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CELEBRATION OF ACHIEVEMENTS OF INDIAN CHEMICAL INDUSTRIES

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Molecular Engineering Of Imidazo[1,2-A]Pyridines: As Gateway For Dual State Emissive Organic Materials For Optoelectronics And Bioimaging

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Abstract Category

Material Science

Abstract

Luminescent dyes represent a pivotal class of compounds with versatile scaffolds, offering immense potential across various applications.¹⁻⁵ These dyes, characterized by properties such as Dual State Emission (DSE) and Aggregation Induced Emission (AIE), are highly coveted for their utility in optoelectronics, bioimaging, sensors, and polymeric materials. However, realizing these properties often entails intricate structural designs and complex synthetic routes.

This study introduces a series of luminescent molecules based on the imidazo[1,2-a]pyridine framework, meticulously synthesized and structurally engineered to exhibit both DSE and AIE properties. Photophysical investigations reveal that these compounds emit across a broad spectrum of the visible range, from blue to red, with exceptional quantum yields. The solid-state luminescent properties were further examined by fabricating OLED devices for optoelectronic applications. These devices demonstrated promising results, achieving high External Quantum Efficiencies (EQEs) with minimal roll-off.

Furthermore, the AIE properties of these compounds were explored for bioimaging applications. The luminogens effectively penetrated cancer cells, binding to the nucleus and cytoplasm with high fluorescence intensities. This work provides a strategic approach for researchers to design novel luminescent materials through structural engineering, paving the way for a wide range of applications.

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Microwave triggered conformational perturbation and aggregation of bovine beta-Lactoglobulin: An enigma towards non-thermal effect

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Abstract Category

Green Chemistry

Abstract

The non-ionizing Microwave Radiation plays a pivotal role in electronic communication starting from radar, satellite, Bluetooth devices to wifi bands specially using the internet of latest 5G technologies (<6 GHz). Nonetheless microwaves are deployed for heat generation in chemical reactions in the field of microwave/green chemistry. A comparative study has been performed on thermal and microwave induced non-thermal conformational changes at the secondary and tertiary level of β -lg structure to ensure the non-conventional heating can produce any perturbation with analogous thermal range.

Both the fluorescence and circular dichroic studies revealed the conformational changes of β -lg. Both SDS-PAGE and native-PAGE study was carried out to identify the higher oligomers and the isocratic-HPLC was used to characterize the oligomers/aggregates.

Morphology study of the aggregates was also performed with the help of FE-SEM technique. In fact conformational change related neurodegenerative disorders such as amylopathies including Alzeimer's, Parkinsons and Creuzfeld-Jakob diseases could be envisioned in context of microwave and sustainability.

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Hollow Micropores in Organic Cage Nanocapsule as a Size Exclusion Gate: Cage Entrapped Pd(II)-catalyst for Efficient Cross-Coupling Reaction

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Abstract Category

Catalysis

Abstract

Hollow porous organic capsules (HPOCs) containing an active catalyst feature nanoscale cavities that offer the advantages of a nanoreactor. These capsules also separate the catalysts from the reaction medium through pores that function as a size-exclusion barrier. Designed with specific molecular weight cutoffs, these HPOCs provide the benefits of semipermeable membrane separation, supporting a sustainable chemical process that avoids energy-intensive separation methods.

We have developed a hollow, porous organic nanocapsule for encapsulating Pd(PPh₃)₂Cl₂ as the catalyst, aiming to combine the benefits of heterogeneous catalysis with the conditions typical of homogeneous catalytic processes. Reports on permeability control in self-assembled polymer nanocapsules are limited to molecules with molecular weights over 5000 Da and typically show long-term retention of encapsulated catalysts. Among various heterophase polymerization methods, miniemulsion polymerization has emerged as a versatile technique for encapsulating both hydrophobic and hydrophilic reagents effectively.

In the case of Suzuki coupling reactions using Pd(PPh3)2Cl2 as the catalyst, the size difference between the standard catalysts, reagents, and products is minimal—just a fraction of a nanometer. In this study, we developed a porous organic nanocapsule with selective molecular cutoff properties, providing a platform that meets these specific requirements. The low density, high surface area, broad pore tunability, and exceptional chemical/thermal stability of these hollow porous organic capsules with selective molecular cut-offs make them an attractive choice for catalyst encapsulation and the development of sustainable processes.

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Kinetics of Butane Deep Oxidation on Commercial Noble Metal Catalyst

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Abstract Category

Catalysis

Abstract

The largest emissions of individual Volatile Organic Compounds (VOCs) are of butane, toluene, pentane, propane, ethanol, and 'white spirit'. VOCs including hydrocarbons like butane, are major air pollutants posing environmental and health risks. Effective mitigation through converting VOCs requires advanced catalysts such as Pt, Pd, Au, Ru, and Rh supported on mixed metal oxides. This study evaluated a noble-based industrial commercial catalyst for butane combustion under varied temperature, GHSV, and butane concentration conditions. The catalyst achieved complete butane conversion at low temperatures with high stability over prolonged use. Kinetic studies highlighted the role of Pt dispersion on alumina in enhancing butane activation and catalytic activity. These findings demonstrate the potential of noble-based catalysts for industrial applications in hydrocarbon combustion and VOC control, offering sustainable solutions for energy and environmental challenges.

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UNVEILING GREEN CHEMISTRY: EXPLORING SUSTAINABLE PRACTICES FOR A GREENER FUTURE

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Abstract Category

Green Chemistry

Abstract

Green Chemistry, or sustainable chemistry, minimizes environmental impact while maximizing efficiency and safety in chemical processes. It aims to design products and processes that reduce or eliminate hazardous substances.

Phase Transfer Catalysis (PTC) uses catalysts like quaternary ammonium salts to transfer reactants between immiscible phases. This enables reactions under mild conditions, reducing energy use and waste.

lonic Liquids (ILs), molten salts with low volatility and tunable polarity, are green alternatives to traditional solvents. Their negligible vapor pressure and recyclability make them valuable in biomass conversion, catalysis, electrochemistry, and separation technologies.

Sonochemistry uses acoustic cavitation to drive reactions, generating reactive species through ultrasonic irradiation. This creates localized heating and pressure, accelerating chemical transformations under mild conditions, minimizing energy input and enhancing reaction rates.

Microwave Irradiation (MWI) enables rapid and selective heating through dielectric heating. Polar molecules absorb electromagnetic radiation, converting it to thermal energy, promoting homogeneous heating and faster reaction kinetics.

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Green tea polyphenols inhibit Helicobacter pylori virulence factors CagA and VacA: A Computational Study[†]

Suraj Mali

D.Y. Patil University (Deemed to be University), Navi Mumbai, India

Abstract Category

Food Chemistry

Abstract

Helicobacter pylori (*H. pylori*) is a bacterium that infects the stomach lining, contributing to various gastrointestinal disorders. *H. pylori* infection is a major cause of peptic ulcers and chronic gastritis, affecting a significant portion of the global population. *Helicobacter pylori*, a prevalent bacterium infecting nearly half the global population, induces chronic stomach inflammation leading to severe gastric conditions, including ulcers, cancer, and MALT lymphoma. Early detection and treatment of *H. pylori* infection are crucial in managing associated digestive health issues and preventing complications like stomach ulcers and gastric cancer. Green tea flavonoids (GTFs), particularly Epigallocatechin Gallate (EGCG), exhibit anti-*H. pylori* actions. EGCG has been shown to inhibit H. pylori growth and colonization, possibly by disrupting bacterial cell membranes and interfering with essential bacterial enzymes. Additionally, the antioxidant and anti-inflammatory properties of green tea flavonoids may contribute to their potential in combating H. pylori-induced gastric inflammation and related gastrointestinal disorders. In current study, we found Epigallocatechin gallate (docking score: -198.72 kcal/mol) and Theaflavin-3-gallate (docking score: -177.19 kcal/mol), as inhibitors of *Helicobacter pylori* virulence factors CagA and VacA, respectively as assessed with in-silico modules. Our results point towards the potentials of such GTFs to inhibit *H. pylori* agents.

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Development of curcumin integrated smart pH indicator, antibacterial, and antioxidant waste derived *Artocarpus lakoocha* starch-based packaging film

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Abstract Category

Food Chemistry

Abstract

Ensuring food freshness remains a critical challenge for both consumers and the food industry. This study introduces a pH-sensitive intelligent food packaging solution using a curcumin-infused starch film (F1). The starch was derived from waste seeds of *Artocarpus lakoocha* (NS-MJF) and subjected to various modifications, including autoclave heat treatment (S1), osmotic-pressure treatment (S2), and citric acid treatment (S3). The native starch was further utilized to create the curcumin (2.5% w/w)-based film (F1). Comprehensive analyses of the starches were performed, including solubility, color evaluation, biodegradability, oil absorption capacity, and moisture content. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) revealed favorable microstructural properties. Incorporating curcumin enhanced the contact angle and elongation at break of the films. Additionally, antioxidant and antimicrobial properties were evaluated, alongside real-time monitoring of chicken fillet freshness. These findings highlight the potential of pH-responsive biopolymer films in intelligent poultry packaging, advancing food preservation and safety.

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DESIGN, SYNTHESIS AND ANTITUBERCULAR EVALUATION OF SOME NOVEL MOLECULES

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Abstract Category

Green Chemistry

Abstract

Tuberculosis (TB) remains a major global health threat, causing approximately 1.4 million deaths annually. This study focused on developing new anti-tubercular agents targeting InhA, a crucial enzyme in mycobacterial fatty acid synthesis. Four series of 3-substituted phenyl-1-(2-substituted phenyl-5-(pyridin-3/4-yl)-1,3,4-oxadiazol-3(2H)-yl)-prop-2-en-1-one derivatives were synthesized using a microwave synthesizer.

In silico ADMET studies were conducted using SwissADME, and docking studies were performed targeting InhA (PDB ID 4TRN). The anti-tubercular activity of the synthesized compounds was evaluated in vitro against Mycobacterium tuberculosis (Mtb H37Rv) using the Microplate Alamar Blue Assay (MABA) method, with concentrations ranging from 250 μ g/mL to 0.49 μ g/mL.

The results showed varying levels of sensitivity and resistance at different concentrations. Some compounds (e.g., 7g) exhibited activity even at lower concentrations (0.98 μ g/mL). Most compounds displayed sensitivity at higher concentrations and resistance at lower concentrations. Docking studies revealed comparable binding interactions to the native ligand, NADP, with notable docking scores.

These findings suggest that the synthesized compounds, incorporating a 2,3-dihydro-1,3,4oxadiazole scaffold with an imine linkage, have the potential to be developed as novel antitubercular agents due to their comparable activity to standard drugs and similar binding interactions with InhA. Structure-activity relationship (SAR) analysis provided insights for future optimization of these lead compounds.

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Nanoporous MCM-48 as a carrier for antidiabetic drug, Metformin Hydrochloride

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Abstract Category

Drug Delivery

Abstract

Metformin Hydrochloride (MTF), a Class III biguanide derivative drug is widely used to treat Type 2 diabetes mellitus (T2DM). However, due to its low bioavailability and short half-life, frequent dosing is required. These limitations can be addressed by designing a controlled drug delivery system (DDS) for MTF. Amongst various DDSs, mesoporous silica nanoparticles (MSNs) have been explored due to their unique properties like ordered porosity, high surface area, and adsorption capacity. The cubic MCM-48 type of MSNs (nMCM-48) has gained significant attention due to its unique bicontinuous channel networks.

This work consists of designing a DDS based on nMCM-48 and its characterization by various techniques. In vitro release study of MTF/nMCM-48 was carried out in pH-1.2 and pH-7.4 at 37 °C under stirring condition followed by evaluation of release kinetics and mechanism supported by dissolution studies. Furthermore, when compared to commercially available formulation, Glycomet-250, MTF/nMCM-48 exhibits more controlled release. Moreover, considering the anti-cancer potential of MTF, this work demonstrates that MTF/nMCM-48 can be used to treat T2DM patients having genetic history of cancer.

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Synthesis of Graphene Quantum Dots from Agricultural Waste for Pharmaceutical Drug Delivery

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Abstract Category

Drug Delivery

Abstract

The conversion of agricultural waste into carbon-based products is a pressing need. Graphene and its derivatives, owing to their high graphitic degree, increased surface area, strong electrical conductivity, and biocompatibility, are gaining attention in diverse fields. Agricultural waste materials, such as sugarcane bagasse, rice husk, and tea waste, serve as low-cost precursors for synthesizing graphene. This study proposes a simple, cost-effective method for synthesizing graphene quantum dots (GQDs) from agricultural waste, focusing on their application in pesticide detection, sensing, and drug delivery systems.

The research aims to synthesize biocompatible GQDs using plant sources, particularly M. indica leaves, through a microwave-assisted method. The GQDs will be characterized systematically to evaluate their properties, stability, cytotoxicity, and potential for drug delivery, specifically for diabetic treatments.

The experimental approach involves extracting leaf powder with ethanol, followed by microwave heating to synthesize GQDs. Various characterization techniques, including transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), fluorescence spectroscopy, and UV-ViS spectroscopy, will be used. Stability and toxicity studies will be performed, including temperature and pH variations and MTT assays to assess cellular viability.

In addition, the GQDs will be tested for drug delivery applications, with encapsulation efficiency (EE) and in-vitro release profiles evaluated using modified dialysis. This study aims to provide a sustainable, cost-effective approach for drug delivery, demonstrating the potential of GQDs synthesized from agricultural waste in pharmaceutical and environmental applications.

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India's First Antibiotic Nafithromycin - An Innovation Through Public-Private Collaboration

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Abstract Category

Drug Delivery

Abstract

More than 2 million deaths happen globally each year due to drug resistant pneumonia of which 23% occur in India. Nafithromycin is a novel lactone ketolide antibiotic derived from erythromycin recently approved for the management of community-acquired bacterial pneumonia (CABP) in adults [1, 2]. Nafithromycin offers improved patient compliance and with just 3 doses is 10 times more potent than azithromycin, also effective against multi-drug resistant isolates of bacteria.

Nafithromycin development has taken approximately ₹500 crores investment, 14 years research, with multi-centric clinical trials spanning Europe, U.S., and India. The drug was found safe *in vitro*, *in vivo* followed by human trials and has no substantial drug or food interactions with negligible gastrointestinal side effects, making it a great treatment option [2,3].

This antibiotic is India's first indigenously developed antibiotic against antimicrobial resistance (AMR). It has been developed through collaboration of Biotechnology Industry Research Assistance Council (BIRAC), Department of Biotechnology, Government of India under Biotechnology Industry Partnership Program (BIPP) and the Pharma company Wockhardt which will be marketing the drug under the trade name Miqnaf[®].

The success of Nafithromycin represents an example of public-private collaboration in the area of healthcare innovation and is a testimony to India's emergent innovation abilities for demanding healthcare challenges. Nafithromycin development is a significant milestone for India's Pharmaceutical industry and a major step forward in the fight against antimicrobial resistance (AMR).

This poster shall review the available published data on Nafithromycin, its role in infection management and data from the different trans-national clinical trials.

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Biogenic synthesis and evaluation of metallic nanoparticles for synergistic antifungal effect

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Abstract Category

Nanomaterial/nanotechnology

Abstract

The noble metals with beneficial health effects are used for synthesis of metallic nanoparticles. The biological methods, Bioreduction and Biosorption for synthesis involve application of microorganism, enzymes and plant products. Green synthesis does not involve use of high pressure, energy, temperature or toxic chemicals. These are cost effective, eco-friendly and easily scalable methods as compared to physical and chemical methods of synthesis.

In this research, Punica granatum (pomegranate) is used as a medium for synthesis of Silver Nanoparticles (AgNPs). The aqueous extract of fruit peel is characterised by TLC, UV Spectral Analysis, Total phenolic content and screened for Anti-fungal activity.

Optimization parameter used for formulation development are volume of extract, concentration of Metal salt, incubation time and temperature. The green AgNPs were characterized for particle size, Zeta potential and by Scanning Electron Microscopy, Inductively coupled plasma atomic emission spectroscopy and In vitro antifungal assay

The developed formulation is useful in overcoming resistance shown towards existing synthetic antifungal drugs. It shows synergistic effect in the treatment of difficult to treat fungal infection as combined effect the natural extract and silver. The AgNPs exhibited enhanced antifungal activity when compared to pure extract and silver used alone. It is effective in lesser dose owing to its nanosized. It can also provide sustained and controlled release

Synthesized nanoparticles can be effectively incorporated into various dosage forms like gel and transdermal patch etc. The aqueous extract of the Punica granatum peel, a waste material was successfully used to reduce and stabilize the silver nanoparticles.

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Three New MOFs, Same Spacers: Synthesis, Characterizations and Selective Gas Adsorption :Application with ws-Carbon Nanomaterials

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Abstract Category

Nanomaterial/nanotechnology

Abstract

The abstract outlines a research focus on the rational design of coordination polymers (CPs) and metal-organic frameworks (MOFs)¹ with specific properties. Aromatic carboxylic ligands are emphasized for their versatility in constructing MOFs, with a discussion on their coordination modes and impact on network robustness. The use of mixed ligands²⁻⁴ is explored, offering potential advantages in pore tuning and structural diversity. Trimesic acid and pyridyl N,N'-donor spacer ligands are highlighted for their contributions to structural diversity and selective adsorption properties^{5,6}. The research group's specific focus on porous coordination polymers for selective CO₂ adsorption is outlined, emphasizing the critical importance of addressing environmental concerns related to rising atmospheric CO₂ levels. Finally, three coordination architectures generated through intelligent ligand combinations and solvothermal methods are presented, along with characterization techniques and selective gas sorption studies.

Moreover, here we utilize for the very first time the common tree barks for the development of water-soluble carbon nanomaterials. Thus, the available wood bark of Jack fruit, Betel-nut and Guava trees were taken for the preparation of carbon based nano-materials. The carbonization of the raw materials was followed by acidification. After certain process steps the acid-free slurry was heated and filtered. The filtrate was dried on the water bath to yield water soluble carbon nanomaterials. Then the nanomaterials added with MOFs separately. The carbon nanomaterials were characterized by the different spectroscopic techniques. The MOF-nanomaterials show remarkable enhancement in growth rate of common gram plants

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The Alchemy of Materials: A Century of Indian Chemical Innovation

SWAPNIL UPADHYAY

VIT, BHOPAL, India

Abstract Category

Material Science

Abstract

Material science stands as a transformative pillar of modern innovation, driving advancements across diverse domains by unlocking the fundamental principles governing materials. Recent progress has redefined possibilities, addressing critical global challenges such as energy sustainability, advanced healthcare, and environmental preservation. The rise of perovskite solar cells, achieving power conversion efficiencies exceeding 25%, marks a paradigm shift in renewable energy, while 2D materials like graphene and transition metal dichalcogenides promise breakthroughs in electronics, photonics, and thermal management.

State-of-the-art characterization techniques, including atomic-resolution electron microscopy and synchrotron-based methods, have unveiled intricate atomic-scale phenomena, paving the way for precision-engineered materials. Simultaneously, the advent of high-entropy alloys (HEAs) with exceptional mechanical properties and next-generation solid-state batteries with energy densities surpassing 350 Wh/kg exemplify the leap toward high-performance and sustainable solutions. Additive manufacturing further redefines production landscapes, enabling bespoke designs with unparalleled efficiency and minimal waste.

The integration of computational modeling and machine learning has accelerated material discovery, predicting novel compounds and optimizing their properties with unprecedented accuracy. Efforts in sustainability have fostered the development of biodegradable polymers and enhanced recycling technologies, addressing the pressing need for circular economies.

Material science's confluence of fundamental research and applied innovation positions it at the forefront of shaping a resilient and technologically sophisticated future. As the field evolves, it not only drives the frontiers of knowledge but also underscores its indispensable role in forging a sustainable, high-tech global society. This synergy ensures its enduring significance in addressing humanity's most pressing challenges.

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Chiral Cinchona Organogel Mediated Chiral Inorganic Nanostructure for Asymmetric Michael Addition

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Abstract Category

Catalysis

Abstract

Asymmetric Heterogeneous Michael addition of dialkyl malonates over substituted chalcones is crucial for synthesizing pharmaceutically relevant synthons and chiral drugs. In the past two decades, two heterogeneous catalysts have been reported in this context, but they pose challenges like metal leaching, yield/ee balance, side product formation and less activity towards heteroaromatic substrates. Unlike Poly-amide homogeneous catalysts, carbamides are bio-degradable and if heterogenized over metal matrix, can offer the same activity as poly-amide systems.¹ *Cinchona* was dimerized by hexamethylene di-isocyanate and later N-alkylated by hexyl bromide to form carbamide (L2) and carbamide gemini surfactant (L3), which interestingly formed gels under toluene. NiO/L3 with particle size 22 nm and its corresponding enantiomer was synthesized through N₂H₄/NaOH.² The developed composite NPs posed as efficient nanocatalysts for chiral asymmetric Michael addition reaction. The NiO/L3 catalyst afforded Michael addition of dialkyl malonates over chalcones in the presence of K₂CO₃ and binary solvent (H₂O : PhMe 4:1 v/v), within 16 h at room temperature with yields of ~92% and ee of ~90%, for over 30 distinct aromatic, heteroaromatic and bulky substrates, for over 7 catalytic cycles with minimal Ni leaching. The mechanistic study confirmed the crucial presence of NiO and carbamide surfactant for the best results, and the composite catalyst showed (+) non-linear effect.

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Kinetic and isotherm studies for removal of lead using bentonite and bentonite activated charcoal mixture

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Abstract Category

Interfacial/surface science

Abstract

The present study is aimed at devising a low cost and eco- friendly method of lead removal from aqueous medium. A comparative study of removal of Pb (II) by bentonite and bentonite activated charcoal mixture (I:I) was done. Batch experiments were done to find optimum condition as a function of variables such as pH, agitating time, initial concentration of Pb²⁺ adsorbent doses. The results showed that experimental results were the best fit for Langmuir isotherm. The kinetic studies confirmed the pseudo-first order reaction. The bentonite was characterised by TGA, DTA, XRD, and FITR. The maximum adsorption maximum adsorption capacity was evaluated to be 99.97 percentage. Further uptake capacity by bentonite activated charcoal mixture was almost same as the bentonite. Bentonite activated charcoal mixture has emerged as a potential adsorbent of lead (II) ions from aqueous medium

Keyword: Bentonite, activated charcoal, adsorbent, lead.

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Next-Generation Ni-Cu-Zn/CeO₂ Catalyst for Sustainable CO₂ Conversion

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Abstract Category

Catalysis

Abstract

We designed and synthesized a Ni-Cu-Zn/CeO₂ catalyst featuring remarkable activity and stability, due to unique electron density distribution, achieved through the strategic integration of defects and SMSI. This catalyst demonstrated exceptional performance, achieving a CO productivity of 49,279 mmol g^{-1} h⁻¹ at 650 °C—a nine-fold improvement over the best-reported catalysts. It also delivered outstanding CO selectivity of up to 99% and remarkable stability, with activity remaining unchanged even after 100 hours on stream at 500 °C. We then undertook a comprehensive series of studies to understand why this combination of trimetallic sites and defective ceria outperforms the reported catalysts. The underlying mechanism was rigorously investigated using in-situ TEM, in-situ STEM-EELS, and in-situ HERFD-XANES, revealing the crucial role of electron shuffling and SMSI between the trimetallic NPs and the CeO_2 surface. The catalyst's extraordinary activity and stability arise from the synergistic interplay among the Ni-Cu-Zn sites and their SMSI with the defected ceria support. HERFD-XANES and *in-situ* EELS data confirmed the role of ceria oxygen vacancies in both CO₂ activation and coke suppression during catalysis. *In-situ* TEM imaging under catalytic conditions captured the movement and growth of active trimetallic sites, showing that their diffusion and sintering ceased once SMSI was established. In-situ FTIR spectroscopy and DFT studies suggested an integrated direct dissociation and a redox pathway, facilitated by hydrogen across various active sites.

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Air-Stable Plasmonic Nanoreactors of 'Black Gold' for Sunlight Driven Acetylene Semi-Hydrogenation

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¹Tata Institute of Fundamental Research, Mumbai, India. ²The University of Tokyo, Tokyo, Japan

Abstract Category

Catalysis

Abstract

In general, catalysts for reduction are unstable in the presence of air. A plasmonic reduction catalyst that is stable only in air has been described in this work. A highly active, selective and particularly airstable plasmonic reduction catalyst for acetylene semi-hydrogenation was developed by loading Ptdoped Ru nanoparticles on black gold (DPC). With over 90% selectivity and ethene productivity of 320 mmol g⁻¹h⁻¹ of ethene, the DPC/RuPt catalyst outperformed nearly all previously reported catalysts. The critical role of co-existing metal oxide and metal phase was evidenced by high catalytic activity and longterm stability for at least 100 h, which could only be achieved by providing continuous airflow along with the reactant feed. Plasmon-mediated simultaneous reduction and oxidation of the active site during the reaction were responsible for the unprecedented stability of the catalyst which was demonstrated by various spectroscopic analyses (XPS, EXAFS, and XANES). FDTD simulations showed a five-fold enhancement in the electric field as compared to pristine DPC due to the near-field coupling between the RuPt nanoparticles and DPC. Higher KIE in light implied the contribution from the non-thermal effects along with the photothermal activation of the reactants as a result of plasmonic activation. Insitu FTIR studies provided insight into the molecular reaction mechanism over the oxide surface and highlighted the role of the intermediates in determining selectivity. The integration of advanced spectroscopic techniques and simulations provided deep insights into the catalyst's behavior and mechanism, showcasing its potential for practical applications in sustainable catalysis.

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Surface-modified NiFe2O4 nanoparticles for the production of biodiesel from fatty acids and microalgae lipidsDunaliella salina

Kalluri VS Ranganath, Manisha Pandey

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Abstract Category

Renewable energy

Abstract

The current global energy demand is primarily met by fossil fuels, which contribute to environmental issues. A sustainable alternative is biodiesel, a renewable fuel obtained from biomass rich in lipid content synthesized by transesterification of cooking oil and lipid extracts of microalgae. Due to high viscosity, virgin oils or lipids cannot be used directly in diesel engines [1]. Transesterification reaction, facilitated by chemical (alkali/acid) or biochemical (enzyme) catalysts, helps in converting vegetable oils into biodiesel thereby reducing the viscosity, thus turning the product compatible for use as fuel. The study investigates the catalytic transesterification of oil and lipid extracts from *Dunalliela salina* using NiFe₂O₄ modified by 4,4'-Biphenyldisulphonic acid (BPDSA), analysing catalyst properties using various techniques and studying methyl oleate esterification.

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The SEPLO Process: A New Approach to Safety Management

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Abstract Category

Process hazard safety

Abstract

1. Introduction:

Chemicals are vital but pose risks during manufacturing. This paper explores challenges and introduces the SEPLO process, enhancing safety, operational efficiency, and profitability in the chemical industry.

2. Material and Methods:

This research paper draws upon Author's 43 years of experience in the chemical industry, transformed in his book "Earn or Burn Your Profits." It introduces the SEPLO process to enhance safety and operational efficiency in chemical plants. Combining practical experience, stakeholder input, and systematic analysis, the SEPLO process is developed through real-world applications, addressing gaps in traditional safety management approaches.

3. Significant Results and Discussion

The Chemical Manufacturing Business (CMB) offers profit and societal benefits but faces risks due to hazardous materials and accidents with severe consequences. Traditional safety systems often fail, seen as burdens rather than assets. The SEPLO process integrates safety into operations, aligning it with business goals to ensure safe, profitable plant operations and bridge the gap between safety and profitability.

Key benefits of the SEPLO process include: applicable throughout the plant lifecycle and across all stages of business growth, Can be implemented at any pace, Intrinsic Integration into core business functions, Continuous Synchronization among core business assets, and Focus on Results - safe and efficient plant operations.

4. Conclusion:

The SEPLO process is the ultimate step-by-step tool for achieving safe and efficient plant operation, alleviating the environment and enhancing profits.

References

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Plasmonic Black Gold Photocatalysts for Green and Sustainable Applications

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Abstract Category

Nanomaterial/nanotechnology

Abstract

Plasmonic nanomaterials, particularly dendritic plasmonic colloidosomes (DPCs), have gained significant attention for their exceptional catalytic performance in various reactions, such as CO₂ reduction, alcohol oxidation, hydrogenation etc. These materials, often referred to as "black gold," are capable of generating thermal and electric hotspots under light, making them highly effective catalysts. However, the conventional multi-step synthesis process for DPCs is complex, time-consuming, and not scalable for industrial applications. This limitation has hindered their widespread use in catalytic processes despite their promising potential.

Recent advancements have introduced a novel one-pot synthesis approach for DPCs, significantly reducing the synthesis time and simplifying the process. This new method not only improves the efficiency of the synthesis but also enhances the scalability of DPCs, making them more suitable for large-scale industrial applications. Furthermore, the incorporation of active metals such as Pt-doped Ru and Ni has been shown to further boost the catalytic performance of DPCs, expanding their applicability in various reactions, including hydrodechlorination and CO oxidation.

The integration of these advancements offers a scalable, sustainable solution for catalytic processes, with significant implications for environmental and industrial applications. By improving the synthesis and enhancing catalytic performance, plasmonic nanomaterials, particularly DPCs, hold immense potential in addressing critical challenges in energy conversion, and other industrial catalytic processes. This research represents a significant step toward the practical application of plasmonic nanomaterials in sustainable and efficient catalytic technologies.

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Development of Multiphysics Simulation Tool for Electrolyzer, Battery and Fuel Cell – Design Optimization and Risk Assessment.

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Abstract Category

Electro Chemistry

Abstract

The increasing demand for sustainable energy solutions has driven the need for faster technology development and accelerated design optimization in electrochemical systems such as electrolysers, batteries, and fuel cells. Considering the risk associated with such systems, it's vital that proper risk analysis is carried out in the design stage itself. This demands for advanced tools capable of simulating complex processes as these systems involve intricate interactions among multiple physical phenomena, including electrochemistry, multiphase and reactive flow, electric current distribution, heat transfer, and structural mechanics. An innovative multiphysics simulation tool tailored to address these challenges is developed. This tool integrates comprehensive modelling capabilities to provide an in-depth understanding of system behavior under diverse operating conditions. By bridging the gap between design and performance optimization, the tool facilitates the development of efficient, reliable, and sustainable energy systems while assessing the risk associated with the systems. This paper highlights the unique features of this simulation tool, its underlying physics, and its potential applications in advancing the development of green hydrogen production, energy storage, and fuel cell technologies without compromising on the safety.

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A Century of Pickering Emulsions: Discovery and Innovation in Pickering Interfacial Catalysis

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Abstract Category

Catalysis

Abstract

Over the last century, chemistry has undergone remarkable transformations, shaping modern science and technology.

Both the quality and span of life have immensely increased due to latest inventions and innovations in chemistry. At the same time there were also many challenges to be addressed. For example, carrying out chemical reactions in benign and renewable solvents and with high activity and selectivity to a desired product became a central theme of 'green chemistry' objectives. While alternate green solvents were being tried, the concept of catalysis became the magic wand to bring about selective conversions under ambient conditions.

While surfactants stabilized emulsions were being used for a long time, S. U. Pickering, a British scientist in 1907, came up with the idea of stabilizing emulsions with solid particles. In the first phase, these emulsions were used for carrying out organic reactions in the dispersed phase, curiosity and the ever ready mind set of researchers recognized another opportunity. The very same solid particles used for stabilization were made to play the role of catalysts as well. This integrated approach led to the concept of Pickering Interfacial Catalysis –since the stabilising solid itself acts as a catalyst, the process is devoid of the use of multiple reagents and reaction steps. In this study, we present a MgO-PIC system for Knoevenagel condensation of benzaldehyde and malononitrile as a model reaction scheme.

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Prowess of sustainable scale up for synthesis of a coumarin intermediate

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Abstract Category

Green Chemistry

Abstract

Scaling up a chemical reaction from the lab to a plant involves numerous technical challenges, such as effective mixing to avoid dead zones and maintaining reaction kinetics under low heat transfer conditions. A well-structured workflow demonstrated herein, uses Mettler Toledo's Automated Lab Reactors (ALRs) with Dynochem's Mixing Web App (MWA) to streamline mixing calculations and create effective scale-up recipes, ensuring success **'right the first time'**. To demonstrate this efficacy of this approach, we synthesized a coumarin intermediate which exhibits high quantum yield, visible region luminescence, and thermal stability. Thus, it has wide range of industrial applications like chemosensors, fluorescent probes, OLEDs and laser dyes. This investigation simplifies scale-up studies sustainably!

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Elucidating the Intricacies of Inverse Hydride Shuttle Catalysis in the Construction of Chiral Azabicyclic Scaffolds

Damanpreet Kaur

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Abstract Category

Catalysis

Abstract

Chirality is vital in pharmaceutical design, and achiral organocatalysts offer a sustainable method for synthesizing chiral alkaloids.[1] Boron-based frustrated Lewis pairs (FLPs) enable reversible hydride transfer, advancing inverse Hydride Shuttle Catalysis (i-HSC). This study computationally explores the exciting work experimentally performed by Maulide et al. [2] and successfully established the mechanism for inverse Hydride Shuttle Catalysis (i-HSC) with FLPs, revealing their potential to achieve high Diastereo- and enantioselectivities without relying on chiral catalysts, thus advancing sustainable asymmetric synthesis. Building on our group's extensive work in analyzing complex reaction mechanisms, [3] this study is the first to uncover the mechanistic insights of the i-HSC pathway.

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Selective Monoarylation of Aqueous Ammonia with Aryl Chlorides under Aerobic Conditions

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Abstract Category

Catalysis

Abstract

The direct arylation of ammonia is a crucial synthetic protocol with applications in pharmaceuticals, materials, and agrochemicals.[1] Nearly 20-25 % of pharmaceuticals feature a link between an aromatic ring and a nitrogen atom.[2] Despite its potential, challenges like ammonia's strong coordination with metals and the need for expensive catalysts have hindered its development.[3] Herein, we report a sustainable, air-stable catalyst capable of efficient, selective monoarylation of ammonia with aryl chlorides in aqueous medium under mild conditions without cocatalysts or ligands with low loading of catalyst

References

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Sustainability: Role of Chemical Sciences in Green Energy

Shristi Singh

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Abstract Category

Green Chemistry

Abstract

This paper explores the role of green chemistry in promoting sustainability and addressing global environmental challenges. Green chemistry emphasizes the design of chemical processes and products that minimize harmful substances, thereby contributing to a cleaner environment and more efficient energy systems. By examining the principles and methodologies of green chemistry, including the integration of renewable materials and energy-efficient processes, the study highlights its importance in achieving sustainable development. It also explores how green chemistry intersects with global initiatives such as the "energy trilemma" and the circular economy, focusing on reducing greenhouse gas emissions and improving resource efficiency. The study underscores the potential of chemical sciences in advancing sustainable technologies, including energy storage solutions and waste reduction methods. Through a comprehensive analysis of key practices, this paper demonstrates how green chemistry can shape a resilient, eco-conscious future by fostering innovation and aligning with global sustainability goals.

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The comparison of physicochemical features and catalytic activity of synthesized mesozeolites for the esterification reaction of dibutyl itaconate

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Abstract Category

Catalysis

Abstract

In this research, an effort has been made to transform microporous zeolite H-BEA to hierarchical zeolite (MDYK, MCYK, MTYK) by employing controlled desilication post modification in the presence of dodecyl trimethylammonium bromide (DTAB), cetyltrimethylammonium bromide (CTAB), tetradecyltrimethylammonium bromide (TTAB) and yeast. It involves comparison of the physicochemical properties and catalytic activities of synthesized mesozeolites. Hierarchical H-BEA catalysts were prepared through controlled desilication followed by room temperature recrystallization. The physicochemical characteristics of the samples were analyzed using various techniques such as SEM, wide and low angle XRD, FT-IR, TGA, NH₃-TPD, and N₂ sorption isotherm analysis. The catalytic activities of the developed mesozeolites (MDYK, MTYK, MCYK) were evaluated in esterification of biomass derived itaconic acid (ITA) with *n*-butanol. The study involves optimizing reaction parameters such as the molar ratio of IA to *n*-butanol, catalyst concentration, and reaction time.

Upload Extended Abstract File

Synthesized cellulose nanocrystals from agricultural waste and utilized as flow improver in waxy crude oil

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Abstract Category

Flow chemistry

Abstract

The formation of wax or paraffin deposits in pipelines at lower temperatures, especially in the winter, poses major challenges for the upstream petroleum sectors when crude oil is produced or transported. More than a few mitigation methods are employed to address these issues, however, Pour Point Depressants (PPDs) can be a practical and economically feasible solution to improve the cold flow characteristics of crude oil. Nevertheless, the majority of the commercially synthesized PPDs on the market are developed from either hazardous chemicals, or nonbiodegradable, and pose environmental risks. So, the current study has concentrated on extracting natural biopolymer, particularly cellulose from sugar cane bagasse, easily accessible agricultural waste. The microcrystalline cellulose is then converted into nanocrystals following acid hydrolysis. The synthesized nanoparticles are further transesterified using a fatty ester obtained from sesame oil and applied as PPD (SOPE-CNCs) to ensure the flowability of Indian waxy crude oil. The SOPE-CNCs nanoparticles were treated with Indian waxy crude oil at varying dosages from 100 to 500 ppm. The pour point was depressed by 15°C after incorporating 200 ppm of SOPE-CNCs, and crude oil tends to perform like a Newtonian fluid after modified cellulose nanoparticles are doped. After adding 200 ppm SOPE-CNCs nanoparticles, a viscosity reduction of more than 90% was seen at 30°C, particularly near the pour point. Tests of biodegradability confirmed the environmental friendliness of SOPE-CNCs nanoparticles and highlighted its potential as a long-term substitute for conventional PPDs.

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Triazine-Carbazole Conjugates pH-Responsive Covalent Organic Polymers and their Energy Storage Application

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Institute of Chemical Technology, Matunga, India

Abstract Category

Material Science

Abstract

1. Introduction: Porous organic polymers have received considerable attention and have emerged with promising potentials due to their heteroatom-containing structures and high surface areas, which can offer high electrochemical performance in energy applications. Bis-carbazoles are a class of molecules with numerous applications in organic electronics, sensors and high thermal stabilities making them a suitable candidate for this study. We report synthesizing a series of novel 2D carbazole–triazine-based COPs by varying the reaction time to study the effect on factors like surface, pore size, and pore diameter.

2. **Significant Results and Discussion:** COPs were synthesized using carbazole-triazine rings as a core for preparing the monomers which were polymerized to form the COPs. They were thoroughly characterized by techniques like IR, SEM, BET, CHN, SSNMR, XRD.Synthesized COPs exhibit a real-time reversible response in the visible spectrum in the presence of acidic and basic fumes. Upon protonation with acidic fumes resulted in protonation of polymers which was studied using Dielectric constants with temperatures from RT to 100°C which demonstrated an increase in proton conductivity with increase in temperature. This property of protonation-deprotonation was used for application in the field of energy storage. A study of protonated and non-protonated forms of the polymers demonstrated good energy storage capacity without the use of any binders. These materials showed excellent cyclic stability upto 90% retention of specific capacitance after 5000 cycles.

3. **Conclusion:** Synthesized COPs therefore show varying surface areas with changes in reaction conditions along with being pH-responsive. The proton-conducting property was well-explored energy storage application.

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Innovative Chemical Solutions for Refinery and Fuel Applications: Advancements by HPCL R&D Centre

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Abstract Category

Material Science

Abstract

The HPCL R&D Centre is a leader in developing innovative chemical solutions for the refining, fuel, and marketing sectors. Using advanced research and facilities, it has created a range of high-performance chemicals, including refinery process chemicals like neutralizing and filming amine corrosion inhibitors to protect against CDU and DHT overhead corrosion. It also developed antifoulant additives for heat exchangers, wax modifiers for refining, demulsifiers for oil-water separation, and viscosity-altering additives for bitumen. In fuel additives, the centre has created lubricity enhancers, multifunctional additives, and pour point depressants to improve fuel performance. Additionally, it produces corrosion inhibitors for pipelines and LPG combustion additives to enhance efficiency and reduce emissions. These innovations support HPCL's goals of sustainability, operational excellence, and technological leadership.

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Utilization of Nickel-supported catalysts for the synthesis of biomass-derived value-added chemicals

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Abstract Category

Catalysis

Abstract

Lignocellulosic biomass is a cost-effective and abundant resource for biofuels and value-added chemicals. Catalytic hydrogenation of platform chemicals (furfural and levulinic acid) and reducing sugars (glucose and xylose) using non-noble nickel-based catalysts provides a sustainable route to produce compounds like furfuryl alcohol, tetrahydrofurfuryl alcohol, cyclopentanone, y-valerolactone, xylitol, and sorbitol vital for industries such as pharmaceuticals, polymers, and flavors. Nickel catalysts, supported on materials like clays and apatites, exhibit high surface areas and metal-support synergy, facilitating selective transformations. Catalyst preparation methods, including wet impregnation and coprecipitation, enhance nickel dispersion and support interactions. XRD and HR-TEM analyses of Ni/Organoclay and Ni-HAP confirmed nanoscale features, while BET analysis indicated mesoporosity and increased surface area for co-precipitated Ni-HAP. TGA-DTA analysis revealed CTAB-Ni interactions in Ni/organoclay, enhancing performance. Hydrogenation reactions conducted in high-pressure autoclaves demonstrated excellent selectivity and yield. These catalysts enable diverse reaction pathways, including dehydration, hydrogenation, and decarboxylation. Controlled conversion of furfural and levulinic acid to valuable derivatives like furfuryl alcohol and y-valerolactone highlights the significance of optimizing catalyst support, such as organoclays and hydroxyapatite. Reusability studies confirm their structural stability, underscoring economic and practical viability. Nickel-supported catalysts thus present a promising, sustainable approach for biomass conversion to industrially relevant chemicals.

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Catalytic performance and kinetics for the synthesis of N-isopropylaniline using organoclay

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Institute of Chemical Technoloy, Mumbai, India

Abstract Category

Catalysis

Abstract

Catalytic performance and kinetics for the synthesis of N-isopropylaniline using organoclay was developed and validated across a range of temperatures. The catalyst was synthesized and thoroughly characterized to determine its structural and morphological properties, revealing synergistic effects of nickel and organoclay that enhance its potential in organic synthesis. To the best of our knowledge, the reductive alkylation of aniline using Ni/Organoclay has not been previously reported, and kinetic modeling for this reaction remains scarcely explored. This study addresses the gap by systematically investigating the kinetics of aniline reductive alkylation with acetone using Ni/Organoclay as the catalyst. The influence of key reaction parameters, including temperature, pressure, catalyst loading, reactant mole ratio, agitation speed, and reactant concentrations, on the reaction kinetics was thoroughly examined. The kinetic analysis included the determination of critical parameters such as reaction rates, activation energies, and heats of adsorption. A series of rate equations were derived to fit experimental data from batch reactor studies. The Langmuir-Hinshelwood-Hougen-Watson (LHHW) model, based on competitive associative adsorption and surface reaction between the Schiff base intermediate and hydrogen as the rate-limiting step, was found to accurately represent the experimental observations.

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Synthesis of sorbitol by the hydrogenation of glucose using a nickel-based catalyst

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¹ICT, Mumbai, India. ²NCL, Pune, India

Abstract Category

Catalysis

Abstract

In this study, we investigated the hydrogenation of glucose to sorbitol using a Ni/bentonite catalyst. The catalyst was prepared via the wet impregnation method and analyzed using various techniques to assess its surface morphology, surface area, metal content, and pore size. We examined several reaction parameters, including temperature, hydrogen pressure, metal loading, and catalyst loading, achieving a glucose conversion rate of 91% and sorbitol selectivity of 95%. To study the glucose hydrogenation process, we applied kinetic models such as the Eley–Rideal and Langmuir–Hinshelwood–Hougen–Watson models.

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Utilization of Hydroxyapatite catalyst in Organic Synthesis

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Abstract Category

Catalysis

Abstract

The production of chiral amines, such as (R)-3-aminobutanol, is crucial for synthesizing small-molecule drugs but often faces challenges like limited substrate compatibility and low catalytic efficiency. A novel method addresses these issues by employing nickel-hydroxyapatite (Ni-HAP) as a catalyst to synthesize 3-aminobutanol from 4-hydroxy-2-butanone. Ni-HAP, an eco-friendly and efficient reagent, enables the conversion of oximes into amines under mild conditions. This method provides significant advantages, including reduced costs by eliminating the need for expensive catalysts and offering reaction conditions conducive to large-scale industrial applications. Its environmentally sustainable approach minimizes ecological impact, aligning with the principles of green chemistry. When applied to the synthesis of pharmaceutical compounds like dolutegravir sodium, this methodology streamlines drug development, combining scalability with economic and environmental benefits. The process represents a critical advancement in chiral amine production, supporting innovation and sustainability in modern pharmaceutical manufacturing

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One pot, two-step synthesis of 2-(subs.)-1H-benzimidazoles using wet copper slag as magnetically separable and recyclable catalyst.

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Abstract Category

Catalysis

Abstract

This work describes the first-ever use of Wet copper slag for 2-(subs.)-1*H*-benzimidazoles synthesis. It is a by-product of the copper refining and smelting processes utilized as a basic catalyst in the present work. Wet copper slag is prepared by immersing a natural copper slag in water to improve the hydroxyl group and, hence, basicity. Iron oxide content in the copper slag helps provide the basic environment and uses surrounding air for the successful oxidative condensation of imines and ophenylenediamine. Various aldehydes reacted well with *p*-anisidine for imine synthesis. Further reaction with substituted o-phenylenediamine and o-phenylenediamine gives desired 2-(subs.)-1*H*-benzimidazoles in environmental-friendly ethanol: water (9:1) as solvent at 85 °C within 40 to 60 min. The present method showed critical advantages of mild reaction conditions, wide availability, recyclability, and magnetic separability of a Copper-slag with moderate to excellent product yields. Overall, the present approach offers a promising route for the efficient and sustainable synthesis of 2-(subs.)-1*H*-benzimidazoles, which have a wide range of applications in various fields, including pharmaceuticals, agrochemicals, and materials science.

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Elimination of Aniline Blue from Synthetic Medium using Water Hyacinth Root: Batch Study

Shraddha Sinha, Subhasis Roy, Sudip Kunar Das

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Abstract Category

Waste Management

Abstract

In the present study, Water Hyacinth (WH) Roots are used as a bio-adsorbent to remove Aniline Blue (AB) in the Batch process. WH is an aquatic plant; hence the roots can adsorb dyes from running water and stagnant water. Adsorption tests were carried out in batch mode, with various operational parameters such assolution pH, initial dye concentration, adsorbent dosage and contact time being investigated to improve the process. At a pH of 5 and a dye concentration of 100 mg/L, the highest adsorption was reported, which were regarded ideal operating conditions. At various temperatures, different isotherm models such as Langmuir, Freundlich, Temkin, and Dubinnin-Radushkevich were utilized to explore adsorption equilibrium. By fitting the obtained adsorption data to the Freundlich isotherm model, the multilayer adsorption process was confirmed. Furthermore, fitting adsorption kinetic data to several kinetic models, such as pseudo first order, second order, and intraparticle diffusion types, shows that AB adsorption on WHR surface fits the pseudo second order kinetic model well. Various thermodynamic parameters, such as standard entropy (ΔS°), Gibbs free energy (ΔG°) , and enthalpy (ΔH°) , were also experimentally analysed, revealing that the adsorption process was both exothermic and spontaneous. Finally, the adsorbent's adsorption mechanism was elaborated, and a regeneration method for repeated usage was investigated. WHR, it can be inferred, may be a cost-effective and locally available option. Safe disposal of the adsorbent was carried out through incineration process and ash transportation to road construction site.

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Synthesis of Bioactive Glass Ceramics in the Calcia-Alumina-Silica (CAS) System -Effect of reinforcement by addition of nano-Zirconia

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Abstract Category

Material Science

Abstract

In 1969, Larry L Hench invented the Bioglass[®] 45S5, and since then, bioactive glass and glass ceramics have been established as essential biomaterials. A good amount of research has been devoted to studying the effect of deploying various additives to enhance the physical, mechanical and chemical properties of these materials. ZrO₂ - containing glass and glass ceramics have shown promising outcomes due to their excellent reinforcing properties. In this present work, a set of 3 nano-ZrO₂ containing bioactive glass and glass ceramics of composition 37.5 nano-SiO₂-(17-X) Al₂O₃-26.5CaO-11.5CaF₂-7.5P₂O₅-X nano-ZrO₂ (where, X= 0.75, 1.7, 2.7, all in mol %) were synthesised by using melt-quenching and subsequent sintering techniques. Standard characterisation procedures of FTIR, XRD, SEM/TEM, DTA/TGA and Vickers hardness tests were performed to examine the chemical and crystalline phase composition, crystallisation characteristics, mechanical strength, structure and surface morphologies. The in vitro bioactivity was determined by immersion in simulated body fluid (SBF) solution and bio-compatibility was examined by cytotoxicity assessment. Fluorapatite (Ca₅(PO₄)₃F) and Anorthite (Ca(Al₂Si₂O₈)) at higher sintering temperature of 1000°C constituted the primary crystalline phases. Adding nano-titania with nano-zirconia enhanced the glasses; thermal stability, the glass ceramics; micro-hardness and bioactivity. The formation of nano meter-size hydroxyapatite (HAp) on the glass-ceramics samples due to immersion in SBF confirmed the good bioactive nature of the samples. The non-toxic nature of the samples towards living cells was demonstrated by cytotoxicity assessment.

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Zirconium oxide nanoparticles catalysed chemo selective reduction of α -keto esters and amides

Anuprita Mathkar

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Abstract Category

Catalysis

Abstract

This study reports the hydrothermal synthesis, comprehensive characterization, and catalytic evaluation of zirconia nanoparticles with various phases for chemoselective reduction of α -keto esters & amides. These nanoparticles exhibited remarkable catalytic activity in highly chemoselective reduction reactions in which monoclinic zirconia NP's show excellent efficiency, particularly in the reduction of α keto esters and amides utilizing NaBH4 as the reductant and methanol/ethanol as environmentally benign solvents. A significant advancement is demonstrated through the achievement of 83-99% conversions for α -hydroxy esters and α -hydroxy amides in a remarkably short time frame of 20-25 minutes. Furthermore, the ZrO2 nano-catalyst demonstrates remarkable reusability, maintaining catalytic activity through five consecutive cycles without significant decline. A combination of FE-SEM, XRD, EDX-elemental mapping, FTIR, BET analysis, and Ammonia TPD techniques was employed to investigate the morphology, thermal stability, crystal structure, and surface acidity of fresh ZrO2 NP's. The TPD results reveal that M-ZrO2 exhibits superior acidic properties compared to T-ZrO2. Furthermore, the catalyst is easily recoverable and may be reused five times without significantly decreasing reactivity

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Synthesis of Alk-2-ynl Weinreb Amide via Pd/Cu- catalysed Oxidative Carbonylation of Terminal Alkynes

Bharati Mourya, sandip gadge, Bhalchandra Bhanage

Institute Of Chemical Technology, Mumbai, India

Abstract Category

Catalysis

Abstract

Synthesis of alk-2-ynl-Weinreb Amide via Pd-catalyzed oxidative carbonylation of terminal alkynes and N,O-dimethylhydroxylamine hydrochloride at room temperature under low CO/O2 pressure reported for the first time. This protocol offers tolerance of various functional groups under mild reaction conditions. The protocol incorporates aromatic and aliphatic substituted alkynes through a one-step oxidative carbonylative route toward the desired alkynyl Weinreb amide, which are of significant synthetic importance as valuable building units.

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Selectivity Tuning Using Rh/PTABS Catalytic System for the Hydroformylation of Eugenol

Rupali Prajapati, Anant Kapdi, Rajesh Sahu, Bhalchandra Bhanage

Institute of Chemical Technology, Mumbai, India

Abstract Category

Catalysis

Abstract

Rhodium catalyzed hydroformylation of eugenol was carried out by using PTABS (4-(1,3,5-triaza-7-phosphaa damantan-1-ium-1-yl)butane-1-sulfonate) as a water-soluble ligand and CTAB (cetyltrimethylammonium bromide) as a phase transfer agent. The reaction conditions had a direct impact on the chemoselectivity of the system, which was capable of the formation of a variety of products; nevertheless, aldehyde yields of up to 93% were obtained with appropriate selectivity tuning. The inclusion of a water-insoluble promoter ligand, xantphos along with PTABS improved the regioselectivity of the system manifold and accelerated the reaction through interfacial catalysis. Various parameters such as catalyst precursor concentration, temperature, Rh/PTABS ratio, syngas pressure, CTAB concentration and volume of the aqueous phase were evaluated with 80 °C, 25 bar pressure for 1.5 h being the optimized reaction conditions. This catalytic system could be recycled for up to three consecutive cycles.

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Furfural: An Efficient Platform Molecule as a CO Surrogate in Palladium Catalysed Synthesis of α , β -Alkynylamides

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Abstract Category

Waste Management

Abstract

Biomass-derived furfural was used as a CO surrogate for the first time in the oxidative Ndealkylation/carbonylation of various aliphatic and cyclic tertiary amines with terminal alkynes to produce alk-2-ynamides. This reaction employed O_2 as an ideal oxidising agent and used a Pd/C catalyst with KI as an additive in a base free and ligand free condition. Notably, the selective sp³ C-N bond cleavage of tertiary amines led to its potential application as an amine source. The typical and simple route provides another option for producing a broad variety of alk-2-ynamide derivatives in environmentally friendly and efficient way under mild conditions. This method also displays notable reusability.

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Fe-Catalyzed, Solvent-Controlled, Switchable Routes for the Domino Construction of 2,4-Disubstituted and 4-Substituted Quinoline Scaffolds

Prafull Jagtap, Bhalchandra Bhanage

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Abstract Category

Catalysis

Abstract

In this report, we unveil a highly efficient novel protocol for the domino synthesis of 2,4-disubstituted and 4-substituted quinoline scaffolds. The developed strategy involves earthabundantFe-catalyzed, solvent-controlled, switchable routes for the selective construction of 2,4-disubstituted and 4-substituted quinoline frameworks, achieved by using either trifluoroethanol(TFE) or methanol (MeOH) as a solvent. By employing TFE as a solvent in Path A, the alkyne itself serves as a dual synthon through Fe-catalyzed in situ C(sp)–C(sp) bond cleavage, enabling the synthesis of two important molecules: 2,4-disubstituted and 4-substituted quinolines. Later, upon switching the reaction medium from TFE to MeOH for Path-B, only 4-substituted quinolines were obtained extensively. In this Path-B, Fe-catalyzed oxidation of methanol was observed and heremethanol functioned as both a solvent and an environmentally benign carbon source. Both of these strategies were utilized to prepare a broad range of mono- and di-substituted quinoline derivatives. In the application section and for practical utility, the scale-up studies, along with the photophysical properties of the synthesized quinoline moiety are also demonstrated.

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Iridium-Catalyzed Electrooxidative Annulation of Naphthol with Acrylate via C-H Bond Activation for the Synthesis of Naphtho[1,8-bc]

Nilam Patil

Institute of Chemical Technology, Mumbai, India

Abstract Category

Electro Chemistry

Abstract

This work discusses the synthesis of naphtho[1,8-bc]furan derivatives using an iridium-catalyzed electrochemical coupling of naphthols and acrylates. Ir-catalyzed electrochemical C-H annulation takes place inside a supporting catalysis manifold, enabling electrooxidative C-H acrylation via weak O-coordination. This application provides a practical approach for generating a variety of naphtho[1,8-bc]furan derivatives in high to moderate yields.

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Ionic Liquid Catalysed Synthesis of Benzimidazolone from Ortho-Phenylenediamine in the presence of Carbon Dioxide as a carbonyl source under solvent free condition.

Satish Chauhan, Bhalchandra Bhanage

Institute Of Chemical Technology, Mumbai, India

Abstract Category

Catalysis

Abstract

In this study, we report the synthesis of 2-benzimidazolone derivatives from o-phenylenediamine using carbon dioxide as a carbonyl source under mild reaction conditions, facilitated by bifunctional protonic ionic liquids (PILs) as catalysts. We synthesized six PILs by reacting the superbases 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) with proton donors such as Trifluoroethanol (TFE), Cyclopropane carboxylic acid (CPCA), and 2,2,2-Trifluoroacetic acid (TFA). Among the synthesized ionic liquids, [TBDH+][TFE-] proved to be the most effective catalyst, achieving high conversion rates of o-phenylenediamine to 2-benzimidazolone at 1 bar CO₂ pressure and 60°C. The reaction conditions were optimized, and the use of [TBDH+][TFE-] PIL resulted in excellent product yield, demonstrating its superior catalytic performance. Notably, this PIL catalyst could be reused for up to six cycles without significant loss of activity, highlighting its excellent stability and recyclability. The process was carried out under mild, solvent-free conditions, offering a greener alternative to traditional methods that often require high temperatures, pressures, or expensive catalysts. This method provides an efficient, sustainable, and environmentally friendly approach for synthesizing 2-benzimidazolone derivatives, which have significant applications in pharmaceuticals and materials science. The use of CO₂ as a feedstock not only reduces greenhouse gas emissions but also contributes to the development of valuable compounds with high industrial relevance.

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Vanillin Hydrogenation in aqueous phase over Ruthenium catalysts

Manisha Sapate, Prakash Vaidya

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Abstract Category

Catalysis

Abstract

In this study, the catalytic aqueous phase hydrogenation of Vanillin (VL) to Vanillyl alcohol (VA) was investigated with a focus on optimizing catalyst support, active metal type, and processing parameters. Conducted in a 100 ml stainless steel batch reactor, the study aimed to enhance the Conversion, selectivity and yield of vanillin hydrogenation. Reactions were performed under various conditions, including temperatures of 318-338 K, VL concentrations of 16.4-65.7 mM, hydrogen pressures of 0.69-2.07 MPa, catalyst loadings of 0.2-0.8 kg/m³, and a reaction time of 1 hour. High-performance liquid chromatography (HPLC) analyzed the products. Ruthenium-based catalysts supported on different carbonaceous materials were synthesized and characterized using techniques such as XRD, BET, SEM. The CNT-supported catalyst achieved a conversion rate of up to 98%, with a VA selectivity of 70% and a yield of 68%. In comparison, the carbon-supported catalyst showed a conversion of up to 88%, maintaining the same selectivity of 70% and a yield of 61%.

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Enhanced Selectivity in Phenol Alkylation Using Modified Clay-Based Catalysts: A Sustainable Approach

Aishwarya Poman, Paresh Kamble, Virendra Rathod, Lakshmi Mannepalli

Institute of Chemical technology, Mumbai, India

Abstract Category

Catalysis

Abstract

This study investigates the alkylation of phenol with tert-butanol (TBA) over modified clay catalysts to synthesize p-tert-butylphenol (PTBP), a valuable intermediate in resins, pharmaceuticals, and antioxidants. Bentonite was modified via ion exchange with Fe, Zn, and Zr to enhance catalytic activity. Fe-bentonite exhibited the highest performance among the catalysts, achieving 100% TBA conversion and 81% PTBP selectivity under optimized conditions (80°C, 10:1 phenol: TBA molar ratio). Catalyst characterization using SEM, XRD, BET, and FTIR revealed significant surface and structural modifications. Reaction kinetics followed a first-order model, with an activation energy of 8.82 kcal/mol, highlighting efficient catalysis. Catalyst reusability was demonstrated over three cycles with negligible performance loss. These findings establish Fe-bentonite as a sustainable, eco-friendly catalyst for industrial phenol alkylation.

Upload Extended Abstract File

Process intensification for synthesis of 2-ethylhexyl acrylate using heterogeneous catalyst.

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Abstract Category

Catalysis

Abstract

Acrylic esters are highly versatile monomers extensively utilized in manufacturing coatings, adhesives, textiles, and plastics. Their production predominantly involves the esterification of acrylic acid with various alcohols. This study explores process intensification for the esterification of acrylic acid (AA) with 2-ethylhexanol (2EH) to produce 2-ethylhexyl acrylate (2EHA) using ultrasound-assisted technology. The reaction was conducted in a batch reactor under atmospheric pressure, with Amberlyst-15 dry ion exchange resin as a heterogeneous catalyst. The effect of various reaction parameters has been studied for the activity of the reaction. The comparative study between conventional and ultrasound-assisted approach have been performed. A comparative analysis of conventional and ultrasound-assisted esterification revealed that the ultrasound-assisted approach is more efficient, achieving superior catalytic activity with reduction of reaction time.

Upload Extended Abstract File

One-Pot Synthesis of Aldimines via Single Screw Extrusion: A Mechanochemical Approach

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Abstract Category

Green Chemistry

Abstract

This study presents a one-pot synthesis of aldimines via single screw extrusion (SSE), employing a mechanochemical approach that operates under solvent-free conditions. The method enables the direct condensation of aldehydes and primary amines, providing a sustainable and efficient route to aldimines. Amine substrates such as cyclohexanol amine, the methyl ester of L-phenylalanine, and ethylenediamine were successfully employed, yielding products in good to excellent yields. The methodology was further validated by scaling up the reaction, demonstrating its feasibility for both laboratory and industrial applications. Thermal studies using differential scanning calorimetry were conducted to compare the grinding method with the extrusion approach, highlighting the enhanced efficiency of the SSE technique. The synthesized compounds were characterized using a range of analytical tools like IR, GC-MS, NMR, single crystal XRD and HRMS. The use of single screw extrusion as a mechanochemical tool provides a straightforward, one-pot solution that can be applied to a wide range of organic syntheses.

Upload Extended Abstract File

A Comparative study between ZIF-Co-Microneedles and ZIF-Co-67 nanozymes: H2O2 detection and unlocking the intrinsic peroxidase activity

Santosh Sethi

Institute of Chemical technology, Mumbai, India

Abstract Category

Biotechnology & Biochemical engineering

Abstract

Nanozymes, a novel class of metal-organic frameworks (MOFs), offer exceptional catalytic activity, mimicking natural enzymes while being cost-effective and efficient. This study presents the synthesis, characterization, and comparative analysis of the peroxidase-like activity of two nanozymes: ZIF-Co-Microneedles and ZIF-Co-67, for the detection of hydrogen peroxide (H₂O₂), a critical biomarker in biomedical diagnostics. ZIF-Co-Microneedles were synthesized by mixing Co(NO₃)₂·6H₂O, 2methylimidazole, PVP, and PEG in water, while ZIF-67 was prepared using $Co(NO_3)_2 \cdot 6H_2O$ and 2methylimidazole in methanol. Both nanozymes were characterized using SEM, DLS, UV-VIS, and FTIR, confirming their successful synthesis and structural attributes. ZIF-67 exhibited a polyhedral morphology with a particle size of ~600 nm, whereas ZIF-Co-Microneedles displayed a rod-shaped structure (1–2 μ m length, ~400 nm diameter). The peroxidase-like activity was evaluated using TMB and H_2O_2 under optimized conditions of pH, temperature, and solvent. Both nanozymes demonstrated high catalytic efficiency with outstanding repeatability (coefficient of variation <10%). The limits of detection for H_2O_2 were 26 nM for ZIF-Co-67 and 29 nM for ZIF-Co-Microneedles. ZIF-Co-67 exhibited superior activity and sensitivity, making it a promising candidate for H₂O₂ detection in biomedical applications. This study highlights the potential of MOF-based nanozymes in enzymatic catalysis and their promising application in biosensing and diagnostics.

Upload Extended Abstract File

Novel Low-Bandgap Organic Dyads Derived from Diketopyrrolopyrrole for Efficient Single-Component Organic Solar Cells

Narayanaswamy Kamatham

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Abstract Category

Renewable energy

Abstract

In order to attain high performance in single-component organic solar cells(SCOSCs), it requires the designing of light-harvesting structures that can absorb light across a wide range from visible to near-infrared (NIR) wavelengths. In this investigation, two novel dyad materials, denoted as SPS-BF-Full and SPS-BT-Fullare designed and synthesized, consisting of covalently linked benzofuran (BF)and benzothiophene (BT) functionalized thiophene–diketopyrrolopyrrole (TDPP)as donor and N-methyl fullero[60] pyrrolidine as the acceptor, respectively. The incorporation of a phenyl bridge between TDPP and fullero[60] pyrrolidine enhances light absorption in SPS-BF-Full and SPS-BT-Full, resulting to a high short-circuit density (JSC). Consequently, the SCOSCs utilizing SPS-BT-Full and PS-BF-Full attained overall power conversion efficiency (PCE) of 6.28 and 7.35%, respectively. The high photovoltaic performance of OSCs utilizing SPS-BF-Full is mainly attributed to its higher external quantum efficiency and balanced hole and electron mobility ($\mu_e/\mu_h = 1.39$), along with improved charge carrier extraction, revealing more effective charge transport in comparison to SPS-BT-Full counterparts.

Upload Extended Abstract File

Visible Light-Induced Denitrogenative Annulation Reaction of 1,2,3-Benzotriazin-4(3H)-ones with Alkenes and Alkynes via Electron Donor-Acceptor (EDA) Complex Formation: A Sustainable Approach to Isoindolinones and Isoquinolinones Synthesis

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Abstract Category

Catalysis

Abstract

An efficient method for the synthesis of isoindolinone and isoquinolinones from 1,2,3-benzotriazin-4(3H)-ones under visible light is described. The reaction of 1,2,3-benzotriazin-4(3H)-ones with activated alkenes such as acrylonitrile, vinyl ketone, acrylates and vinyl sulfones in the presence of DIPEA under blue led light irradiation gave the isoindolinones in good to high yields. In a similar manner, the reaction of aromatic terminal alkynes with 1,2,3-benzotriazin-4(3H)-ones gave 3 substituted isoquinolinones. This method avoids the use of any metal- and external photocatalysts and is believed to proceed via an electron-donor acceptor (EDA) complex formation facilitated by DIPEA and 1,2,3-benzotriazin-4(3H)-ones. The practical applicability of these reactions is also demonstrated by performing gram scale synthesis of isoquinolinones and isoindolinones. Moreover, the utility of this method was showcased through the synthesis of anxiolytic drug pazinaclone analogue in high yield.

Upload Extended Abstract File

Chlorosulfonic acid activated peanut husk carbon for dye removal

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Abstract Category

Waste Management

Abstract

Activated carbon obtained from peanut husk is used for removal of methylene blue (MB) a cationic dye from an aqueous solution. The batch adsorption study was performed to identify the effect of initial concentration, pH, temperature, contact time and adsorbent dosage on the adsorptive capacity of MB. This bio-sorbent was characterized by BET analyzer, SEM analysis and FT-IR spectroscopy. The adsorption data was analyzed based on models of adsorption isotherms, Langmuir, Freundlich, and Redlich Peterson. Equilibrium data for adsorption fitted with Langmuir adsorption isotherm model implying that the adsorption is monolayer with adsorptive capacity of 119 mg/g. The dye removal was found to enhance with an increase in bio-sorbent dosage, time and decrease with initial dye concentration and temperature. The pseudo first order and pseudo second order kinetics models was studied for kinetics MB adsorption. The rate of adsorption inveterate to pseudo second order kinetics with good correlation. The kinetic and thermodynamic parameters are evaluated and are discussed.

Upload Extended Abstract File

Catalytic Solvolysis-Hydrolysis of Rigid Polyurethane Foam: A Green Approach for Polyol and Aniline Recovery

Vinayak Kadam

Institute of Chemical Technology, Mumbai, India

Abstract Category

Waste Management

Abstract

Chemical recycling of waste rigid polyurethane foam (RPUF) offers a sustainable pathway toward green chemistry and circular resource utilization by recovering high-value polyols and aromatic amines. Achieving rapid degradation and efficient separation of products under mild conditions remains a significant challenge. This study presents a catalytic solvolysis strategy using sodium ethoxide, enabling the selective cleavage of carbamate and urea bonds in RPUF. Various alcohols were explored as solvolysis agents to optimize the process. Complete degradation of RPUF was achieved at 190 °C within 2 hours, yielding polyether polyols and aromatic amines as primary products. The reaction system was uniquely designed to facilitate product separation. Following centrifugation, the system segregates into three distinct phases: the upper layer containing polyol alcohol solution, the middle layer comprising solid benzene derivatives, and the lower layer holding the catalyst solution. This simple phase separation significantly streamlines the recovery and purification of degradation products, minimizing energy consumption. This work underscores the potential of catalytic solvolysis as an effective and environmentally friendly approach for RPUF recycling. It provides valuable insights into the development of sustainable degradation mechanisms and efficient product separation technologies for polyurethane waste management.

Upload Extended Abstract File

In situ nanotechnology - Sustainable low energy Nanoengineering for nanomedicine applications

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Abstract Category

Drug Delivery

Abstract

In Situ Nanotechnology (ISN) is a revolutionary amazingly simple low energy approach to develop drug loaded nanoparticles. It relies on addition of a solution of drug, nanocarrier material and stabilizers into a predefined aqueous medium to generate a ready to administer nanoparticulate dispersion. This technology has been proven for a range of drugs including curcumin, baicalein, Betulin, tamoxifen, Primaquine and Amphotericin B. This method ensures nanoscale particle size, high entrapment efficiency, and enhanced stability while eliminating complex processing steps.

Using this innovative approach, Mitocurcumin Lipomer (MitoCur-Lipo) was designed as a mitochondria-targeted oral nanocarrier. Optimized for gastrointestinal transport through balanced hydrophobic and hydrophilic properties, MitoCur-Lipo enhances mitochondrial accumulation. The formulation exhibited a particle size of ~230 nm, EE >98%, PDI <0.2, high drug loading. Stability studies confirmed >95% drug content with no significant particle size change under accelerated and long-term conditions.

MitoCur-Lipo showed a significantly lower IC₅₀ (0.75 μ M), a 2.17-fold reduction compared to MitoCurcumin (1.63 μ M), and a 52-fold reduction compared to Curcumin (69.54 μ M). MitoCur-Lipo demonstrated a 9-fold reduction in survival fraction and significantly enhanced apoptosis in A549 cells at lower concentrations compared to mitocurcumin. Antiangiogenic studies using the Zebrafish tail fin regeneration assay revealed MitoCur-Lipo's superior efficacy compared to MitoCur, Cur-Lipo, and Curcumin, attributed to targeted mitochondrial delivery facilitated by the lipophilic TPP cation with added advantage of In Situ technology.

Our study demonstrates a simple ISN approach for development of MitoCur-Lipo with desired physicochemical characteristics and high anticancer activity in cell lines.

Upload Extended Abstract File

Waste to Wealth and Safer Bio-based Flame Retardant: A Novel Approach Towards Phosphorus-Functionalized Chitosan-Banana Pseudo-Stem Composite

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Institute of Chemical Technology, Mumabi, India. Bajaj College of Science Wardha, Wardha, India

Abstract Category

Material Science

Abstract

In response to the growing need for eco-friendly flame retardants, researchers have developed bio-based solutions for applying flameretardant finishes to cotton cloths. The current work presents an innovative phosphorus-functionalized chitosan-banana pseudo-stem composite (P-CBPS), which is applied to cotton cloth through a layer-by-layer technique (P-CBPS-C). The P-CBPS-C was wellcharacterized using XPS, SEM, TGA, and FTIR. Additionally, we explored the application of banana pseudo stem sap (BPS) and chitosan combined with banana pseudo stem sap (CBPS) as coatings on cotton fabric (BPS-C and CBPS-C). P-CBPS-C exhibited remarkable flameretardant properties, maintaining its size and shape upon exposure to flame, producing minimal smoke, and resisting ignition for more than 140 s, in contrast to the control cloth (C-C), BPS-C, and CBPS-C samples, which were completely consumed by the flame. C-C burned away in just 5 s, while BPS-C and CBPS-C samples lasted 35 and 60 s, respectively, leaving behind a small amount of char residue. The effectiveness of the flame retardancy of P-CBPS-C was rigorously assessed through tests such as the Limiting Oxygen Index (LOI) and the Vertical Flammability Test (VFT). The LOI value increased from 17.76% for the C-C to 48.44%, and the VFT showed a residual char length of 1 cm, demonstrating its promise in fire protection. This study represents an initial effort to create a P-CBPS composite using a cost-effective and simple method, proving its effectiveness as a flame-retardant material.

Upload Extended Abstract File

Mechanistic Perspectives on the Production of 4-Propyl Phenol via Hydrogenation and Demethoxylation over Ni-Co/Al-SBA-15 Catalysts for the Catalytic Valorization of Eugenol Derived from Renewable Resources

Harsha Dhanwani

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Abstract Category

Catalysis

Abstract

The depletion of resources in the modern period has made the hunt for sustainable substitutes for traditional fuel sources more pressing. Fuel and energy derived from biomass are viable options with much smaller carbon footprints, reducing their negative effects on the environment. One important phenolic molecule that comes from lignocellulosic biomass is eugenol, which offers a chance to produce sustainable energy. This work uses a unique NiCo/Al-SBA-15 heterogeneous catalyst to convert eugenol into 4-propylphenol, a multifunctional chemical used as a disinfectant, flavoring agent, and antioxidant. 100% conversion and 93% yield of 4-propylphenol were achieved under the conditions of 230 oC and 30 bar pressure in an isopropanol medium. Numerous reaction optimization factors were examined, and the catalyst's efficacy and activity were assessed through the use of comprehensive characterisation procedures. The kinetic model was created, and an Arrhenius plot analysis was used to determine the activation energy. The catalyst's resilience and reusability increase its economic feasibility, while the process's clean, green characteristics establish environmental sustainability. By addressing the global need for renewable energy sources with less of an impact on the environment, our research helps to establish cleaner and more effective pathways for the usage of biomass.

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Development of a Predictive Model for Caproic Acid Extraction Efficiency Using Artificial Neural Networks

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Visvesvaraya National Institute of Technology, Nagpur, India

Abstract Category

AI in Chemical synthesis

Abstract

This work addresses the challenge of optimization of caproic acid extraction efficiency, E%. The process involved is critical for various applications in the fields of biofuels, food additives, and fragrances. Chemical extraction by its nature involves complexity due to the presence of several interacting variables such as KD, solvent, and extractant. Traditional experimental attitudes toward optimizing these processes are lengthy, time consuming, and resources demanding. This has motivated the investigation of data-driven ML techniques that present a systematic means for analyzing and predicting outcomes under various conditions with minimum experimentation.

The study Utilizes Artificial Neural Networks (ANNs) to model E% based on a curated dataset refined after originating from peer-reviewed literature. Explainable AI (XAI) techniques, such as SHAP (Shapley Additive Explanations) and Permutation Feature Importance highlighted K_D as the most significant feature, followed by solvent and extractant types. The ANN model was compared with Linear Regression and Support Vector Regression (SVR), demonstrating the effectiveness of ML models in capturing the complexity and non-linearity in chemical processes.

This work is motivated by the need to develop predictive tools that not only reduce the experimental burden but also provide insights into the underlying factors driving extraction efficiency. By integrating model XAI techniques, the study ensures that the predictions are transparent and actionable. The proposed methodology has the potential to significantly advance chemical process optimization and serve as a foundation for future research in related extraction systems.

Keywords: Chemical Extraction, Machine Learning, Explainable AI, Regression

Upload Extended Abstract File

Greener synthesis of 2, 5-Furan dicarboxylic acid via base-free oxidation of 5hydroxymethyl furfural using carbon supported noble metal catalysts

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Abstract Category

Green Chemistry

Abstract

2,5-Furandicarboxylic acid (FDCA) is frequently promoted as a bio-based substitute to the prevalent petroleum-derived terephthalic acid which is used for making polyethylene terephthalate (PET). Current limitations for commercial production of FDCA include the use of excess amount of base additives, resulting in formation of sodium salt of FDCA and humins which necessitates further purification and down streaming. In this work we have compared catalytic activity of carbon supported ruthenium and platinum catalysts for 5-hydroxy methylfurfural oxidation to FDCA in a base-free environment. 2% Ru/C achieved 99.3% conversion of HMF with 21.6% FDCA selectivity using 0.5 mM HMF, 15:1 HMF:Ru at 393 K, 1200 rpm and 0.68 MPa of oxygen under aqueous base-free conditions in 10 hours. Whereas, labmade 3.4% Pt/C based catalyst gave higher yield of 94 % at milder reaction conditions of 368K temperature, 0.35MPa oxygen pressure, catalyst loading of almost 80:1 HMF:Pt ratio using 10 times higher HMF initial concentration. This research provides a greener approach by using carbon supported noble metal catalysts which allow aqueous phase oxidation where FDCA is sparingly soluble, enabling easier product separation unlike non-noble catalysts. The base-free reaction approach helps reducing exotherm, minimize by-products such as humins, reducing color formation and total dissolved solids, enhancing the overall process efficiency, safety and greenness; giving FDCA yield of 94% with carbon balance of 99.4% using lab-made 3.4% Pt/C catalyst.

Upload Extended Abstract File

Low-Energy Free Electrons as Eco-Friendly Agents for Chemical Activation and Reactivity Engineering.

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Abstract Category

Green Chemistry

Abstract

Investigation of collisions between electrons and neutral molecules is of high importance for understanding and development of many naturally and technologically occurring processes.¹ The activation of molecules and controlling the outcome of reactions is a central issue in chemical research. Low-energy electron beam is a physical tool that can achieve this as they are able to precisely dissociate specific bonds of a molecule. They can also initiate the formation of new bonds between two reactants to yield a more complex product or the formation of specific reactive molecular species. ^{2,3}

Upon the resonant capture of a very low-energy electron into an intermolecular bonding combination of π^* orbital of the π -stacked pyridine molecules, they are stabilized but become reactive species. Additionally, the capture of a second electron generates two nucleophilic centers at the nitrogen sites.

Upload Extended Abstract File

A Dual-Action Approach to Mosquito Control: Harnessing Mosquitoes Affinity for Light with Metofluthrin's Lethality

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Guru Tegh Bahadur Institute of Technology, New Delhi, India

Abstract Category

AI in Chemical synthesis

Abstract

Vector-borne diseases transmitted by mosquitoes represent a significant global health challenge, with particular impact in urbanized regions. Recent research has demonstrated that conventional mosquito control methodologies, which typically target single sensory mechanisms, exhibit limited efficacy in contemporary urban environments. The World Health Organization's epidemiological data indicates a concerning trend, with dengue virus cases alone ranging from 100 to 400 million annually in the past two decades.

The limitations of traditional control methods, particularly in densely populated urban areas, necessitate the development of more sophisticated intervention strategies. Current household mosquito repellents, whether targeting olfactory or phototactic responses in isolation, have proven inadequate for comprehensive vector control. This inadequacy is especially evident in congested residential environments, where mosquitoes continue to find novel breeding grounds despite conventional intervention measures. [1]

This study presents an innovative approach that integrates dual sensory targeting: combining mosquitoes' documented attraction to specific light wavelengths with the proven efficacy of metofluthrin vaporization. This methodology represents a significant advancement over single-modality systems, offering enhanced vector control while maintaining environmental safety parameters suitable for indoor deployment.

The research examines the theoretical foundations and practical applications of this integrated approach, with particular emphasis on its potential for creating vector-free indoor environments. By synthesizing established technologies in a novel configuration, this work addresses critical gaps in current mosquito control strategies while maintaining rigorous safety standards.

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Cascade upgrading of biomass-derived levulinic acid to γ-valerolactone (GVL): a biofuel precursor over carbon-based catalysts

Kamleshwar Patle, Jayant Ekhe, Kailas Wasewar

Visvesvaraya National Institute Of Technology Nagpur, Nagpur, India

Abstract Category

Catalysis

Abstract

The cascade upgrading of biomass-derived levulinic acid (LA) to γ -valerolactone (GVL) represents a promising approach for sustainable biofuel production. Biomass-derived γ -valerolactone (GVL) is an important high-quality liquid biofuel or value-added chemical and green solvent for various reactions, commonly produced by levulinic acid's hydrogenation. This transformation involves the hydrogenation of LA to intermediates such as 4-hydroxyvaleric acid (4-HVA), followed by intramolecular cyclization to GVL. The design of high-performance catalysts with superior catalytic universalities is a particularly fascinating and important task since it may be used to manufacture GVL easily and practically. Carbon-based catalysts, including functionalized activated carbons, carbon nanotubes, and graphene-based materials, have garnered significant attention for this process due to their tunable surface chemistry, high surface area, and potential for metal dispersion. Carbon-based catalysts derived from biomass or different organic compounds have a large specific surface area, and plenty of oxygen-containing functional groups can be modified with the various metals, providing the effective characteristics for the cascade hydrogenation-lactonization of alkyl levulinates into GVL.

This paper provides an overview of carbon-based catalysts for LA-to-GVL conversion, emphasizing the roles of surface functionalities, porosity, and functionalization with metal in enhancing catalytic performance. Special attention is given to the synergistic effects of Lewis acidic sites and Brönsted acidic sites supported on carbonaceous materials, enabling selective hydrogenation and acid-catalyzed lactonization. Reaction mechanisms, catalytic pathways, and structure-performance relationships are discussed to provide insight into catalyst design. Challenges like catalyst deactivation, scalability, and integration with green hydrogen sources are addressed.

Upload Extended Abstract File

Exploring Rock Art: Insights into Paint Composition and Weathering Effects through Raman Spectroscopy

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Abstract Category

Material Science

Abstract

Humans have left their mark on the landscape through various forms of inscriptions, decorations, or structures since prehistoric times, including rock art paintings (RAP) and petroglyphs. RAP stands as a remarkable human artistic accomplishment that not only deepens our understanding but also evokes respect, admiration, and excitement in those who experience it. The paint used in RAP was created by mixing pigments with natural binders [1]. Pigment identification is conducted for various purposes, such as understanding the materials and technologies used by ancient peoples, determining optimal preservation methods, ensuring accurate restoration and conservation, verifying the authenticity of artifacts, tracing the provenance of materials, and examining changes in materials and techniques over time [2,3]. Vibrational spectroscopy, particularly Raman spectroscopy, provides molecular structural information hence it is ideally suited for the analysis of inorganic archaeological materials. As, the future of rock art research depends on adopting rigorous scientific methods and fostering a mindset that supports objective testing and verification of hypotheses; This study aims to replicate the paint composition reported in literature, characterize it using Raman spectroscopy, and computationally model the composition to validate the experimental results. Additionally, it seeks to address the research gap in data, as real-time Raman spectra are often complex and affected by background noise from various factors. Moreover, an electron was introduced into the modeled compound to account for its presence in the environment, which can occur due to climatic reasons and may act as a potential weathering agent.

Upload Extended Abstract File

Green synthesis of Ni-Pd NPs over casted on MnO2 nano-rods: Intelligent catalytic support in low temperature fuel cells with optimal Ni inclusion

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Heritage Institution of Technology, Kolkata, India

Abstract Category

Renewable energy

Abstract

Despite vigorous efforts toward mitigating environmental issues, the situation is worsening due to impending energy demand all over the world. In this respect, fuel cell have emerged as one of the best green energy alternatives. Bio-ethanol has become one of the aspiring fuels in direct ethanol fuel cell (DEFC), which bear the advantage of faster reaction kinetics, better water management, and fuel flexibility in ambient environment.

However, due to the difficulty in C-C and C-O bond cleavages, leads to sluggish kinetics within the fuel cell. The present article involves designing, architecture, and fabrication of advanced nano-structured, Pt and carbon-free electrochemical materials, that provide opportunities for ameliorating conductivity, cycling stability, effective surface area, and redox kinetics in DEFC operating, at room temperature. The objective of the present study is to successfully eliminate Pt as well as carbon from the catalyst matrix exploring relatively cheaper elements across the periodic table functionally efficient in energy harvesting.

The two major trials in this investigation include (i) optimal loading of transition co-metals Ni reinforced onto Pd and (ii) replacing meso-carbon by transition metal/ceramic oxides like MnO₂ as support materials for the metal NPs. The synthesis of the binary PdNi/MnO₂ in different metal/co-metal compositional ratio involved cost effective green technique without using solvents and aggressive reducing agents. MnO₂ nano-rods were prepared through solid phase synthesis, while Pd-Ni NPs were over casted on MnO₂ by sono-chemical method. The synthesized catalyst structures were validated in alkaline DEFC by evaluating the electrochemical output parameters.

Upload Extended Abstract File

An efficient ex-situ method for synthesizing 1,2,4-triazolidine-3-thiones using thiosemicarbazide has been developed. This metal-free, ambient-temperature process enables late-stage modification of biologically active compounds. Employing a biodegradable catalyst, it ensures high atom economy, adheres to green chemistry principles, and demonstrates recyclability with significant therapeutic potential.

Vivekanand gavali

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Abstract Category

Green Chemistry

Abstract

An efficient ex-situ method for synthesizing 1,2,4-triazolidine-3-thiones using thiosemicarbazide has been developed. This metal-free, ambient-temperature approach allows late-stage modification of 1,2,4-triazolidine-3-thione-based multidirectional biological activity compound. It supports the rational design of novel agents. The 1,2,4-triazole ring is a pivotal heterocyclic structure widely used in agrochemicals and pharmaceuticals, underscoring the need for efficient, scalable synthesis methods with versatile applications. The process employs a biodegradable catalyst, ensuring high atom economy and adherence to green chemistry principles, enhancing the sustainability and efficiency of the reaction. The method demonstrates notable recyclability of the catalyst, contributing to both environmental and economic benefits, while maintaining significant biological activity potential across multiple therapeutic targets.

Upload Extended Abstract File

Aqueous phase reforming of glycerol using bimetallic copper-containing catalysts

Gargi Borkar, Prakash Vaidya

Institute of Chemical Technology, Mumbai, Mumbai, India

Abstract Category

Green Chemistry

Abstract

Clean energy is an important pillar on which the sustenance of future generations stands. H_2 , with its capacity to carry energy, has become an alternative to conventional fossil-based fuels. Aqueous phase reforming (APR) has emerged as a "greener" process with low temperatures and aqueous-based feeds to reform biomass-derived oxygenates. Glycerol, a surplus by-product of the biodiesel industry, is a conducive substrate for hydrogen production. Hence, an attempt has been made to reform synthetic glycerol, as a model compound of crude glycerol, using bimetallic copper-containing catalysts. Platinum and nickel, known for their capacity to cleave C-C bonds from organic molecules, have been added to a dehydrogenating agent: copper on mesoporous ceria-based support. The addition of these catalysts and the action of parameters including reaction temperatures up to 255°C, reaction periods reaching 4.5 hours, varied catalyst loadings and feed concentrations have been experimented with to produce H₂ via APR. The maximum selectivity of H_2 was 80% when Ni-Cu on mesoporous CeO₂ was used as a catalyst, while it was 79% when the novel bimetallic Pt-Cu was used. All reactions were carried out in batch mode. Characterization of catalysts showed their high surface areas, stability and crystallinity with welldispersed metallic species on the surfaces. Using green solvent, that is water and utilizing waste, followed by a few other green chemistry principles, APR tags itself with greenness, circularity and a producer of highly pure hydrogen for a well-conserved future.

Upload Extended Abstract File

Key Challenges in Electrochemistry for the Production of Green Hydrogen

MAINAK RAY

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Abstract Category

Electro Chemistry

Abstract

The anomalous climate change over the past few decades "reflected in fact" from melting Alfotbreen Glaciers to Air's CO₂ concentration beyond 420 ppm exclaim the reduction of fossil fuel usage and incorporating sustainable and clean technologies, which are essential to accelerating the decarbonization goal. Coupling of Sustainability and favorable economics requires technical advancement and scaling up the process; without it, sustainability can't progress much for large-scale implementation.

Upload Extended Abstract File

Optimization and Kinetic Modeling for Levulinic Acid Production from Sugarcane Bagasse: Experimental Validation and Aspen Plus Simulations

Madhuri Kininge, Parag Gogate

ICT, Mumbai, India

Abstract Category

Renewable energy

Abstract

This work explores the use of acid-catalyzed hydrolysis to produce levulinic acid (LA) from pretreated sugarcane bagasse (SCB), a lignocellulosic biomass. Important variables such as reaction Time, temperature, acid concentration, and solid-to-solvent ratio, RPM that affect the conversion of cellulose and hemicelluloses into LA, formic acid (FA), and acetic acid (AA) has investigated. Aspen Plus simulations and experimental data were used to evaluate the kinetic models for the breakdown of glucose, xylose, and arabinose, which shed light on the reaction processes and ideal circumstances. At 200°C, 4% sulfuric acid concentration, and a solid-to-solvent ratio of 1:60, the maximum LA production (36-40%) and 500 RPM was attained. When compared to traditional procedures, the utilization of biomass that had been ultrasound-pretreated greatly increased LA production. These results aid in the optimization validated the experimental results were found close agreement in conversion efficiencies and yields.

Upload Extended Abstract File

Indole-linked 1,2,3-triazole hybrids as cytotoxic agent targeting EGFR receptor.

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Abstract Category

Drug Delivery

Abstract

Resistance to chemotherapy is an obstacle in cancer treatment. Getting a promising anticancer lead is daunting task. To overcome this problem, the heterocyclic skeletons such as indole and 1,2,3-triazole scaffolds were explored extensively in present study. Better chemical reactivity, greater receptor affinity, and low toxicity make heterocyclic moleties the first choice synthon in drug discovery process. Among heterocycles, indole is one of the most promising moieties. Several indole derivatives were reported as anticancer compounds such as Sunitinib, and Osimertinib. The 1,2,3-triazole is another wellknown heterocyclic scaffold with anticancer property. Epidermal Growth Factor Receptor (EGFR) plays a key role in cancer development. Its over expression, has been observed in different cancer types. In this context, the crystal structure of EGFR (PDB ID: 6P8Q) was considered as the target structure and a series of indole linked-1,2,3-triazoles were synthesized and screened for EGFR inhibitory effect^{1,2}. Among synthesized derivatives, molecule SK-03 found to be potent against L1210 (IC₅₀: 3.0 \pm 0.9 μ M), CEM (IC₅₀: 1.5 \pm 0.6 μ M) and HeLa (IC₅₀: 3.4 \pm 0.6 μ M) cell lines. Intrinsic and extrinsic apoptotic pathways activation was observed during the study. No genotoxicity was found. Molecular docking showed interaction of synthesized derivatives with MET790, LEU788, and ALA743 amino residues of EGFR-6P8Q receptor. Molecule SK-03 found potent derivative against all three tested cell lines. Further study warrant to establish it as potential lead against cancer.

Upload Extended Abstract File

In situ catalytic upgradation of methane in biogas by CO2 hydrogenation - A sustainable approach

Priyanka Shivde

institute of chemical technology, mumbai, India

Abstract Category

Green Chemistry

Abstract

With the goal to meet energy demands and carbon emissions, CO_2 hydrogenation offers a sustainable method of turning CO2 from biogas into synthetic natural gas or methane. CO2, a primary component of biogas, can serve as a basis for hydrogenation, which generates additional CH4, which in turn produces more biomethane. In this work, the upgradation process was investigated by a multifunctional catalyst using a fixed-bed reactor. A multifunctional catalyst was developed by combining mixed metal oxides support for methane synthesis for CO_2 activation. Under different conditions, the catalytic activity was assessed in a fixed-bed reactor, and gas chromatography was used to study the product distribution. With a CO_2 conversion of 70–80% at 300–350°C and atmospheric pressure, the catalyst exhibited remarkable activity and selectivity towards methane. With minimum byproduct formation, the multifunctional nature of the catalyst allowed for selective methane production and improved CO_2 activation.

Upload Extended Abstract File

Green solvent-based Extraction techniques for the Recovery of Biochemicals from aqueous solutions

Ashwini Thakre, Kailas Wasewar

VNIT, Nagpur, India

Abstract Category

Green Chemistry

Abstract

Prolonged use of solvents has harmful impacts on the environment and entire surviving things. Solvent losses represent a major portion of organic pollution, and solvent removal represents a large proportion of process energy consumption. To counter these issues, a range of greener or more sustainable solvents have been proposed and developed over the past three decades. Using environmentally friendly solvents offers a promising avenue for promoting sustainability in various industries. Green solvents, including vegetable oils, ionic liquids, deep eutectic solvents, supercritical fluids, biobased solvents, switchable solvents, and liquid polymers, offer several advantages compared to the traditional solvents in the present time. These solvents possess low toxicity, biodegradability, and reduced environmental impact, making them highly desirable for extraction processes. By minimizing solvent waste and reducing the environmental impact, green solvent-based methods align with the principles of green chemistry, making them a promising option for industries aiming to reduce their ecological footprint. Conventional extraction techniques often involve the use of large amounts of organic solvents, high temperatures, long extraction times, and complex equipment. Green extraction techniques such as microwave-assisted, ultrasound-assisted, or enzyme-assisted methods can overcome these drawbacks. Green technology coupled with the use of green solvents, such as deep eutectic solvents and ionic liquids, industries can actively contribute to sustainable development, minimize environmental harm, and support the transition towards an eco-friendlier future. In the present work, various green approaches have been analyzed and discussed for the recovery of biochemicals such as organic acids, essential oils, and bioactive compounds from aqueous solutions.

Upload Extended Abstract File

Coconut Coir and its Acid-Treated Variants for the Removal of Crystal Violet Dye: Adsorption-Desorption Study, Isotherm, and Kinetic Models

Tamasha Chatterjee, Indrajit Ghosh, Sudip Kumar Das

Univsesity of Calcutta, Kolkata, India

Abstract Category

Waste Management

Abstract

Coconut coir and its acid-treated forms are used in a batch study to extract crystal violet (CV) dye from an aqueous solution. Three variants are used - untreated (UCC), treated with phosphoric acid (PCC), and treated with sulfuric acid (SCC). BET, SEM, and pH PZC analysis are used to characterize adsorbents. The acid-treated variants with a larger BET surface area had better ability to remove dye. The optimum dose for UCC, PCC and SCC is 5 g/L, while the optimum pH is 3 for PCC, 4 for SCC, and 3 for UCC. PCC and SCC, the initial dye concentration is 50 mg/L for all adsorbents, and the contact times are 120 min for UCC, 120 min for PCC, and 90 min for SCC. At the lowest temperature, 303 K, CV dye goes away to the maximum amount. The pseudo-second-order kinetic model fits the Langmuir and Temkin isotherm model quite well. UCC, PCC, and SCC adsorbents have adsorption capacities of 78.25 mg/g, 95.33 mg/g, and 85.47 mg/g for 303 K, respectively. Compared to film diffusion, intraparticle diffusion is more prevalent. By using the Dubinin-Radushkevich (D-R) isotherm model, physisorption is estimated. A spontaneous, favourable, exothermic reaction is indicated by thermodynamic analysis. The most promising desorbing agent for recovering more than 90% of the CV dye is glacial acetic acid (50% to 100%). Particularly in third-world countries' rural areas, small to medium-sized industries effluent containing CV is treated using raw coconut coir and its acid-processed varieties.

Upload Extended Abstract File

Waste Water Treatment using Bio Flocculant Okra Gel

Saurabh Pardeshi

School Of Engineering And Applied Sciences, Kalyan Campus, kalyan, India

Abstract Category

Waste Management

Abstract

This review paper looks at how well the bio-flocculant from okra gel works for treating wastewater, which is an important way to tackle environmental pollution caused by poor wastewater handling. The research uses numbers to evaluate how well okra gel helps sediments settle in different wastewater types, comparing it to regular flocculants. Key results show that okra gel boosts sedimentation rates and lowers chemical oxygen demand (COD) more effectively than traditional methods, indicating it can make treatment better overall. These findings matter especially for healthcare because better wastewater management is essential to prevent waterborne diseases and protect public health. By supporting a sustainable and eco-friendly product like okra gel, this study not only addresses environmental issues but also helps public health efforts. The potential effects of this research reach further into environmental biotechnology, where using natural bio-flocculants might change treatment methods, resulting in more effective, affordable, and environmentally friendly wastewater treatment options. This work highlights the need to include new biotechnological methods in wastewater management systems to create cleaner water and improve community health.

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Deuterium Labelled Compounds by H–D Exchange Using Heavy Water for Improving Pharmacokinetics

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¹Bombay College of Pharmacy, Mumbai, India. ²Bhabha Atomic Research Center BRIT/BARC, vashi, India

Abstract Category

Green Chemistry

Abstract

Medicinal chemists employ bioisosterism in drug discovery process to optimize the efficacy and safety of small molecules. This approach involves substituting one substructure with another to improve physicochemical properties while preserving biological activity. For example substituting the hydrogen atom with deuterium can significantly alter a number of pharmacological properties.

Deuterium, being a stable hydrogen isotope, has diverse applications in the field of new drug discovery programs. Incorporating deuterium enhances metabolic stability and can significantly improve drug efficacy and safety, facilitating the development of deuterated analogues of commercially available medications.

The most common reaction in deuterium chemistry is Hydrogen/Deuterium (H/D) exchange. The C-D bond is 6 to 10 times more stable than a C-H bond, making it more resistant to cleavage. This slow rate of bond cleavage leads to the kinetic isotope effect (KIE) which alters the pharmacokinetic properties and allows lower doses or reduces frequency of doses to achieve the desired effects in patients.

We have developed efficient and straightforward deuteration techniques for important scaffolds, biomolecules, and pharmaceuticals. These methods employ heavy water as a deuterium source and heterogeneous catalysts such as Pd/C, Pt/C, Ru/C, Rh/C and NaBD₄. Selective deuteration reactions have been conducted under both conventional and microwave conditions under nitrogen atmosphere. The obtained deuterium labeled products have been confirmed using LC-MS, ¹H-NMR. The synthesized compounds include phenol-d₃, p-nitrophenol-d₂, 4-hydroxycoumarin-d₃, valproic acid-d₁₀, chalcone-d₁ and uracil-d₁ for better metabolic stability.

Upload Extended Abstract File

Sonophotocatalytic Degradation of Organic Pollutants Using Visible-Light-Responsive TiO2-Based Catalysts

B. Neppolian

SRM Institute of Science and Technology, Chennai, India

Abstract Category

Nanomaterial/nanotechnology

Abstract

Titanium dioxide-based and other visible-light-responsive photocatalysts have proven effective for degrading organic pollutants in water and wastewater, utilizing sunlight as an energy source. Additionally, the role of ultrasound in both nanoparticle synthesis and pollutant removal, when combined with photocatalysis (sonophotocatalysis), has been extensively studied. Binary metal oxide photocatalysts, supported by materials such as graphene oxide and graphitic carbon nitride, have demonstrated remarkable efficiency in achieving complete oxidation of organic pollutants. Various solution and operational parameters affecting photocatalysis and ultrasound processes are optimized based on the specific nature of the pollutants. Furthermore, modifications such as band gap tuning and defect engineering of the photocatalysts significantly enhance their efficiency. The synthesized photocatalysts are meticulously studied with advanced instrumentation to examine their intrinsic and extrinsic properties, elucidating the mechanisms involved in photocatalysis. Studies on the stability, recyclability, and commercial feasibility of these catalysts indicate their potential as a viable alternative for large-scale treatment of organic pollutants.

Upload Extended Abstract File

Biochemistry of Dark Fermentation for the Industrial Bio Hydrogen Production

MAINAK RAY

HPCL-MITTAL ENERGY LIMITED, BATHINDA, India

Abstract Category

Biotechnology & Biochemical engineering

Abstract

In recent years, non-fossil-based hydrogen/bio hydrogen (H2) production has gained attention. These efforts aim to limit Grey Hydrogen production and expedite the decarbonisation goal. Dark fermentation is a fermentative conversion method of organic substrate. Multitudinous bacteria shepherd organic polymers to organic acids and alcohols, followed by H2, engendering acidogenic bacteria. Also, few organisms produce H2 under stress conditions. Microbes and their biochemical mechanisms are complex puzzles, but they have the potential for H2 production; technological advancement and more R&D are needed for commercial development.

Upload Extended Abstract File

Engineering Insights into Thermal Plasma Processing for Plastic Waste Management - A Review

Karan Sharma

Institute of Chemical Technology, Mumbai, India

Abstract Category

Waste Management

Abstract

The increasing accumulation of plastic waste due to its non-biodegradability and enhanced standard of living poses a significant global environmental challenge. Current thermochemical waste management techniques, such as pyrolysis and gasification, offer partial solutions that are accompanied by issues such as secondary pollutant formation, operational inefficiencies, and poor scalability. Thermal plasma-assisted processes operating at extreme temperatures of 1500 –5000°C, emerge as a promising alternative, leveraging high-energy plasma arcs to achieve complete waste destruction and its conversion into syngas and inert slag while marginalizing hazardous byproducts like dioxins and corrosive tar. Although waste plasma processing techniques have existed for around four decades, they have seen limited and unsustainable commercialization attempts due to high capital requirements, proprietary technology, and suboptimal reactor designs. The scalability of plasma technologies depends on optimizing energy efficiency and feedstock variability, which can be achieved through prudential reactor design. This review aims to provide a foundational framework for designing efficient, plasma systems for sustainable plastic waste management, approaching the challenge through the lens of chemical reactor design. By applying core chemical engineering principles such as reaction kinetics, heat and mass transfer, and reactor design to advance the scale-up of plasma technologies for plastic waste treatment. The paper highlights studies and innovations aimed at tackling key obstacles in waste plasma processing, including electrode erosion, uneven heat distribution, and inadequate material mixing. Additionally, the authors discuss in detail the role of modeling studies and strategies to bridge the gap in experimental work and advance fundamental understanding.

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Prussian white cathode material for Sodium-ion battery

Vickrant Gharat

Institute of Chemical Technology, Mumbai, India

Abstract Category

Material Science

Abstract

The growing demand for sustainable energy storage solutions has increased the search for efficient, cost-effective, and environmentally friendly battery technologies. In this regard, lithium-ion batteries (LIBs) offer many advantages: high energy density, long life cycle, and high efficiency. However, LIBs are more expensive, and their disposal is difficult. Sodium-ion batteries (SIBs) are great economical alternatives to LIBs for large-scale energy storage devices because of their abundancy, low cost of sodium extraction, and sharing similar properties with Li. The performance of the battery depends largely on the cathode active material. In this context, Prussian white as a cathode material has received great interest from researchers in recent times for its application in low-cost SIBs. Prussian white (PW) is a fully reduced and sodiated form of Prussian blue, and while its potential is widely recognized, its synthesis remains challenging task. Researchers explore methods for synthesizing Prussian white, including co-precipitation method, mechanochemical method, and hydrothermal method. Among these, the co-precipitation method is the most promising method for SIBs because of its simplicity, scalability, and control over particle size. This paper emphasizes the recent advancements in Prussian white analogues, focusing on synthesis techniques and characterization.

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Understanding the Synthesis of Indomethacin–Saccharin Cocrystals by Anti-Solvent Co-crystallization

Soham Deshmukh

INSTITUTE OF CHEMICAL TECHNOLOGY, MUMBAI, India

Abstract Category

Material Science

Abstract

Indomethacin (IMC), a widely used Nonsteroidal anti-inflammatory drugs (NSAID), known for its therapeutic efficacy. However, there are certain issues with how efficiently it functions within the body. It doesn't dissolve well in water, it have limited solubility and also have low bioavailability. In recent years, co-crystallization rises as one of the most promising approach for improving the solubility of a drug. This review study provides an in-depth review of the developments in IMC cocrystals, highlighting how they improve shape, solubility, dissolution rates, and bioavailability in comparison to raw IMC through antisolvent method. In this study, all the co-crystallization methods are explored while antisolvent method is studied in detail. The study also explore the different types of solid forms formed during co-crystallization. Using the anti-solvent approach, methanol was almost the only solvent among those tested to successfully produce highly pure IMC–SAC co-crystal powders. Techniques like X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) are used to study the crystal structures of IMC cocrystals, while differential scanning calorimetry (DSC) is used to analyze their thermal behavior. This review focuses on the most recent developments in IMC cocrystals, highlighting how they gistoly dissolving rates, and bioavailability.

Upload Extended Abstract File

Engineering Aspects of ZIF-67: Investigating Kinetics and Strategies for Scalable Synthesis

Aaush Bhardwaj Singh, Manishkumar Yadav

Institute of Chemical Technology, Mumbai, India

Abstract Category

Material Science

Abstract

Zeolitic Imidazolate Framework-67 (ZIF-67), a metal-organic framework, has attracted considerable interest due to its high surface area, open crystal structure, and tunable crystal pores. This research primarily utilizes ZIF-67 as a model material to develop a comprehensive methodology for determining the kinetics of metal-organic frameworks (MOFs) and formulating scale-up strategies for large-scale production. The study focuses on the development of a simple, efficient, and economically viable synthesis method for ZIF-67, with an emphasis on scalability and ease of production. A novel aspect of this research is the investigation of formation kinetics, which has not been reported for any MOF to date. The work also explores the effects of various parameters, including different molar ratios of Hmim/Co, solvents, and aging time, on the morphology and specific surface area of the crystals. It also measures the intensification effect of using surfactants on the settling time of the crystals. Additionally, the impact of hydrodynamic factors such as impeller type and speed on the structural and physical properties of ZIF-67 is examined. By optimizing these parameters, the study aims to enhance reproducibility and provide practical insights into the engineering aspects of ZIF-67 production. The work facilitates the transition of ZIF-67 from laboratory-scale research to industrial-scale production.

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VENT SIZING FOR INTEGRATION OF PROCESS SAFETY AND GREEN CHEMISTRY

Jasbir Singh, <u>Vilobh Shete</u> H.E.L India, Mumbai, India

Abstract Category

Process hazard safety

Abstract

Combination of green chemistry and process safety represents a promising approach to managing risks and promoting sustainability in the chemical industry. These two fields, mutually, offer comprehensive solutions that aim to eliminate hazards at the source, rather than merely controlling them.

Adoption of green chemistry and process safety together is not without challenges, such as the need for investment in technology and process redesign, and the paradigm shift required from traditional hazard control to proactive hazard elimination. Moreover, there is a need for ongoing education, research, and development to advance the application of principles and designing the processes to its optimum limit of operation.

One such design parameter that needs to be taken very seriously is Vent Sizing. Sizing of a relief device using presently recommended methods (e.g. DIERS) frequently leads to extremely large and expensive vents. The presentation discusses methodology that leads to a simple but much improved method for vent sizing, fully allowing for two-phase release of the gas—liquid mixture. A number of examples are presented which lead to interesting conclusions about the influence of green chemistry variables.

Upload Extended Abstract File

Synthesis of commercially important esters using non-noble metal catalyst

Rushikesh Pagare

institute of chemical and technology Mumbai, Mumbai, India

Abstract Category

Catalysis

Abstract

The synthesis of products is commercially vital for esters, Pharma intermediates, and chemicals using non-noble metal catalysts in mild conditions. The study of catalyst characterization techniques includes FTIR, Raman, P-XRD, HR-TEM, XPS, and nitrogen adsorption-desorption. GCMS, GC and HPLC confirm products. Using the characterization found that active acidic and basic site. All catalysts contain biomass waste to support the reduction of environmental pollution. In this Paper, synthesis of ester for Fragrance, bio-fuel and Bio-surfactant, Amine and amide synthesis to pharmaceutical intermediate.

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La Nanorod and Octahedral Mn and Co Spinel Synergistic Efect for Selective Oxidation of Alcohol to Aldehyde

Kajal Pawar

Institute of chemical technology, mumbai, India

Abstract Category

Catalysis

Abstract

The La nanorod and cobalt-manganese spinel were synthesised by an improved sol–gel technique for the selective oxidation of

alcohols. The active sites of the catalyst were demonstrated using parameters and a recycling study. Moreover, the catalyst was

characterized by Raman spectroscopy, X-ray photoelectron spectroscopy, Fourier transform infrared spectra, X-ray difraction,

and surface analysis to examine the impact of La addition on the structural and morphological characteristics of CoMn₂O₄.

La is introduced into CoMn₂O4, which decreases the activation energy; therefore, CoMn₂-xLaXO₄ selectively oxidizes alcohol

at lower temperatures. Higher benzyl alcohol to benzaldehyde conversion was observed for the CoMn1.96La0.04O4 catalyst.

The catalyst was further also examined for the selective oxidation of other alcohols. The various commercially important

substrates like 2-bromo benzyl alcohol, furfuryl alcohol, etc. undergo selective oxidation using a catalyst was also been

investigated. The mechanistic aspects of the catalyst with active sites have been explained using Raman and ATR-FTIR

adsorption study.

Upload Extended Abstract File

Synthesis of esters using modified waste copper slag: a sustainable approach for waste valorisation

Bhagyashree Megha

Institute of chemical technology, Matunga, Mumbai, India

Abstract Category

Catalysis

Abstract

The active sites of waste copper slag were moulded using BaO and used as a catalyst for the esterification reaction without solvent. Various concentrations of BaO were doped over the copper slag and investigated for the esterification of various model components of flavour, fragrance and biofuel. The catalyst was characterized by X-ray photoelectron spectroscopy, attenuated total reflectance -Fourier transform infrared spectroscopy, surface area analysis and X-ray diffraction to examine the impact of BaO addition on the structural and morphological characteristics of BaO_x/Cp-Sl. BaO increases the grain size and enhances the BaO_x/Cp-Sl catalyst's activity and selectivity to flavour, fragrance and biofuel. The BaO_{2.5%}/Cp-Sl catalyst showed the maximum conversion of oleic acid to the methyl ester. The esterification of various commercially important substrates like geraniol, citronellol, menthol, isoamyl acetate, palmitic acid and waste cooking oil using a catalyst has been explained in detail. The kinetic study of the esterification has been explained with TON and TOF. The mechanism pathway of the catalyst with various active sites of waste copper slag has been explained using adsorption studies.

Upload Extended Abstract File

Synthesis of Nanohybrids of 2D Co-Fe-LDH NSs and 1D FCNTs For High Performance Hybrid Asymmetric Supercapacitors

Shraddha Pawar¹, Shweta Talekar¹, Prashant Sawant¹, Hemraj Yadav², Jayavant Gunjakar¹

¹D. Y. Patil Education Society ,Kolhapur, Kolhapur, India. ²Shivaji University ,Kolhapur, Kolhapur, India

Abstract Category

Material Science

Abstract

1D carbon nanotubes (CNTs) with high electrical conductivity and electrochemical stability are employed as a hybridization matrix to improve the electrode performance of layered double hydroxides (LDHs). A cobalt-iron-LDH hybridized with a CNTs channel leads to anchored Co-Fe-LDH-CNTs (CC) self-assembly with a high surface area, mesoporous morphology, high electrical conductivity, and high charge transfer kinetics. The structural study using X-ray diffraction (XRD) reveals formation of well-crystalline hexagonal layered Co-Fe-LDH-CNTs structure. The nature of chemical bonding of CC nanohybrids are probed using Fourier transform infrared (FTIR) spectroscopy. The CC nanohybrids display enhanced specific capacity with high-rate characteristics compared to pristine Co-Fe-LDH, signifying the crucial role of CNTs as a hybridization matrix for improving the electrode performance of LDH materials.

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Chemical Conversion Approach for Thin Films of Magnesium-Aluminium-Layered Double Hydroxide Nanosheets: Room Temperature NO₂ Sensing

Shweta Talekar¹, Prashant Sawant¹, Shraddha Pawar¹, Hemraj Yadav², Jayavant Gunjakar¹

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Abstract Category

Material Science

Abstract

1. Introduction:

Detection of the very minute amount of gas analytes using chemiresistive gas sensors is attractive owing to their high sensitivity, long-term stability, weather tolerance, lower cost, portability, minimum maintenance, less effort in fabrication, simple electronic constructions, and capability to sense various hazardous gases [1, 2].

2. Material and Methods:

The preparation of magnesium-aluminum-layered double hydroxide (MA-LDH) thin film by chemical conversion of magnesium oxide (MgO) thin film.

3. Significant Results and Discussion:

The chemically converted MgO thin films lead to the formation of hexagonal MA-LDH thin films with interconnected nanosheet-like structures. Furthermore, the resulting MgO and MA-LDH sensors are studied for different oxidizing and reducing gases. The MA-LDH resistive electrode works as a NO₂ gas sensor at room temperature (RT). The optimized MA-LDH sensor response to NO₂ is 54.18 % for 100 ppm, a quick response time, a detection limit of 0.1 ppm, and a long duration time at RT. Of prime interest is the MA-LDH sensor, which displayed a high relative humidity effect on the response of NO₂ sensing. The excellent NO₂ sensing performance and remarkable response improvement of MA-LDH are ascribed to the gas adsorptive reactive sites by interconnected nanosheet-like structures.

4. Conclusions:

The excellent NO₂ sensing performance and remarkable response improvement of MA-LDH are ascribed to the gas adsorptive reactive sites by interconnected nanosheet-like structures.

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An efficient Nickel-Iron bimetallic nanoparticles as heterogeneous catalysts for Hydrodeoxygenation of a lignin model compound(Vanillin)

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Visvesvaraya National Institute of Technology (VNIT), Nagpur, Nagpur, India

Abstract Category

Catalysis

Abstract

This study presents that bimetallic nickel-iron nanoparticles, synthesized via a straightforward onepot hydrothermal, co-reduction method, exhibited excellent activity and selectivity in the hydrodeoxygenation of vanillin to creosol. To investigate the catalytic performance of Ni_xFe_y bimetallic nanoparticles, HDO reactions were performed in alcohol starting from lignin-derived vanillin. The efficient catalytic activity of Ni_xFe_y BMNPs is ascribed to the synergistic actions of Ni and Fe bimetallic composition. The catalysts has high thermal stability and reusability, furthermore, the catalytic potential of Ni_xFe_y bimetallic nanoparticles was demonstrated starting from vanillin to produce creosol.

Upload Extended Abstract File

Water Delamination Ultrathin 2D Nanosheet of Cobalt Doped Ni-Fe-LDH for OER

Prashant Sawant¹, Shweta Talekar¹, Shraddha Pawar¹, Hemraj Yadav², Jayavant Gunjakar¹

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Abstract Category

Material Science

Abstract

1. Introduction:

The water-splitting process is considered a crucial reaction to enable the storage of intermittent solar and wind energies as chemical energy sources, specifically oxygen and hydrogen [1]. In the watersplitting process, the oxygen evolution reaction (OER) is the main obstacle due to sluggish kinetic reaction. However, the slow rate and considerable excess potential of the four-electron transfer reactions needed to perform the water-splitting process constrain the OER [2].

2. Material and Methods:

The cobalt-doped NiFe-LDH was synthesized by the co-precipitation method.

3. Significant Results and Discussion:

Layered materials have recently gained tremendous importance in various electrochemical applications due to their intercalative and exfoliable nature. The controlled synthesis plays an important role in delaminating layered material into single layers without damaging its physicochemical properties. This report uses a co-precipitation method to synthesize Co-doped Nickel-Iron-Layered Double Hydroxide (Ni-Fe-LDH). Afterward, stable exfoliation of Co-doped Ni-Fe-LDH is achieved in water and confirmed by the Zeta potential. The structural analysis confirms the formation of hexagonal Ni-Fe-LDH as well as Co-doped Ni-Fe-LDH (JCPDS card 40-0215). XPS spectra show the presence of Co in the Ni-Fe-LDH. The selected area electron diffraction pattern (SAED) confirms the single-layer exfoliation of material. The film of exfoliated nanosheet is prepared by the electrophoresis method. The nanosheets film showed good electrocatalytic properties for the OER application.

4. Conclusions:

The doping and NSs thin film of exfoliated nanosheets remarkably enhance the OER performance.

References

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Synthesis of Zinc Aluminium Layered Double Hydroxide by Co-Precipitation Method

Mayura Medhekar¹, Sayali Kulkarni¹, Monali Jalak¹, Hemraj Yadav², Jayavant Gunjakar¹

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Abstract Category

Material Science

Abstract

Introduction:

Layered double hydroxides (LDH) exhibit an excellent catalytic activity for various application. The structure of LDH can be represented by the chemical formula $[M^{2+}_{1-x} M^{3+}_x (OH)_2]^{x+} [A_{x/n}]^n$.mH₂O, where m is the interlayer water, A^{n-} are the hydrated interlayer guest anions and $x = M^{3+}/(M^{2+}+M^{3+})$ is the layer charge density or the molar ratio. M^{2+} are divalent cations (e.g., Co^{2+} , Ni^{2+} , Zn^{2+} , Ca^{2+} , Mn^{2+} , Fe^{2+} , and Mg^{2+}) that are octahedrally coordinated to six OH⁻ hydroxyl groups and can be substituted by trivalent cations M^{3+} (e.g., Al^{3+} , Ga^{3+} Fe³⁺, Ti^{3+} , Cr^{3+} , In^{3+}) in the brucite-like $M^{2+}(OH)_2$ layer [1].

Material and Methods:

In this work, zinc-aluminium layer double hydroxide (Zn-Al-LDH) in nitrate form is synthesized by simple co-precipitation method.

Significant Results and Discussion:

The pristine Zn-Al-LDH shows well-resolved (003), (006), (009), and (110) Bragg reflections. The calculated lattice parameters a = b = 0.303 nm and c = 0.88 nm for pristine Zn-Al-LDH are in good agreement with the lattice parameters of the nitrate-intercalated LDH phase [2].

Conclusions:

The XRD analysis confirms the formation of Zn-Al-LDH in hexagonal crystal structure (JCPDS Card No.: 38-0486). This report highlights scalable synthesis approach of Zn-Al-LDH.

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An emerging class of material: High entropy layered doubled hydroxide for water splitting

Ganesh khande

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Abstract Category

Material Science

Abstract

The efficiency of the oxygen evolution reaction (OER) is significantly influenced by the properties of electrocatalysts, highlighting the importance of developing highly effective catalysts. Layered double hydroxides (LDHs) are considered promising candidates for OER due to their unique structural and electronic characteristics. High-entropy materials (HEMs) bring benefits such as high entropy, lattice distortion, slow diffusion, and the cocktail effect, which can improve active sites and optimize the interaction with reaction intermediates. By combining the strengths of these two material types, we propose the synthesis of high-entropy layered double hydroxides (HE-LDHs) through a straightforward coprecipitation method, offering exceptional OER electrocatalytic performance.

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Synthesis and Characterization of Ceramic Membrane and its Application in Microalgae Harvesting

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Institute of Chemical Technology, Mumbai, India

Abstract Category

Biotechnology & Biochemical engineering

Abstract

Microalgae filtration using ceramic membranes is gaining serious interest among researchers compared to polymeric membranes. Ceramic membranes offer advantages over traditional polymeric membranes, including strong material, high-temperature and chemical resistance, and effective filtration. They are suitable for processing large volumes of microalgae cultures. However, their high initial costs and membrane fouling have limited their widespread use. Fouling, caused by the build-up of organic matter and cells, reduces membrane performance and increases operational costs. Also, the cost of harvesting microalgal solutions remains a serious concern. Thus, membrane filtration is considered a cheap and best alternative compared to other alternatives. This study provides an experimental approach of using kaolin clay-based ceramic membrane for harvesting microalgae, which includes synthesis by pressing method, characterization using TGA, SEM and XRD, microalgae cultivation, flux analysis studies, and different analyses that can be done, which is mentioned in materials and methods. The key approaches used by the research community to harvest microalgae with membranes are then discussed, with a special focus on the innovative developments that have been made to enhance filtration efficiency and fouling analysis through pore-blocking techniques.

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Enhancing OER activity in electrochemical water splitting using MoS₂-MoO₃ composites on Ni-Co LDH supports

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Institute of Chemical Technology (ICT), Mumbai, India

Abstract Category

Electro Chemistry

Abstract

Developing an efficient electrocatalyst for oxygen evolution reaction (OER) and is critical for advancing towards an era powered by Hydrogen. In this study, we investigated the catalytic performance of MoS₂-MoO₃ composites, and Ni-Co layered double hydroxides (LDH), across varying MoS₂-MoO₃ ratios (0%, 33%, 50%, and 67%). The focus is on understanding the influence of sulfur-oxygen (S-O) interactions, sulfur and oxygen vacancies, and specific interaction of both the supports with MoS₂-MoO₃ composites on catalytic activity. X-ray Photoelectron Spectroscopy (XPS) was employed to understand the underlying interactions between support-composite and identify the optimal composition for maximizing OER activities. Subsequently, SEM were employed to understand results from a morphological point of view, and lastly, XRD was used to gain insights into crystal structure and phases. Preliminary results and the literature survey indicated that support material significantly enhances catalytic performance through vacancy formation and metal-support interactions. This systematic approach provides insights into the design of cost-effective and highly efficient catalysts for future renewable energy applications.

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Evaluation of face mask efficacy in filtering pesticide aerosols for improved air quality and health protection

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Abstract Category

Interfacial/surface science

Abstract

Farmers are at a high risk of inhalation exposure when handling pesticides. Indian farmers mostly rely on cloth or kerchiefs tied around for pesticide protection, with limited use of commercial respiratory protective equipment (RPE). Scientific data on the pesticide filtration efficiency of RPEs commonly used by farmers is scarce. Studies revealed that 74% of farmers knew the need to wear protective gear when handling pesticides. The most frequently used safety equipment included face masks, which had 58.48% usage as protective gear. RPE protects against pesticide inhalation and subsequent absorption through the respiratory system. Since several pesticides are classified as organic vapors and pesticide spraying through nozzles produces fine particles, it is recommended that pesticide handlers should wear at least a respirator during the handling of pesticides, but most farmers wear RPE made of fabric, which would not protect against pesticides and several RPEs and check for their filtration efficiency from the method followed by simulating real-world conditions with pesticides. The results will provide insights into the adequacy of different RPEs in protecting farmers from pesticide exposure, helping to improve safety guidelines.

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