Hildebrand relationship, the stoichiometry of the host-guest complexation has been estimated. The incorporation of OFX inside the cavity of β -CD was revealed from fluorescence anisotropy measurement. The effect of temperature on the Stern-Volmer quenching constant (K_{SV}) and binding constant (K) has been analyzed and a suitable mechanism has been proposed for the nature of quenching. Using Vant-Hoff equation

and Gibbs-Helmholtz equation, thermodynamic parameter change of enthalpy (ΔH), entropy (ΔS), and Free Energy (ΔG) has been determined, a negative value of ΔH and positive value of ΔS validate that hydrophobic interaction between drug and quencher and negative value of ΔG suggest the complex is spontaneous in nature.

PP-73

Assessment of Ground Water Quality for Rural Areas of Paradeep-City

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The most essential material for the survival of human civilization is water. The role of water in different spheres of life is well known to us. The various role played by the water itself is also the primary cause of its pollution. The study of nature and extent of pollution of water is of great relevance owing to its significance in our survival. The scope of pollution depends primarily on the source of water like Surface or Ground. The scope is comparatively less in the case of ground source, but the threat perception is more. This is mostly due to its use for drinking purpose throughout rural India. So we are interested to study the nature and extent of water pollution around the rural areas of Paradeep city. Water pollution is related to various health hazards and has also been studied extensively. The sample collection domain is presented through a map involving different areas like Siju village of Kujanga Block, Rangiagarh village near Paradeep New Railway Station, Udayabata Village near GOA Carbon factory, and Atharabanki of Paradeep. Various parameters like pH, total hardness, temperature, total alkalinity, turbidity, TDS, DO, COD, BOD, TSS, Fluoride, Chloride, Phosphate, Sodium, Potassium, Iron, and Zinc will be analyzed. The comparisons of values of above mentioned Physico-Chemical parameters using WHO and Indian standards will give us a clear insight into the quality of its appropriate role for drinking and domestic purposes. The results of the study establish the need for suitable treatment before its use.

Synthesis and Characteristics of TiO₂ grafted Chitosan based Novel Superabsorbent Hydrogel

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Superabsorbent materials are three-dimensional network types of hydrophilic substances that have the propensity to soak up and preserve the huge capacity of water or aqueous solutions. They can intake a very high quantity of water a hundred to thousand times more extent in comparison to their original weight within a certain period without suffering any break up even after the application of some pressure. Broadly, such superabsorbent hydrogels have enormous applications in disposable diapers, female personal care products and also in the agricultural field. Due to the presence of different types of monomeric and polymeric units, these superabsorbent hydrogels can show excellent absorption behavior. Chitosan also contains different types of potential and active functional moieties like one - NH₂ group as well as primary and secondary -OH groups. Generally, these functional groups are biocompatible with various organic and inorganic compounds due to the presence of free lone pairs of electrons, which are always ready for making bonds through the electrostatic force of attraction and weak intermolecular hydrogen bonding. So here TiO₂ has been used for the modification of this chitosan by using a very simple and reasonable methodology. Finally, the synthesized superabsorbent material has been characterized for unique behaviours related to their water absorption capacity as well as swelling properties and reusability. Also, their surface characteristics have been studied by using FTIR, SEM, and XRD. From this water absorbency propensity, this synthesized biomaterial can prove its candidature as a superabsorbent hydrogel in various fields by solving various environmental-related issues.

Keywords: Chitosan, Grafting, Titanium dioxide, superabsorbent, hydrogel.

Coumarin-based fluorescent dyes for highly selective imaging of actin proteins

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Very recently, the luminophores which show aggregation-induced emission (AIE) behavior have been meticulously employed for bio-imaging applications to visualize various bio-molecules and organelles.

Imaging methods are indispensable tools to elucidate the structure and function of biomolecules in cells, tissues, and animals. Thus, many biomolecular trackers developed to track several biomolecules in both *in vitro* and *in vivo* systems. Amongst various biomolecules, actin is the major cytoskeletal protein present within the living organism. The amount of actin and its organization varies from cell to cell. Actin helps to maintain the cell shape by contributing to functions like cell adhesion, cell movement, and cell division. Further, it plays a crucial role in vesicular trafficking and also undergoes rearrangement to form highly ordered structures to perform a specific function in many sensory organs. Alteration in the actin organization leads to deformation of cells resulting in the malfunction of the organs. Thus, understanding the pattern of actin and its related cellular functions greatly relies on its visualization, which is primarily carried out by using optical fluorescence microscopy techniques. This is generally performed by fusing the fluorescent probes to different actin-binding domains (ABD). However, the cross-linking/fusion of fluorescent probes to an actin-binding domain adds further complexity to actin labeling. *This triggers the quest to develop direct actin labelling fluorescent molecules, which would eventually avoid cross-linking between the probe and actin-binding domain through complex chemical synthesis steps.* In this regard, we have designed and synthesized two coumarin-based fluorescent Schiff base molecules (**Dye-A and Dye-B**) which showed aggregation-induced emission (AIE) characteristics in DMSO/Water (Buffer) medium with bright reddish-yellow fluorescence signal around 566 nm in their emission spectrum. By taking the advantage of novel AIEE feature, we herein report a competent and convenient procedure for bioimaging application of the dye (**Dye-B**) for the target actin proteins in the gut cells and eye of a model organism *Drosophila melanogaster*. The most significant outcome of this study is that the dye binds with the actin protein without any actin-binding domain and emits red fluorescence.

Keywords: Coumarin, Fluorescence, AIE, Imaging, Actin protein.

PP-76

Fluoride ion sensing by a coumarin–fluorescein bichromophoric dyad *via* through-bond energy transfer (TBET)

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The development of synthetic receptors that can sense the presence of anionic species in micromolar concentrations through a dual mode detection comprising chromogenic as well as fluorogenic sensing

has been attracting a great deal of interest in recent years. Among the anionic species, the role of fluoride ions is unique in the field of environmental, chemical, and medical sciences. Despite many reports on fluoride sensors, there is a paucity of receptors that work on dual-mode detection of fluoride ions using chromogenic and fluorogenic sensing. In this context, we have successfully synthesized a bichromophoric dyad that represents an ideal TBET system having coumarin as the donor and fluorescein as the acceptor fluorophore. The bichromophoric dyad demonstrates the detection of fluoride ions in parts per billion (ppb) concentration level (22.8 ppb) with high selectivity *via* a TBET emission signal at 548 nm with a diagnostic bright yellow color fluorescence output. Based on UV-visible, fluorescence, ¹H NMR and DFT studies, it is shown that the fluoride ion induces the opening of the spirolactam ring of the fluorescein moiety and provides a π -conjugation link between the donor and acceptor units enabling a TBET phenomenon with a larger pseudo-Stokes shift of 172 nm.¹

Reference:

1. S. K. Padhan, V. K. Mishra, N. Murmu, S. Mishra and S. N. Sahu, RSC Adv., 2020, 10, 28422–28430.

PP-77

Exploration and investigation of various solid forms of Dichlorphenamide

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The drugs available in the market have low solubility and stability, which get expired soon. Even under certain chemical and physical conditions, it could get transformed into undesired forms. Therefore, there is a specific need to prepare stable formulations of drugs with good dissolution rates. Diclofenamide (or dichlorphenamide (DCF)) is a sulfonamide and a carbonic anhydrase inhibitor of the meta-disulfamoylbenzene class. It is used for the treatment of acute angle closure glaucoma. However, its weak solubility and slow rate of dissolution restrict its therapeutic applicability. Here we have carried out a complete solid-state screening experiment of the drug Diclofenamide, to explore various forms with useful physicochemical features. As a result, we got two new polymorphic forms (i.e., Form II and III) and one dioxane-solvated structure (DCF.dioxane) by the crystal growth under different crystallization conditions. These solid forms were characterized by Powder X-Ray Diffraction (PXRD),

Single Crystal X-ray Diffraction (SCXRD), Field Emission Scanning Electron Microscope (FE-SEM), Thermogravimetric analysis (TGA), and Differential Scanning Calorimetry (DSC). Variable-temperature PXRD (VT-PXRD) and various solvent media were used for studying the relative stability of the newly produced solid forms. Most of the forms remained stable at higher temperatures, but DCF. dioxane changed to Form III. A similar trend was also seen in various solvent environments but DCF. dioxane converted to Form II. For studying the physicochemical properties of all the solid forms, the solubility studies were done at pH1.2 and pH 6.4 media. In comparison to the parent form, in most cases, it is observed an increase in molecular salt solubility. This research implies that a better solubility of obtained DCF forms might aid in the creation of novel DCF formulations.

Keywords: Polymorphism, Solvates, Hydrogen bond, Solubility, Stability

PP-78

Recent Advancements in Applications of Nanomaterials in Civil Engineering

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This study presents a comprehensive overview of current breakthroughs in the usage of nanomaterials as a concrete performance enhancer. Nanomaterials have recently attracted a lot of interest in improving the mechanical and durability properties of concrete. Nano-silica (nano-SiO₂), nano-alumina (nano-Al₂O₃), nano-ferric oxide (nano-Fe₂O₃), nano-titanium oxide (nano-TiO₂), carbon nanotubes (CNTs), graphene and graphene oxide are examples of such nanomaterials. These nanoparticles can be combined with other reinforcement elements such as steel fibers, glass, rice husk powder, and fly ash to produce cement. It has been observed that the incorporation of such nanomaterials promoted geopolymerization, densifying the microstructure and thus improving the mechanical properties of cement-based materials, such as compressive, tensile, and flexural strength, as well as their water absorption and workability. Furthermore, nanomaterial as a filler agent also aided in the reduction of microholes. The nanoparticles could reduce the porosity of the cement, resulting in a denser interfacial

transition zone. Thus, nanoparticles in cement can be used to build high-strength concrete buildings with longer endurance, reducing the need for maintenance or early replacement. In addition, the integration of nano-TiO₂ and CNTs in cementitious matrices can render self-cleaning and self-sensing characteristics to concrete structures. Nanomaterials offer a tremendous deal of promise for use in smart infrastructure built atop high-strength concrete structures.

Keywords: Nanomaterial; Strength; Durability; Smart infrastructure; Building materials

PP-79

Investigation of thermal and antibacterial properties of Polypropylene and cerium oxide-based nanocomposites

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A study was conducted to evaluate the influence of cerium oxide nanoparticles on the thermal and antibacterial properties of Polypropylene based nanocomposites. Polypropylene/nanoceria nanocomposites with a varied amount of nanoceria ranging from 0 to 3 % were prepared by the solution casting method. The morphological characteristics of the nanoceria were investigated with the help of Scanning electron microscopy and the properties and characteristics of nanoceria and PP nanocomposites were investigated using FTIR spectrophotometry, and thermogravimetry. The TG analysis revealed that the thermal stability of the PP was increased with the addition of nano cerium oxide with increasing the percentage composition. The prepared nanocomposites were also tested for antibacterial activity. For the antibacterial activity test, the gram-positive test was conducted by Staphylococcus aureus and a gram-negative test was performed using the bacteria E. coli. The results showed that the incorporation of a small amount of nanoceria had a significant impact on the final properties of the nanocomposites.

Keywords: Nanoceria, Polypropylene, Nanocomposites, Thermal properties, antibacterial activity

Anticorrosion behavior of nano SiC embedded polyaniline (PANI) nanohybrids on mild steel

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Polyaniline (PANI) is one of the most important conducting polymers which has been studied extensively as sensors, transparent conductors, ESD and EMI protection, electrochromic displays, etc. [1]. This polymer is an important constituent in coatings and recently that it has drawn attention as an effective material for corrosion protection [2]. Herein, nano SiC embedded polyaniline (PANI/SiC) nanohybrids were fabricated through chemical oxidative polymerization of aniline in presence of suspended SiC nanoparticles. The chemical interaction between polyaniline and nano SiC was studied by Fourier transform infrared (FTIR) spectroscopy. An X-ray diffraction (XRD) study was done in order to investigate the structural behavior of polyaniline/SiC nanohybrids. The surface morphology of the fabricated nanohybrid was studied by scanning electron microscope (SEM). The elemental composition of nanocomposites was investigated by energy dispersive spectra. Potentiodynamic polarization measurement of PANI/SiC coated steel showed a large shift in corrosion potential to the anodic region concerning pure PANI. The corrosion inhibition efficiency (IE%) of PANI/SiC coating on mild steel in 3.5 wt% of NaCl, 1 M HCl, and 1 M H₂SO₄ are calculated from the respective Tafel plots, and the calculated all values were above 90 %. The higher IE% of the synthesized nanohybrids indicated the superior anti-corrosion performance on mild steel due to the synergistic effect between PANI and SiC nanoparticles. The enhanced efficiency was attributed to an insulating interfacial layer formed by PANI/SiC coating on mild steel.

Keywords: Nanohybrids, Scanning electron microscope (SEM), Potentiodynamic polarization study.

Reference:

1. Huang, J.; Virji, S.; Weiller, B. H.; Kaner, R. B. Polyaniline nanofibers: facile synthesis and chemical sensors. *J. Am. Chem. Soc.*, **2003**, *125*, 314-315.
2. Yao, B.; Wang, G.; Ye, J.; Li, X. Corrosion Inhibition of Carbon Steel by Polyaniline Nanofibers. *Mater. Lett.* **2008**, *62*, 1775–1778.

PP-81

Physicochemical Properties of Phosphate-Doped Ferrihydrite Mineral: Implications in Understanding Ferritin Iron Core and Bacterial Growth

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Iron, a crucial element, is inextricably intertwined in various stages of living and non-living systems. Its existence in two different oxidation states ($\text{Fe}^{2+}/\text{Fe}^{3+}$) is not only a virtue (involvement in electron transfer) but also troublesome (low solubility of Fe^{3+} at neutral pH and Fenton's reaction by Fe^{2+}). As a solution to this essentiality and toxicity dilemma, nature devised a globular multimeric protein nanocage; ferritin to detoxify and store iron in soluble ferrihydrite bio-mineral form. Native ferritin bio-minerals are associated selectively with variable amounts of phosphate depending upon their source, for instance in animals Pi: Fe ~ 0.1 and in plant and bacteria Pi: Fe $\sim 0.5 - 1.0$, which possibly contributes to their physicochemical properties. Similarly, in nature among various impurities, phosphate adsorption on ferrihydrite is verily observed. Therefore, a comparison of bare and protein-encapsulated phosphate-doped iron minerals may give insights into the impact of phosphate on the structure, stability, and reactivity of iron bio-mineral. So a detailed investigation was performed on number of phosphate-doped ferrihydrite with varied ratios of Pi and Fe, which closely resembles, iron minerals found in animals, plants, and nature. The doped ferrihydrite having almost equal ratios of Pi and Fe exhibited a phase transition with minimal water of crystallization (amorphous nature of the mineral), showed the highest amount of iron release both in the reductive and non-reductive pathway, and also promoted bacterial growth. Hence, the current work justifies the association of phosphate with native ferrihydrite minerals in different proportions.

PP-82

Iodine-TBHP Mediated Efficient Synthesis of α -Ketoamides from Vinyl Azides and Amines under Mild Condition

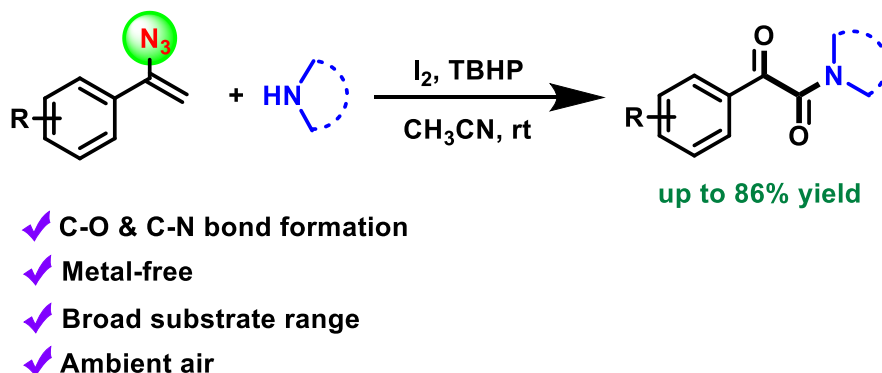
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A convenient and practical synthetic approach for α -ketoamides has been developed under mild conditions. The facile synthesis of α -ketoamides has been accomplished using aryl vinyl azides and secondary amines at room temperature. The inexpensive and readily available iodine and TBHP easily promoted the oxidative amidation process to afford diketoamide derivatives in high yields. This method

involves the synthesis of ketoamide compounds via sequential C–O and C–N bond formation. Moreover, metal-free and aerobic conditions and wide substrate scope are the notable advantages of this protocol.



PP-83

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

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A polyamine-mediated bioinspired strategy to assemble polyoxometalate (POM) (phosphotungstic acid (PTA)/phosphomolybdic acid (PMA)) nanoclusters and glucose oxidase (GOx) generating microsphere structures under very mild reaction conditions are demonstrated. The non-covalent interactions between multivalent anions (citrate ions) and polyamine chains (poly(allylamine hydrochloride), PAH) are keys to the assembly process, which results in positively charged coacervates allowing the assembly of GOx and POM nanoclusters into microsphere structures. As observed in the process, in addition, to having an impact on the size, composition, and textural properties of the spheres, the pH of the reaction medium has a pivotal role in safeguarding the enzyme. The enzyme assay shows that the activity of GOx is totally preserved during the assembly process and the enzyme loading is slightly improved with the increase in the pH of the medium. In contrast, a physical mixture of GOx and POM leads to the inactivation of the enzyme retaining only ~50% GOx activity. The peroxidase-like activity of PTA nanoclusters assembled in enzyme-enzyme microspheres as indicated by maximal velocity (V_{max}) and catalytic constant (K_{cat}) values is improved by 3-5 folds with the increase in the pH, which in turn is attributed to the smaller size of the microspheres facilitating a better diffusion of reactants, intermediates, and products. Importantly, the confinement and proximity of GOx and POM in the

microspheres not only play crucial roles in defining the peroxidase-like activity of POM but also endow high selectivity (by GOx) in detecting glucose at physiological pH conditions. Thus the microsphere assembly while enabling an effective heterogenization of the POM as a nanozyme, simultaneously addresses the issues related to the high cost and instability associated with natural peroxidases.

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

PP-84

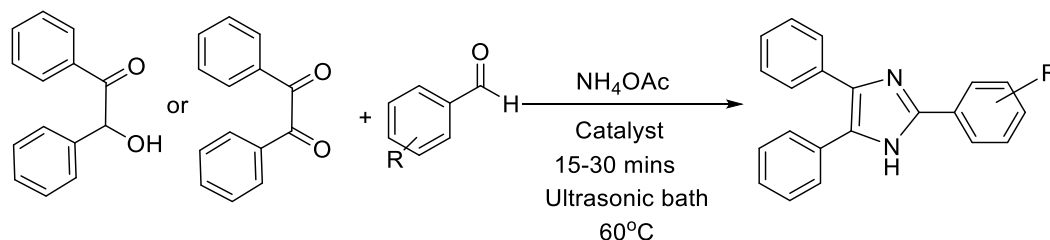
Synthesis of Imidazole derivatives via ultrasonically accelerated organic synthetic methods

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Imidazoles are an essential structural motif in a variety of compounds that are frequently employed in the fields of materials, biochemistry, pharmacology, and medicine. The first imidazole synthesis was reported in 1858. Several synthetic methods of imidazole and its derivatives have been depicted in literature. However, the primary goal of the current effort is to adopt a green method to create the imidazole derivatives using diketone and hydroxyl ketone as precursors. Ultrasonically accelerated organic synthesis has received significant attention in recent years. The ultrasound-assisted preparation of 2, 4, 5-triphenyl substituted Imidazole derivatives are described successfully using GO-NiFe₂O₄ as a magnetic catalyst. Synthesis of imidazole derivatives with excellent yields in short times, a wide range of products under ultrasound irradiation, environmental benignity, and a simple work-up procedure are some of the important features of this protocol. Thus the present work represents the synthesis of imidazole derivatives following ultrasonically accelerated organic synthetic methods with magnetic catalysts. The synthesized molecule has been characterized using IR and NMR spectroscopy. Further confirmation of the molecule using Mass data and Single-crystal XRD is under progress.



Keywords: 2, 4, 5 – triphenyl substituted imidazole, ultrasonic, magnetic catalyst, green method

Synergistic effect of Copyrolysis of Non-Edible Seed Biomass and Waste Plastics

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In the present study, copyrolysis of Tamanu seed (*Calophylluminophyllum*) and waste saline bottles (PP) were carried out in a semi-batch reactor at different temperatures ranging from 400 °C to 550 °C at 25 °C temperature intervals in an inert atmosphere. The objective was to improve the yield and quality of co-pyrolytic oil. For that purpose, waste polypropylene (PP) was mixed with the seeds in 1:1 proportion and pyrolyzed. The copyrolysis results showed that the optimum oil yield of 74.635 wt% was obtained at 475°C while lower temperatures (400 °C) produced more char yields of 29.32 wt%. Thermogravimetric analysis (TGA) revealed that the blending of biomass in PP decreases the thermal degradation temperature of the PP. In addition, a synergetic effect was observed due to the blending of biomass with waste plastics. Fuel properties showed that the oil obtained at optimum temperature has the gross calorific value, specific gravity, and kinematic viscosity of 39.76 MJ/kg, 0.834 g/cm³ and 8.5 cSt respectively. FTIR analysis revealed that the oil contained different kinds of functional groups like alkanes, alkenes, ketones, carboxylic acids, and amides.

Keywords: Copyrolysis; biomass; waste plastics; pyrolytic oil.

Synthesis, Characterization, and Applications of Triazole-based resorcin[4]arene cavitands

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Calix resorcin[4]arene cavitands have been recognized as a highly versatile class of compounds since their first appearance in chemistry around thirty years ago. These cavitands have a bowl-shaped aromatic cavity of molecular dimensions, which can be decorated at the upper and lower rims with a

variety of functional groups, heterocyclic systems, etc. They are efficient molecular receptors for host-guest interaction, pH sensing, chemical sensing, catalysis, and molecular recognition as well as tunable building blocks in the formation of covalent and metallo-supramolecular cages. Literature study reveals that 1,2,3-Triazole derivatives are an important class of five-membered N-heterocyclic compounds known for their potential biological activities. These compounds reportedly exert anti-inflammatory, anticancer, antiparasitic, antimicrobial, antioxidant, antiviral, anti-Alzheimer, and enzyme inhibitory effects, antiplatelet, and antipsychotic. Triazole molecules possess active nitrogen atoms and can go for versatile applications. Thus in the current research work tetra-triazole, dodecameric-triazole-based resorcin[4]arene cavitands have been synthesized using copper(I)-catalyzed [1,3]-dipolar cycloaddition reaction. All the synthesized molecules were characterized by using their FT-IR, ¹H NMR, ¹³C NMR, ESI-MS or MALDI-TOF-MS and wherever possible single-crystal XRD data. The newly synthesized triazole-based resorcin[4]arene cavitands have been subjected for their docking analysis with the DHFR protein of *S. aureus* to evaluate their antibacterial property and furnished excellent results.

Keywords: Calix resorcin[4]arene, Cavitand, Triazoles

PP-87

Synthesis and photophysical studies of imidazole-based donor-acceptor molecules

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In recent years fluorescent imidazole derivatives have got a greater interest among the scientific communities due to their extensive potential applications ranging from pharmaceuticals to optoelectronics. However, the synthetic methodologies capable of producing novel nonsymmetric heterocyclicimidazole derivatives are still scarce.¹ Thus, it becomes a very essential task for the synthesis of such kind of fluorescent imidazole derivatives which have abilities to exhibit dramatic photophysical properties such as; excited state intramolecular proton transfer (ESIPT), intramolecular charge transfer (ICT), aggregation-induced emission enhancement (AIEE), chemosensing and imaging behaviors. In this context, we have synthesized a series of imidazole derivatives that showed unique fluorescent behaviors. It was observed that by adding more phenyl and electron donating group (EDG) i.e. methyl group, to a simple imidazole framework significantly enhances the fluorescence properties

of the molecules by transforming them from a solid non-fluorescent molecule to a brightly fluorescent molecule.

Keywords: Imidazole, Fluorescence, Aggregation

Reference:

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PP-88

Recovery of Sc(III) from Red Mud using different methods: A review

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Scandium is the first of the transition element and occupies an intermediate position between the typical rare-earth elements and the light metallic elements. Its natural abundance in the earth's crust is 130 to 240 µg/g (0.0026 wt%). Scandium recovery from its minerals like thortveitite and sterrettite is uneconomical but ores with Scandium in the range of 0.0002%-0.0005% are considered resources. Scandium can be recovered extensively from secondary sources like uranous deposits, bauxite (red mud), and tailing samples as it exists as isomorphous admixtures. It is called a critical commodity owing to its growing demand, significant technological potential, and complicated purification processes. Red mud contains up to 1700 mg/kg of rare-earth elements (including 120 g/t Sc). Sc recovery from red mud can occur via various pyrometallurgical and hydrometallurgical processes. Pyrometallurgical processes are used to efficiently remove iron from Sc owing to their same physio-chemical properties. Hydrometallurgical processes involve recovery of Sc via leaching, solvent extraction, precipitation, and ion-exchange methods. Selective leaching of Sc from red mud was achieved through neutralization precipitation followed by using dilute mineral inorganic acids. Selective separation of Sc from red mud was also attained using organic acids as leaching agents and ionic liquids as extractants. Further acidic organophosphorus extractants like D2EHPA, HDEHP, and P204 are used for the extraction of Sc from the leach liquors. Ion-exchange adsorption using ion-exchange resins and chelating resins are also used for selective recovery of Sc from red mud leachate. Our emphasis should be on separating Sc from red mud in a sustainable approach through a hydrometallurgical route.

Novel salts of the antiemetic drug domperidone: Synthesis, characterization and physicochemical property investigation

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The solubility and dissolution rate of a drug are important factors in determining its effectiveness and potency. Crystal engineering is a technique for increasing an API's solubility and boosting its physicochemical characteristics. Due to rising R&D costs, the failures of certain popular drug candidates with low aqueous solubility, and the unavailability of newer compounds due to patent limits, the pharmaceutical industry is experiencing a growing crisis in the process of product development. The use of cocrystals, salts, and solvates to increase an API's solubility, dissolution profile, bioavailability, and other physicochemical characteristics is becoming more popular.

Domperidone (DOM) (6-chloro-3-[1-[3-(2-oxo-3H-benzimidazole-1-yl) propyl] piperidin-4-yl]-1H-benzimidazole-2-one) is an antiemetic, galactagogue and gastrokinetic that works by blocking the dopamine receptor D2. Domperidone binds to D2R expressed by peripheral neurons after treatment, inhibiting dopamine binding and D2R-mediated signaling. This antagonist is also used to relieve nausea and vomiting produced by Parkinson's disease medications. DOM comes in a biopharmaceutical classification system (BCS) class II, which implies the drug possesses very low solubility (0.0925 mg/ml). Such poor solubility ultimately leads to low bioavailability in the living being. DOM dosages (30-40mg/d) prescribed are much higher due to its difficulty to cross the blood-brain barrier. In several studies, it is observed that in high-risk patients, DOM has been shown to increase the risk of sudden cardiac death. DOM, in particular, may raise the risk of ventricular arrhythmia and sudden death by causing QT prolongation. Hence, there is a need for a better method for improving DOM solubility, which can overcome not only the issue of bioavailability but also can fill the voids of several limitations associated with it. At 298 K, the value of its pK_a is 7.9. Therefore, following the pK_a rule, the carboxylic acids with pK_a<5 should form salts with domperidone.

A salt variant, domperidone maleate (permotil), is currently on the market, although there are possible safety issues concerning the long-term implications of frequent maleic acid intake. A certain report has presented one report, in which domperidone succinate salt displays enhanced solubility when

compared to two reference commercial products, and Sridhar recently disclosed the hydrogen bonding properties of its four new salts. Since the reported solubility of the synthetic adduct is inadequate, we set out to create novel solid forms of DOM that might improve solubility as compared to the reported structure.

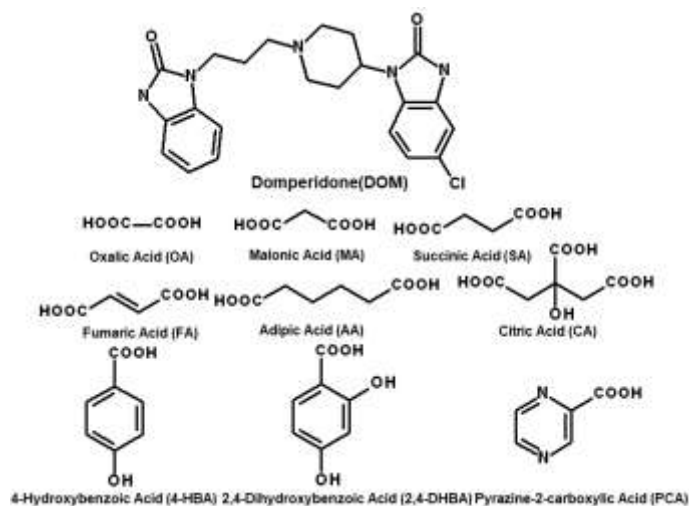


Figure 1: Representation of increase in solubility in case of Domperidone with coformer than parent drug alone.

Keywords: Domperidone, Crystal, Solubility

PP-90

PIFA-Promoted Transamidation of Carboxamides and Carboxylic Acids with Amines

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A simple and efficient method has been developed to exhibit the versatile catalytic behavior of PIFA, a hypervalent iodine for the synthesis of amides. In this method, PIFA [(bis(trifluoroacetoxy)iodo)benzene] has been used as a useful promoter for the transamidation of dimethylformamide (DMF) and dimethylformamide (DMA) with the amines. Besides, this hypervalent iodine smoothly promoted the N-formylation and N-acylation of various aromatic amines with carboxylic acids. Notably, the catalytic amount of PIFA is found to be efficient for both strategies. However, the present protocol involves a metal and solvent-free, mild, eco-friendly condition with a high yield of amide products.

Cations and pH on the quality and formation of silk: A review

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Natural silk synthesis involves systematic biochemical pathways and enzymatic reactions involving the conformation transition of the liquid silk protein to silk fiber and is induced by changes in the cationic concentration. The silk fiber formation in silkworms is induced by shearing and extensional flow from the spinning apparatus of the ducts of the silkworm. Liquid silk is stored as metastable colloidal complexes of heavy and light chain fibroins and silkworms convert it into silk fibers. In pyruvate kinase, Mn^{2+} acts as a cofactor and participates in the binding of substrates. The silk fiber has finer fiber and smaller crystallite size with significant orientations of molecules and hence has high strength. In silkworms the pH value (6.9-4.8) and cation concentration change progressively in the secretory pathways. Protonation of acidic residues, dehydration throughout the length of the gland, and evaporation lead to the dry spinning of silk fiber. In the regenerated silk fibroin, there is a change in the secondary structural transition from the random coil and/or α -helix to β -sheet with the increase in the concentration of K^+ . Ca^{2+} and Mg^{2+} ions induce network formation with the carboxylic acid group and stabilize a disordered state whereas Al^{3+} , K^+ , and Na^+ induce structural changes to a more oriented structure. Ca^{2+} increases the viscosity of silk helps the formation of a salt bridge makes proteins less sensitive to shear alignment and aggregation and provides ideal storage conditions for silk. Li^+ interacts strongly with peptide groups thereby reducing molecular interactions to the extreme, preventing aggregation and dissolving already spun silk. Fe^{3+} interacts with tyrosine and tryptophan residues within the silk, facilitates the conformation transition, and increases strength and mechanical properties. Thus, this review highlights the importance of cations in the formation and structural change in silk to help increase silk productivity.

Keywords: Metal ions, silk fiber, silkworm, pH

PP-92

An Indigenous tool for the adsorption of rare earth metal ions from the spent magnet e-waste: An eco-friendly bio-polymer nanocomposite hydrogel

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Polymer bionanocomposite hydrogel (PNC-hydrogel) has attracted the focus and attention of young and dynamic researchers in water remediation and its purification as well. The acrylic acid and acryl amide functionalized chitosan effectively enhance the usability capacity thousand times in comparison to the virgin biopolymer. The functionalization of the biopolymer is proficient enough for binding the rare earth ions from the wastewater solution and it is done by grafting of biopolymer with a variety of copolymers. Herein, SiO₂nanopowder embedded bionanocomposite hydrogel (SCB-hydrogel) has been prepared. The impact of various parameters such as pH, adsorbate doses, time of contact, the concentration of metallic ions, kinetic parameters with proper isotherms, desorptivity, and reusability of the PNC was studied in batch adsorption mode. The adsorption efficiency by the PNC-hydrogel with increasing concentration of lanthanide ions was observed to be 99% from the waste-diluted water followed by the Langmuir model along with Pseudo second-order kinetics. The adsorption efficiency of these PNCs didn't alter much as with the original in reusability of a maximum of three times. So the PNCs can be effectively used as a novel bio-adsorbent for treatment of wastewater-containing pollutants along with transition rare earth (Nd⁺³, Pr⁺³).

Keywords: Polymer nanocomposite, chitosan, rare earth, adsorption. wastewater, desorption

PP-93

Synthesis of Novel Bio-Based Nanophotocatalysts for Application towards Degradation of Organic/ Inorganic Water Pollutants

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The growth of population, science, technology, and heavy industrialization boosts environmental pollution as one of the most important issues in the past half-century. One of the major environmental

problems is water pollution by different organic and inorganic pollutants has become a challenge for life on earth because of anthropogenic activities. In recent years industrial waste effluents such as phenol, phenolic derivatives, and hexavalent chromium are creating a major problem for aquatic life, human being, and the environment. In this concern, nanometals and their composites have gained profound attention in photocatalytic degradation or removal of toxic pollutants from water due to their chemical reactivity, higher surface area, regeneration efficiency, ample adsorption sites, intriguing catalytic activity, and cost-effectiveness. Synthesis of these nanocomposite photocatalysts through a green approach using plant biomolecules is reported to be the most effective way to synthesize stable nanomaterials, due to the polar-protic-polyphenolic-phytoconstituents present in plant biomass acting as reducing, capping as well as stabilizing agents. Here, we have synthesized different bio-based nanocomposites such as bio-functionalized Fe₃O₄, Au/C₃N₄, and Ag/RGO nano photocatalysts through green routes for the degradation of toxic pollutants like Cr(VI), various phenolic compounds, etc under visible light irradiation. The polar biomolecules of leaf extract of *Averrhoa carambola* were used as natural surfactants in the synthesis of these photocatalysts, which is rich in reducing sugar, proteins, lipids, amino acids, and flavonoids which prevent aggregation of the nanoparticles by increasing the repulsion force between them and stabilize them. The as-synthesized nanocomposites are photoactive, stable, cost-effective, highly reusable, and environmentally friendly.

Keywords: Green synthesis, Polar plant biomolecules, Nanocomposites, Photocatalysis, Water pollutants.

PP-94

Augmentation in the photocatalytic activity of quaternary TiO₂-ZnS-CdS-rGO nanocomposites by the incorporation of novel metal

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An innovative TiO₂-ZnS-CdS-RGO hybrid composite has been synthesized via sol-gel-assisted hydrothermal and solvothermal methods. The addition of Au nanoparticles improves the final composite with the advantages of heterostructure semiconductor/semiconductor junction benefiting the

hole transfer and noble metal as well as graphene favorable for electron transportation. Moreover, the addition of Au nanoparticles helps the composite to achieve absorbance in the visible region. XRD's data confirm the anatase phase of Titania (TiO₂). UV-DRS reports show the absorbance wavelength around 530-550 nm. The composites show an improved photocatalytic degradation of MB (Methylene Blue) under exposure to visible light is reported.

PP-95

Evaluation of ion-solvent interactions of tetracycline hydrochloride in mixed solvents at different temperatures

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Density, ρ , and ultrasonic velocity of solutions of amino acids L-Histidine, L-Valine, and L-Serine in water and aqueous solutions of antibiotic drug tetracyclines hydrochloride (TCH) have been measured at five different temperatures, $T = (293.15 - 313.15)$ K and experimental pressure $P = 101.3$ kPa. The experimentally obtained density and ultrasonic speed values were used to calculate apparent molar isentropic compressibility, [partial molar compressibility, $\overline{K_{s,\phi}^0}$, intermolecular free length, L_f and hydration number, The results obtained from the above properties were used to determine the intermolecular interactions that exist in the said solutions.

Keywords: Ultrasonic velocity, intermolecular interactions; thermoacoustic properties, amino acids, intermolecular free length, tetracyclines hydrochloride.

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PP-96

Synthesis and characterization of Co-Ni-Cu ternary oxides nanoflakes by electrochemical technique.

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An electrochemical technique has been employed to synthesize a cobalt–nickel-copper mixed ternary oxide, via a two-step route involving electrochemical precipitation followed by calcination. A diaphragm cell was used for the electrochemical precipitation /deposition of the ternary metal hydroxide at room temperature from the nitrate bath of the respective metal salts at pH ~ 4. The tertiary metal hydroxides were calcined at 300°C for 2 hours to obtain the respective ternary oxides. The synthesized tertiary metal hydroxides and tertiary metal oxides were characterized by XRD, FTIR, UV-Vis-DRS, STA, and SEM-EDS techniques. The formation phase and crystallinity of synthesized nanoparticles were studied by XRD. The SEM results reveal the formation of nano-flakes that are formed by the combination of rod-shaped nanomaterials. These ternary oxides are quantum dots and exhibit chemoluminescence behavior. The band gap of the prepared Co-Ni-Cu hydroxides and Co-Ni-Cu oxides are found as 2.35eV and 5.12eV respectively, using a UV-Vis-DRS study.

PP-97

Preparation of Biobased Polymer nanocomposite and its study of Gas Permeability.

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Novel biobased polymer nano-composite is attracting increased attention due to their common qualities of being firm, hard, or unable to bend and not easily broken, torn, etc. These properties have been universally adopted in the field of the biomedical, food packaging industry, pharmacology, transportation construction, electronics, and consumer products. Biobased polymer nanocomposites demonstrate an adjustment in composition and structure over a nanomaterial length scale and have been shown over the last few years to provide rare properties increased relative to non-traditional composites. Organically reformed ZnO can be capable of producing reinforcing agents used especially in compounding rubber to improve the physical properties (such as resilience, toughness, and tensile strength). Commercial ZnO nanoparticles were modified by polyhydroxy butyrate (PHB) in an aqueous

system. The hydroxyl groups of nano-ZnO particle surface can interact with carboxyl groups (-COOH) of PHB and form poly(zinc hydroxybutyrate) complex as testified by Fourier-Transform Infrared Spectra (FT-IR). Thermogravimetric analysis (TGA) Indicated that PHB molecules were absorbed or anchored on the surface of nano-ZnO particles which facilitated to hinder the aggregation of nano-ZnO particles. It was found that PHB enhanced the dispersibility of nano-ZnO particles in water. The dispersion Stabilization of modified ZnO nanoparticles in an aqueous system was significantly improved due to the introduction of polymer on the surface of nanoparticles. The modification did partially alter the crystalline structure of the ZnO nanoparticles according to the X-ray diffraction patterns. The enhancement of electrical properties due to the incorporation of ZnO nanoparticles in PHB was observed by The gas permeability of the nanocomposite sample incorporations measured by “gas permeameter”. A considerable amount reduction in gas permeability was observed by measuring ZnO loading and through sonication (The act of applying sound energy to agitate particles in a sample). These disruptions are used for mixing the solution to increase the speed of dissolution of a solid into a liquid and for the removal of dissolved gases from the liquids.

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The efficiency of a natural surfactant in stabilizing a crude-oil-water dispersion

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The price for crude oil is hiking consistently in the global market due to its extensive uses in both industrial and domestic sectors. Consequently, underdeveloped countries like India, which import oil from middle-east countries, are spending lots of their revenue on transportation and purification of crude oil. Since the purification procedure has already been established, the transportation section is only left behind, which needs to be standardized for the minimal expenditure protocol. The present work reports a low-viscosity crude oil-water emulsion was made using saponin from *Acacia concinna* fruits. Varying saponin concentration, crude oil content, pH of the medium, the emulsion's rheology, and stability were examined. The study examined the cost-effectiveness and efficiency of saponin extracted by physical and chemical methods. The propensity of optimal saponin concentration to stabilize was investigated within 30 to 80 percent oil volume fractions. The optimal saponin concentration for the chemical extraction technique was 0.008 g/cc to reduce the viscosity from 1200 mPa.s to 400 mPa.s.(acceptable range) the emulsion containing 80 volume fraction of oil. In contrast, the saponin from the physical extraction method required 0.017 g/cc. The variation of shear stress with the shear rate was investigated to determine the yield stress and fluidity of the emulsion. Saponin's effect on the emulsion's zeta potential before and after treatment suggested the stability mechanism. Studies suggested saponin could outperform commercial additives.

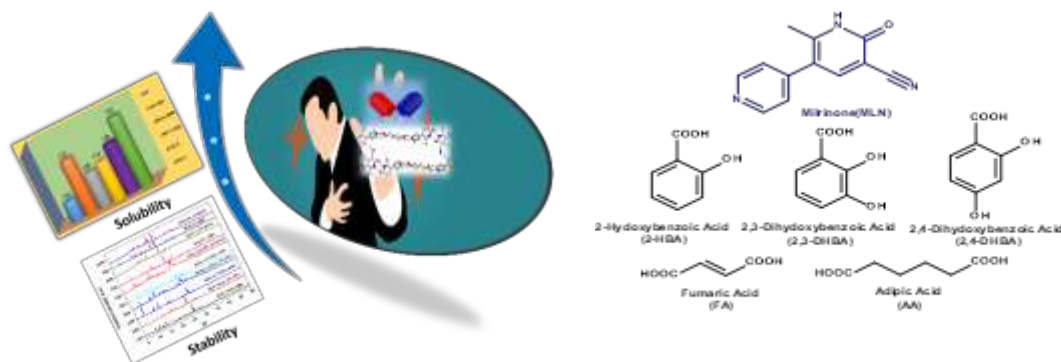
Keywords: Apparent viscosity; Crude oil; Plant-based additive; Rheological behavior; Stabilization of emulsion.

Pharmaceutical novel solid forms of Milrinone with advanced physicochemical properties

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Cardiovascular diseases have recently become the leading cause of mortality across the world. *Milrinone (MLN)*, sold under the trade name Primacor, is a medicine used to treat myocardial infarction in patients but its usage has been linked to major side effects such as it belongs to Bio-pharmaceutical Classification System class II drug of limited aqueous solubility and poor permeability. Five novel molecular solids of the cardioprotective drug MLN with generally recognized as safe co-formers were successfully made using mechanochemical and solution crystallization, including 2-hydroxybenzoic acid, 2,3-dihydroxybenzoic acid, 2,4-dihydroxybenzoic acid, fumaric acid, and adipic acid. The obtained new solid forms of the Milrinone drug molecule were characterized by Powder X-ray Diffraction and Single Crystal X-ray Diffraction, and thermal analysis was performed by Thermogravimetric Analysis and Differential Scanning Calorimetry. It was found that the molecular assemblies developed different kinds of sheet structures, those comprising Adipic acid and 2,3-DHBA-produced channel structures. All molecular adducts showed higher solubility in a milli-Q water medium, as compared to the parent medication. While the parent drug's solubility is 0.61 mg/ml, Adipic acid exhibits an increased solubility of 2.23 mg/ml.



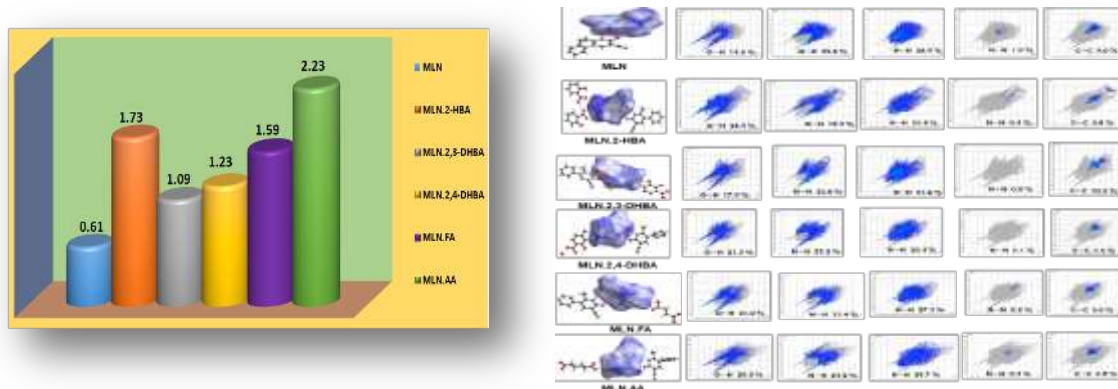


Figure 1: Representation of increase in solubility in case of Milrinone with coformer than parent drug alone.

Keywords: Milrinone, Crystal, Solubility

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PP-100

Evaluation of molecular interactions between amino acids and vitamins in an aqueous system: Acoustic Studies

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Density, ρ , and ultrasonic velocity of solutions of amino acids L-isoleucine, L-valine, and L-alanine in water and aqueous solutions of vitamins have been measured at five different temperatures, $T = (293.15 - 313.15)$ K and experimental pressure $P = 101.3$ kPa. The experimentally obtained values of ultrasonic velocity, u , and density, ρ have been used to calculate the thermoacoustic properties like isentropic compressibility (β_s), Isothermal Compressibility (β_T), Heat capacity ratio (γ), hydration number, n_H , Molar compressibility (W), Acoustic independence (Z), molar sound velocity (R), relative association (RA), intermolecular free length (L_f), relaxation time (τ), Coefficient of thermal expansion (α) and non-linearity parameters. The results obtained by these processes have been used to analyze the presence of

intermolecular interactions existing in the solutions. The effect of the concentration and temperature of the solutions on intermolecular interactions were studied at the same pressure.

Keywords: Density; Speed of sound; amino acids, vitamins, acoustic properties.

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PP-101

Bimetallic Cobalt Nickel Sulfide for Oxygen Evolution Reaction in Alkaline medium

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Hydrogen is an attractive alternative source of energy that can replace fossil fuel-based energy generation. It has high energy density and zeroes hazardous environmental impact. The production of hydrogen by water splitting is an appealing process to produce energy sustainably.¹ The earth-abundant transition metal-based electrocatalysts are economic and are being explored for efficient hydrogen generation from water electrolysis.² Herein, we have demonstrated a non-precious transition metal based bimetallic chalcogenide electrocatalyst, i.e., Cobalt Nickel sulfide by simple hydrothermal method for alkaline oxygen evolution reaction (OER). The structure and morphology were studied using several characterization techniques. The sample exhibited considerably good OER performance at a current density of 10mA cm⁻².

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PP-102

Epichlorohydrin-g-Nanopolyaniline: An efficient pH-sensitive adsorbent for the removal of dyes

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Dyes are considered potential pollutants of water because of their mutagenic, carcinogenic properties. Out of all developing methods to treat contaminated water, adsorption remains propitious method due to its advantages like low cost, eco-friendly, and reusability. Herein, the adsorbent Epichlorohydrin grafting Nanopolyaniline (PANI-g-EC) was synthesised by ring opening reaction of epichlorohydrin by using polyaniline as a nucleophile. The structural properties of the synthesized adsorbent were determined by using techniques like Scanning Electronic Microscopy (SEM), Fourier Transformation Infrared (FTIR), Thermo Gravimetric Analysis(TGA), and X-Ray Diffraction (XRD). The effect of adsorption parameters such as dosages of adsorbent, initial dye concentration, pH, and temperature on the removal of dyes was studied. Thermodynamic parameters (ΔG° , ΔH° , ΔS°) of the adsorption process were extensively studied for a potential application. The adsorption process follows pseudo-second-order reaction kinetics and Langmuir adsorption isotherm.

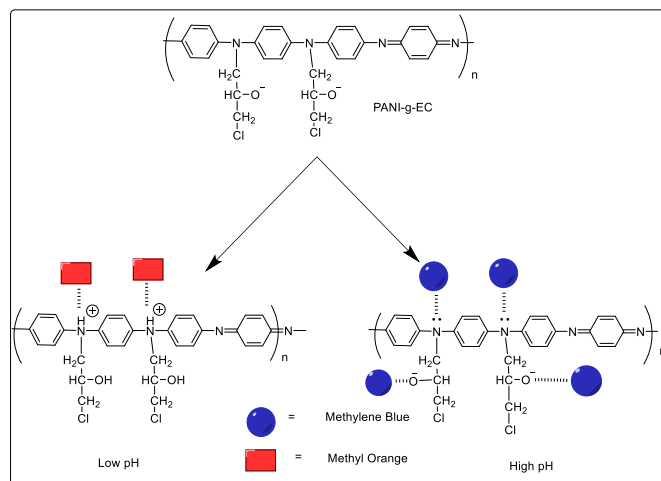


Figure 1: Removal of Methylene Blue and Methyl Orange dyes by PANI-g-EC at different pH

Photocatalytic Behaviour of Calcium Doped Lanthanum Manganite Nanocomposite towards the Degradation of Methylene Blue

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Calcium doped lanthanum manganite $\text{La}_{0.75}\text{Ca}_{0.25}\text{MnO}_3$ having Perovskite structure shows high degree of catalytic efficiency for the removal of Methylene Blue organic dye from its aqueous solution. The sample powder (LCMO) was prepared through the sol-gel technique and was characterized by X-ray diffraction (XRD), Fourier transform 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 shows 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 the required stoichiometric $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ Oxide. The Photocatalytic performance of the nanocomposite for photodegradation of Methylene Blue dye (MB) as an Organic water pollutant, was evaluated over visible light irradiation, at a pH of 4, at a constant dose for several hours. The result showed the photocatalytic efficiency $\text{La}_{0.75}\text{Ca}_{0.25}\text{MnO}_3$ nanocomposite was 69% of the initial dye concentration within 100 min illumination time. The linear increase of photodegradation rate was found in our sample as a function of the time of irradiation, which was confirmed by the study of the optical properties of the resulting aqueous solutions. These findings show convincingly that the $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ photocatalyst possesses great promise for visible light-driven photodegradation of MB dye. The percentage of degradation was calculated using mathematical laws.

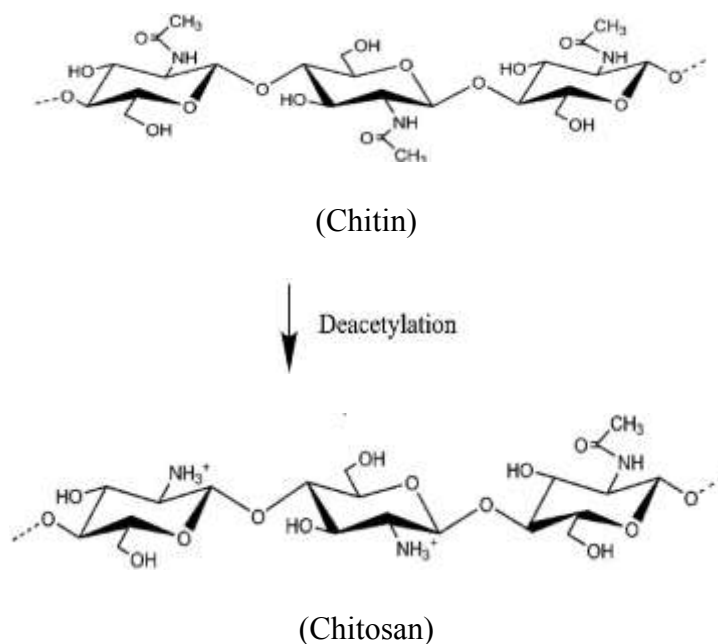
Keywords: Perovskite; Sol-Gel technique; Photocatalyst; Methylene Blue.

Fire retardancy, biodegradability and swelling behavior of porcelain based “Chitosan-g-P(MMA-co-AN)/Chicken Eggshell powder” Nano composite

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Chitosan is a versatile biopolymer and is mainly extracted due to the alkaline deacetylation of another bio-polymeric material chitin. It is a unique bio-polymeric material having excellent biodegradability and antibacterial properties. Chicken eggshell powder is a waste zero-cost biomaterial. A new composite material Chitosan-g-P(MMA-co-AN)/Chicken eggshell powder was prepared by using MMA monomer along with chitosan and nano powdered form of chicken eggshell, reinforced by porcelain and the material obtained was characterized by LOI study, FESEM, FTIR, TGA, its swelling behavior and biodegradability study was also carried out by using proper procedure. The prepared grafted composite material shows a high value of flame retardancy properties along with biodegradability and significant water swelling behavior, which is studied in different time intervals.



$$\text{Deacetylation Degree (DD)} = 16.1(Y - X) FW$$

Where Y and X are two different Inflection points, F= Molarity of base (NaOH taken) solutions, W = molecular weight of the given sample.

Keywords: Bio-Nano composite, water absorbency, fire retardancy, swelling behavior

Evaluation of Carbohydrates as capping and stabilizing agent for Green Silver Nanoparticles

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In recent times, silver nanoparticles (AgNPs) have attracted considerable attention due to their wide range of potential applications in the textile industry, biomedicine, food packaging, the cosmetic industry, clean water technology, energy generation, and information storage. The conventional methods for the synthesis of AgNPs require toxic chemicals as reducing agents and harsh reaction conditions. But, green synthesis of silver nanoparticles is considered one of the promising eco-friendly approaches due to biocompatibility and low toxicity. In the present study, we report a unique, cost-efficient, and green method for the synthesis of carbohydrate-capped silver nanoparticles (AgNPs) using *Ocimum sanctum* (tulsi) leaf extract, for the detection of mercury (II) ions in water. The carbohydrate-capped silver nanoparticles synthesized using the above method were found to be more stable than the corresponding uncapped AgNPs. The optical and structural properties of the nanoparticles were confirmed by different spectroscopic methods such as UV-Visible absorption spectroscopy, Photoluminescence study, X-ray Diffraction (XRD) study, and Scanning electron microscopy (SEM). The synthesized AgNPs were found to be selective colorimetric sensors for the detection of Hg²⁺ ions. The selective detection of mercury (II) ions by the silver nanoparticles were studied using optical absorption spectroscopy. The detection of Hg²⁺ ions was also investigated by designing an optical fiber sensor. From both absorption and optical experiments, it was observed that the limit of detection (LOD) of the sugar-capped AgNPs was superior to the uncapped ones. The sensing ability of the silver nanoparticles towards mercury (II) ions was further examined using filter paper coated with sugar-capped silver nanoparticles. The above study using sugar-capped, highly stable silver nanoparticles provides a simple, cost-effective method for the detection of mercury (II) ions in water.

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P-106

Synergistic Effect of Oxalic Acid and Hydrochloric Acid leaching of Iron from coal fly ash

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The present paper deals with the leaching and the behavior of iron in oxalic acid and hydrochloric acid solutions of coal fly ash samples collected from National Thermal Power Corporation, Angul. To characterize the samples X-ray diffraction (XRD) was used. It reveals the presence of iron. (hematite). Acid leaching techniques were used to minimize iron. This investigation was performed to know the interaction of oxalic acid with hydrochloric acid to attain better performance for iron dissolution in comparison to the absence of oxalic acid. The effect of important factors affecting the leaching, the stirring rate, and the oxalic acid to hydrochloric acid ratio was studied at room temperature i.e 26°C. It was determined that the iron dissolution rate increases with oxalic acid-hydrochloric acid concentration and stirring rate. SEM-EDX analysis confirmed the presence of iron oxides in the sample. Fly ash used in the present study contains 8.34% of iron., It was observed that the leaching of iron increases and then remains constant in Oxalic acid - HCl. From this study, it can be concluded that the optimum leaching conditions are 8 mol dm⁻³ HCl, 300 rpm stirring speed, and 50 °C temperature. At these conditions, 88.7% of the iron is removed from the solution. The iron oxide content of the fly ash was reduced to 0.96 from 8.34% after acid leaching.

PP-107

Assessing the Suitability of a Dicationic Ionic Liquid as a Stabilising Material for Storage of DNA in Aqueous Medium

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This study investigates the potential of a pyrrolidinium-based dicationic ionic liquid (DIL) in stabilizing *ct*-DNA in an aqueous solution by following DNA-DIL interaction. Additionally, to

understand the fundamental aspects of DNA-DIL interaction in a comprehensive manner, studies are also done by employing structurally similar monocationic ionic liquids (MILs). The investigations have been carried out both at ensemble-average and single molecular levels by using various spectroscopic techniques. The molecular docking study has also been performed to throw more light on our experimental observations. The combined steady-state and time-resolved fluorescence, fluorescence correlation spectroscopy (FCS) and circular dichroism (CD) measurements have demonstrated that DILs can effectively be used as a better storage media for *ct*-DNA as compared to MILs. Investigations have also shown that the extra electrostatic interaction between the cationic head group of DIL and the phosphate backbone of DNA is primarily responsible for providing better stabilization to *ct*-DNA retaining its native structure in an aqueous medium.

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PP-108

Monitoring Enzymatic Activity by Amperometry

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The Clark-type electrodes are regularly used to measure oxygen concentration in real-time, both in liquid (dissolved O₂) and gaseous (pO₂) samples, based on the amperometric principle (i.e. the current, measured at a constant voltage, is directly proportional to the concentration of the analyte). There are important metabolic/antioxidative enzymes, that either consume or generate O₂ during its catalytic cycle. For example, glucose oxidase (GOX) catalyzes the oxidation of β-D-glucose to gluconic acid, by utilizing molecular O₂ (one of the substrates) as an electron acceptor. GOX as an enzyme has a wide range of industrial uses such as in food processing, glucose sensing, and fuel cells. This work investigates the enzymatic activity of GOX by using a Clark-type electrode and determines various enzymatic parameters by employing Michaelis-Menten kinetics to the oxygen consumption data. The

kinetics parameters (K_M and k_{cat}) obtained from our amperometry-based dissolved O_2 consumption correlates well with the reported values, obtained by other techniques [1].

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PP-109

Vitamin C derivatives and anti-HIV drugs cocktails potentially effective against SARS-CoV-2: A molecular docking-simulation based validation

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According to current WHO reports, there were 643,379,243 positive cases as of December 7, 2022, with 6,624,181 mortality cases recorded from several SARS-CoV-2 variants. Although existing antibiotics, antiviral drugs, and antiparasitic drugs were used on a repurposing basis in the emergency to control the pandemic without any concrete clinical evidence. Locating more advanced drugs to control newer variants of SARS-CoV-2 with appropriate clinical evidence and side effect studies is still ongoing for FDA approval. We have hypothesized a combinatorial drug approach, taking ten anti-HIV drugs and ten vitamin C derivatives. Initially, the vitamin C derivatives and anti-HIV drugs used as ligands were retrieved from PubChem and the target protein, SARS-CoV-2 main protease (PDB ID: 6Y84), from the protein data bank. Further, assess the potency, toxicity, drug-ability, and pharmacokinetic profiles using several bioinformatics tools, viz., molecular docking by the AutoDock 4.1 software with predicting activity spectra for substances, Molsoft, ProTox, and SwissADME tools. Molecular dynamics simulation was also employed for most potential candidates to assess their binding stability using GROMACS 5.1.4 software. The above computational investigation indicated that 'darunavir with lascorbyl-2,6-dibutyrate or ascorbic acid-2-sulfate' combinations strongly inhibit the SARS-CoV-2-main protease. Mostly, vitamin C derivatives enhanced the anti-COVID activity and might reduce the post-treatment side effects of darunavir in combined formulations. The current study suggests that bioinformatics tools are appropriate for identifying potential candidates in an emergency,

and the selected 'anti-HIV drug-vitamin C derivative' cocktails may be considered less-toxic regimens against COVID-19 treatment with further clinical studies.

Keywords: Coronavirus; Anti-HIV drugs, Vitamin C derivatives; Computer-aided drug design; Combinatorial drug approach; Molecular docking-simulation.

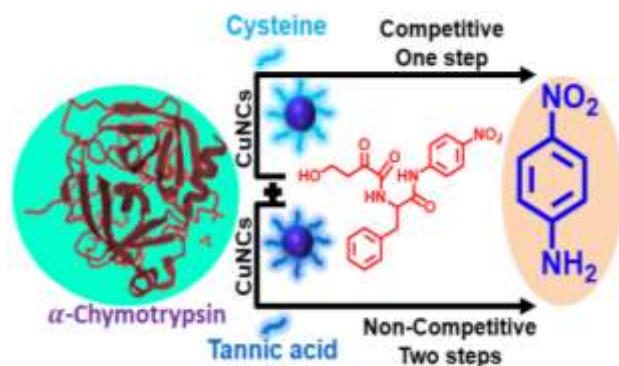
PP-110

Copper Nanoclusters as an Effective Enzyme Inhibitor: Role of Surface Chemistry on the Activity Modulation of α -Chymotrypsin

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The present work is undertaken to find out the suitability of CuNCs on the activity modulation of a model enzyme, α chymotrypsin (α -ChT).¹ This work also aims to highlight the role of surface chemistry corresponding to CuNCs in modulating the activity of α -ChT. For this purpose, two different types of CuNCs having chemically different surface ligands, namely, cysteine (Cys) and tannic acid (TA), have been synthesized. Subsequently, the interaction of these CuNCs with α -ChT has been investigated by employing various spectroscopic techniques at both ensemble average and single molecule levels. Results obtained from enzyme kinetics studies have revealed that both CuNCs act as good enzyme inhibitors. While Cys-CuNCs almost completely diminish the activity of α -ChT through a competitive inhibition mechanism, TA-CuNCs partially reduce the enzyme activity through a non-competitive inhibition mechanism indicating the vital role of surface ligand in the regulation of α -ChT activity. To gain a molecular-level understanding of the enzyme-inhibitor interaction event, fluorescence spectroscopy, ITC measurements, fluorescence correlation spectroscopy (FCS), agarose gel electrophoresis, and circular dichroism (CD) spectroscopy are conducted.² Thermodynamics results obtained from fluorescence titration experiment and ITC measurements have indicated that Cys-CuNCs follow a one-step binding process, whereas TA-CuNCs follow a two-step binding process. Moreover, FCS studies have provided evidence for the interaction of CuNCs with α -ChT at the single-molecule level. Importantly, Circular dichroism (CD) measurements have demonstrated that the basic structure of α -ChT remains almost unaltered in the presence of CuNCs. The outcome of the present study is expected to open up a new possibility of using CuNCs as an effective nanoscale enzyme regulator for various biological applications.



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PP-111

Surface Modification of CsPbX_3 (X = Cl and Br) Perovskite Nanocrystals by Treatment with Imidazolium-Based Ionic Liquids to Enhancing the Stability and Photoluminescence Quantum Yield

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Even though perovskite nanocrystals (PNCs) are quite attractive for optoelectronic applications, issues such as the low photoluminescence quantum yield (PLQY) and poor chemical stability of PNCs remain formidable challenges that need to be tackled. Because ionic liquids (ILs) possess some interesting physicochemical properties, the present study is undertaken to find out the suitability of ILs in obtaining stable and defect-free PNCs. To explore this possibility, the interaction of ILs with PNCs has been investigated by both spectroscopy and microscopy. Studies have demonstrated that a significant enhancement in the PLQY of PNCs can be obtained by post-synthetic treatment of PNCs with chosen ILs. Analysis of time-resolved fluorescence studies, X-ray photoelectron spectroscopy, and infrared spectroscopy data has suggested that ILs help in removing excess lead from the surface of PNCs.

Interestingly, it has also been observed that the chemical stability of PNCs can be increased considerably in the presence of ILs. More interestingly, the investigations have further shown that IL-treated PNCs are stable even at a single-particle level. The outcomes essentially show that ILs can effectively be used in obtaining chemically stable and photostable PNCs with improved photophysical properties.

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PP-112

Synthesis, characterization, and catalytic properties of TiSBA-1

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SBA-1 is a mesoporous silica-based material, possessing a three-dimensional cubic mesopore structure, remarkably high surface area, and good thermal stability, which make it suitable as a solid heterogeneous catalyst. Modifying the purely siliceous framework of SBA-1 with titanium (TiSBA-1) was intended to obtain titanosilicate catalysts—a proven class of solid heterogeneous catalyst employed in several oxidation reactions. TiSBA-1 was directly synthesized via a hydrothermal method and characterized by XRD, TEM, N₂ adsorption-desorption, FT IR, Raman, DR UV VIS, and TG studies. The XRD and TEM showed the formation of ordered SBA-1 materials having mesopore structures. TGA curves of as-synthesized TiSBA-1 gave about 43% of total weight loss noticed in three steps indicating the highly porous nature of the Ti-SBA-1. Nitrogen adsorption-desorption studies indicated a surface area of 1250 m²g⁻¹, pore volume of 0.64 cm³ g⁻¹ and average pore size of ~ 19 Å. DRUV-VIS studies revealed Ti(IV) oxidation state and titanium is located in the silicate matrix in tetrahedral coordination. Raman studies and FTIR spectra of the both as-synthesized and calcined TiSBA-1 samples showed various bands that can be attributed to titanosilicate structure. Catalytic oxidation studies of *veratryl alcohol*, an important lignin model molecule over TiSBA-1, resulted in the formation of two fine chemicals such as veratraldehyde and/or veratric acid. Our studies confirmed the formation of well ordered, stable nanoporous TiSBA-1 catalyst, which can be employed for oxidation of veratryl alcohol under mild conditions.

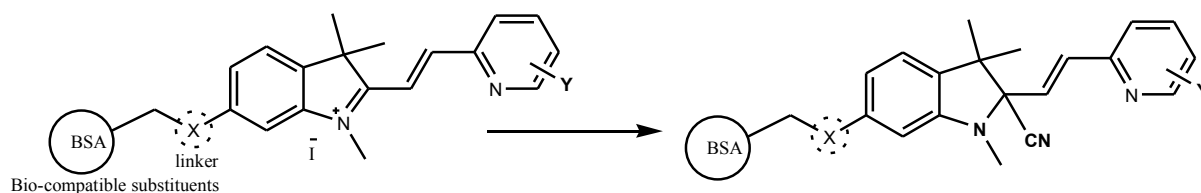
Functionalized Hemicyanine derivatives for cyanide detection

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The recognition of anions has attracted much their important role in biological, chemical, clinical and environmental applications. Anions such as cyanide, hydroxide, phosphate and fluoride play important roles in biological functions [1]. Among them, Cyanide, in its ionic or gaseous form, is extremely toxic beyond critical concentration threshold. It produces cellular respiration in mammals by strongly bind with a ferric ion in the active site of cytochrome system and its binding leads to inhibition of enzyme complex electron transport resulting in decrease cellular utilization of oxygen (hypoxia) and an eventual death [2]. Hence, the essence of real-time detection of these analytes selectively at low concentration level promotes development of detection techniques. Furthermore, developmental concern prevails in improvement of effective detection methodologies of high sensitivity and selectivity for cyanide anion, predominantly executable in aqueous and physiological conditions [3]. One of the viable processes in this context is recognition with fluorescent chemosensors, which has proven to be advantageous in terms of sensitivity, fast response, and operational simplicity [4]. Among many such chemosensors built through various methodological manifestations of design, appropriate componential choice and adequately efficient operative photophysical processes, hemicyanine [5] derivatives are amongst highly promising reactive group for CN^- due to its positive charge character which gives a strong attractive force between indolium group and CN^- ion.

Herein, we have synthesized a series of hemicyanine based molecular probes with tailor-made receptors for effective CN^- interactions. The photophysical signalling responses of the molecular systems were investigated by using different anions, which inferred to a selective cyanide ion response as a function of indolium unit and solvent medium based on the ICT process i.e. mechanism could be rationally interpreted by the nucleophilic addition reaction of CN^- and the polarized $\text{C}=\text{N}$ bond of the indolium group. The results indicated a structural rigidity-driven induction of selectivity and electronic environment-driven modulation in signalling parameters in these probes. The utility of these probes in CN^- detection were evaluated through molecular imaging investigations.



Scheme1: The probe-CN⁻ interaction leading to colour change and perturbation in side-group dependent fluorescence

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PP-114

Cyclodepsipeptides and Indolizidine based bioactive N-heterocycles

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Nature offers interesting examples of different sources of simplest to complex, wide-range of bioactive natural products. *N*-heterocycles based natural products constitute a major portion among such bioactive molecules.

Celebeside A (isolated-2009) is a cyclodepsipeptide with potent anti-HIV activity based natural product. There have been no much synthesis work since its isolation. Among the key steps involved in the synthesis are Evans Aldol, *cis*-epoxide ring opening, alkynol rearrangement to *all-trans-diene* ester among others for the synthesis of non-peptide part of celebeside A which displays potential anti-HIV activity. Indolizidine class of *N*-heterocyclic natural products are distributed in different natural sources with a range of biological activities. Pd-catalyzed cross coupling of cyclopropanols and acyl chloride afforded to achieve several functionalized indolizidine and other *N*-heterocycles based natural products. The method of cross coupling of cyclopropanol with acylchloride provide essay access to get 1,4-diketones which are used as building block to achieve several natural products.

Semi-synthesis of flavor and pharmaceutical grade (-)-menthol from citronellal rich essential oils using novel composites

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(-)-Menthol is a terpene alcohol with a strong minty odour, cooling effect and taste. Menthol is the third most popular flavour after chocolate and orange flavor. It is produced from the *Mentha arvensis* essential oil. It is well recognized for its flavor and also finds application in pharmaceutical industries. (-)-Menthol has a long history of use as topical analgesic. Clinical studies have proved that topical use of (-)-menthol is safe and effective in treating a variety of painful conditions, including musculoskeletal pain, injuries, neuropathic pain and migraine. The Global demand of (-)-menthol crystal is more than 12,000 ton. Thus there is need of a greener process for the production of (-)-menthol from low value essential oils. Recently, our group has developed a two-step catalytic process for selective semi-synthesis of flavour grade (-)-menthol from citronellal-rich essential oils such as *Cymbopogon winterianus* and *Corymbia citriodora* by using novel bi-acidic composite. The bi-acidic Sn-B-NaYZE composite was developed to cyclize 99% of citronellal directly from the essential oils to isopulegol isomers with 99% selectivity via liquid CO₂ medium in 45 min. Further, these isopulegol isomers were reduced to 98% of menthol using 1%Pd/AC at moderate reaction condition such as 40 PSI H₂ pressure and 60 min reaction time in ethanol. The reaction mixture was slowly frozen to -40 °C for trouble-free isolation of the crude menthol. Further, pharmaceutical and flavor grade (-)-menthol was purified from the crude menthol through the esterification process. This isolated (-)-menthol was found to 100% biobased on ¹⁴C radiocarbon-dating to authenticate as nature-identical. This catalytic process is based on greener solvent such as liquid CO₂ and ethanol as the reaction medium. The liquid CO₂ condition is easily attained in normal cylinder pressure. The overall process is consider to be a greener and economically suitable for the production of nature-identical (-)-menthol for flavor and pharmaceutical applications.

Spectroscopic and Biophysical Interaction Studies of novel Ir(F2ppy)₂ N hydroxypiconilamide complex with calf thymus DNA for its potential Application in cancer research

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DNA being the hereditary biomolecule, since the revelation of its structure, this bio-macromolecule has gained undivided attention for the discovery of bio-materials that bind and alter how DNA essentially functions, studying the interplay of which is very much essential for the discovery of potential anti-cancer complexes. Ir(F2ppy)₂ N hydroxypiconilamide is one such bio-material complex whose mode and efficiency of interaction with DNA was scrutinized and this report is the portrayal of the data accumulated in the process. It is an organometallic complex with bidentate cyclometallated ligand. UV-visible spectroscopy was done to confirm the interaction. With increasing concentration of complex, hyperchromic shift was observed. Steady state fluorescence spectroscopy exhibited hypochromic shift with increasing concentration of DNA. A binding constant of 1.4×10^4 was calculated from Stern-Volmer plot, a value somewhat in-between that of classic DNA intercalators and groove-binders. Competitive displacement assay was carried out, displacement of intercalating agent EtBr by the complex confirms an intercalative mode of interaction which was further validated by KI quenching experiment. A significant decrease in K_{SV} was observed in DNA bound state of the complex (03.35) than free Complex (10.53). Increasing salt concentration experiment was executed to verify the presence of electrostatic binding mode, confirming a mixed mode of binding for the Complex with DNA. Raman spectroscopy data analysis revealed a number of Raman shifts was observed by the Complex-DNA interaction. Superoxide generation experiment was performed to investigate DNA damage by photo activated ROS generation properties. Docking studies also revealed preferential binding of the complex at the hydrophobic cavity of site IB with suggestive involvement of hydrophobic forces. The cytotoxicity of Ir(III) complex against cancer cell lines MDA-MB 231, T98G and normal HEK 293t cells were investigated using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-tetrazoliumbromide (MTT) method and the results showed a promising anti-cancer property by the complex.

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Advances in Materials Chemistry and Applications
(OCS-AMCA -2022)
December 18-19, 2022

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