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in the Honour of Prof. Lakshmi K. Kantam

ABSTRACT BOOK

Theme

The Green Shift

Pioneering a Sustainable Chemical Industry

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Serial no.	Title
2	Process intensification for the continuous production of 2, 2-Dimethoxypropane using Fixed Bed Chromatographic Reactor (FBCR)
13	Machine Learning for Predictive and Inverse Modelling of Propionic Acid Extraction Efficiency
14	Role of biomass derived carbon in enhancing the performance of Zinc ion batteries
16	Electrocatalytic performance evaluation of Nickel-iron layered double hydroxide for overall water splitting
18	Biomass Derived Electrocatalyst for Hydrogen Evolution Reaction (Hydrogen Generation)
21	Understanding the Physical and Reactive extraction behavior of Malic Acid.
32	Evaluating filtration efficiency of respiratory protective equipment against pesticide aerosol in agricultural environment.
33	Investigating S–O Interactions in MoS_2–MoO_3 on Ni-Co LDH for Bifunctional OER and HER
42	Transition Metal-Loaded TiO2 Catalyst for Catalytic Thermoliquefaction of Municipal Solid Waste into Carbon-Rich Oil.
44	Catalytic Co-Liquefaction of Organic Biodegradable Fraction of Municipal Solid Waste and Sugarcane Bagasse
47	ONE-POT UPGRADING OF POLYETHLENE AND CO2 INTO AROMATIC CHEMICALS VIA TANDEM CATALYSIS
48	Pathways to Climate Positive Fuels: Experimental and Simulative Exploration of CO2 Conversion
49	Photocatalytic CO_2 Reduction for Sustainable Fuel Synthesis: Experimental and Simulation Approaches
52	An Electrolytic Route to Sustainable Cotton Bleaching with In-situ Oxidant Regeneration
56	AI-Driven Environmental Toxicity Prediction Platform for Sustainable Chemical Manufacturing: A Machine Learning Approach for Early Hazard Assessment of Industrial Chemicals

57	Recoverability-Aware Industrial Operations: Quantifying Degradation Dynamics, Operational Observability, and Recovery Potential
61	A greener approach towards sustainable production of biodiesel from waste frying oil using biowaste-derived *Unio pictorum* shell-*Musa acuminata* peel ash nanocomposite catalyst
66	Electrochemical Pathway for CO2 conversion into Ethanol
68	Analytical Quality by Design optimization of dual RP-HPLC and ion chromatography methods for sustainable determination of edoxaban tosylate: Comparative validation and multi-metric greenness assessment
69	Effect of CaCO3 Concentration and Inoculum Size on Glucose Utilization by Aspergillus oryzae and Aspergillus wentii
71	Extraction of High-Grade Silica from Rice Husk Ash: A Sustainable Engineering Approach
73	Sustainable synthesis of 3,4-dihydropyrimidinone scaffolds as potential antiviral agents
74	Development and Characterization of "Oraalix":A Sustainable, Anhydrous Dentifrice Tablet
75	Analysis of Energy Consumption and CO_2 Emissions in India's Petrochemical Sector
76	Synthesis of Fluorobased pyrazole scaffolds as sustainable design with antiflaviviral potential
77	Cyrene as a bio renewable resource towards synthesis of cyrenyl-quinolinyl chalcone hybrids having antimalarial potential.
78	AI For Air pollution And monitoring Control
82	Microwave assisted intensification of n-octyl acetate synthesis over H5PW10V2O40/FAC catalyst: Kinetic Study
83	Design, Synthesis, Computational Evaluation, and Dual Cu^{2+}/Ag^{+} Sensing Studies of Alkyne-Functionalized Pyrimidine–Chalcone Hybrids
84	Hemp Fiber Inspired Iron Oxide synthesis and application as nanocatalyst fermentive biohydrogen production.
85	Enhancing Bioactive Recovery from Pigeon Pea Seed Coat: A Comparative Evaluation of ultrasound assisted and Conventional Extraction

86	Visible-Light-Driven Reductive C–N Bond Formation of Renewable Aldehydes and Lignin Bio-Oil to Amines
87	Photocatalytic Lignin Valorization through Selective Cleavage of C–O Linkages over Ru-Supported Holey g-C3N4 Nanosheets.
89	MOF-Incorporated Polymeric Membranes for CO2 Capture: A Comparative Literature Review
90	Selective Hydrogenation of Furfural to 2-Methyltetrahydrofuran over Bimetallic Ru–Ni Nanoparticles Supported on Nanocrystalline CeO2
91	Ni NPs decorated ZrO2 Phase-dependent activity for Furfural hydrogenation to yield THFA and CPO selectively
93	Life Cycle Assessment of FDCA Production from Cellulose using Cradle to Gate Approach.
96	AI for Sustainability Evaluation of Waste-to-Value Technologies
98	Nanofiller-Engineered Thin-Film Nanocomposite Membranes for Liquid and Gas Separation
100	Valorization of Lemon Peel Waste into Sustainable Biochar for Green Removal of Acidic Black 1 Dye from Wastewater: Insights from RSM and ANN Predictive Modelling
103	Unveiling the pore characteristics of Indian coal for geological CO2 sequestration and natural gas recovery.
106	A palladium bio-nanocomposite as an efficient heterogeneous catalyst for nitro reduction:a fungus mediated green and sustainable process
113	CO_2 Refinery: Catalytic Pathways for Conversion of Carbon Dioxide into Value-Added Chemicals
116	Dry Reforming of Methane over Nickel-Based Catalysts: Mechanistic Understanding and Catalyst Design
117	Sustainable Conversion of Biomass to Deoxygenated Bio-Oils via Catalytic Hydrothermal Liquefaction
119	Development of a Bio-based Polymeric Surfactant from Epoxidized Mahua Oil and Hydroxyethyl Cellulose
38	Regeneration of High-Quality NMC cathode from Spent Lithium-Ion Batteries

2

Process intensification for the continuous production of 2, 2-Dimethoxypropane using Fixed Bed Chromatographic Reactor (FBCR)

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Abstract Category

Catalytic reaction engineering & scale up

Abstract

2,2-Dimethoxypropane (DMP) is a crucial intermediate in vitamin synthesis and serves as an effective water scavenger. The conventional synthesis of DMP from methanol and acetone is characterized by an equilibrium-limited reaction, yielding water as a byproduct, with equilibrium conversion rates typically below 5%. Traditional batch reactors are highly energy-intensive due to low one-pass conversion rates.

In this study, we introduce a multifunctional reactor, specifically a Fixed Bed Chromatographic Reactor (FBCR), to facilitate the synthesis of DMP. Notably, we explore the innovative use of non-polar solvents to enhance productivity in reactive chromatography. Employing dry Amberlyst-15 as a catalyst, we demonstrate that the FBCR allows for simultaneous reaction and chromatographic separation, resulting in a remarkable 2.5-fold increase in reaction productivity. This approach not only optimizes the synthesis process but also significantly reduces energy consumption, marking a novel advancement in the production of DMP.

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13

Machine Learning for Predictive and Inverse Modelling of Propionic Acid Extraction Efficiency

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Abstract Category

Sustainable Engineering

Abstract

The downstream purification of fermentation-derived products depends on the effective recovery of propionic acid from aqueous streams. Complex physicochemical interactions between solvents, extractants, and aqueous phases complicate conventional evaluation of extraction efficiency (E%), which frequently calls for extended experimental runs, usually lasting several hours. A machine learning (ML) framework was developed in this study to forecast and maximise propionic acid extraction efficiency across four systems: reactive extraction, temperature-based reactive extraction, temperature-based physical extraction, and physical extraction. To determine how operational factors like temperature, pH, extractant concentration, and diluent type affected extraction performance, each system was separately modelled. An inverse design framework was used to infer the best combinations of process variables needed to reach a target extraction efficiency in order to go beyond prediction. By converting ML models from descriptive predictors into active design tools, this method reduces the need for long, iterative laboratory research and permits data-driven experimentation. The study demonstrates that coupling predictive modelling with inverse optimisation provides a practical pathway toward intelligent and adaptive solvent extraction systems for propionic acid recovery, with potential applicability to other short-chain carboxylic acids.

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14

Role of biomass derived carbon in enhancing the performance of Zinc ion batteries

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Abstract Category

Clean Energy

Abstract

Zinc-ion batteries are a promising alternative to traditional battery technologies, offering a potential replacement for stationary energy storage systems. These batteries are safer and cheaper than the existing lithium-ion batteries. Transition metal oxides such as manganese dioxide have been used as the active cathode material in zinc ion batteries, as they can store Zn^{2+} ions effectively. One of the major drawbacks of MnO_2 is the low electrical conductivity. This study focuses on incorporating sustainable biomass-derived carbon from secondary floral waste to enhance the conductivity of MnO_2. Two methods have been used to prepare the composites of MnO_2 with biomass-derived carbon viz., ultrasonication of the precursors in a solvent and growth of MnO_2 on biomass-derived carbon using solvothermal techniques. X-ray diffraction study confirmed the synthesis of α-MnO_2. FTIR studies confirmed the carbon ring-like structure in biomass-derived carbon. The charge discharge studies showed that the growth of α-MnO_2 on the carbon structure performed better as there might be chemical bonding at the metal oxide and carbon interface. The coulombic efficiency of the insitu sample also was 90.9% which will be beneficial for better battery performance.

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16

Electrocatalytic performance evaluation of Nickel-iron layered double hydroxide for overall water splitting

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Abstract Category

Catalysis For Energy

Abstract

Seawater electrolysis is currently a promising technology for efficient green hydrogen production owing to its abundant available resources. The development of a stable electrocatalyst is a prerequisite for the hydrogen and oxygen evolution reaction (HER and OER) activity in electrochemical water splitting. Layered double hydroxides (LDH) have garnered significant interest for the generation of hydrogen and oxygen by virtue of their high surface area, hydroxide-rich surfaces and exchangeable anions. In this work, NiFe LDH has been developed in situ on nickel foam (NF) by the hydrothermal method. XRD study reveals the good crystallinity and structural growth of LDH on NF. The electrocatalytic performance of the synthesized catalyst (NiFe LDH/NF) was studied for HER and OER in simulated seawater. The overpotential was found to be 298 mV at 10 mA/cm^2 for HER, which is quite low compared to OER performance. Whereas, the Tafel slope obtained was 176 mV/dec in HER and 81 mV/dec in OER. The active site density of the catalyst was higher in HER than in OER. Post-chronoamperometry study reveals that the NiFe LDH/NF sustain its structure with improved crystallinity. The HER and OER study paves the way towards employing the NiFe LDH/NF electrocatalyst for overall water splitting.

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18

Biomass Derived Electrocatalyst for Hydrogen Evolution Reaction (Hydrogen Generation)

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Abstract Category

Hydrogen generation And storage

Abstract

Exploring efficient non-noble metal catalyst for the hydrogen evolution to the development of clean and green energy technologies. Herein, we adopted a “waste utilization” strategy by using readily available and inexpensive coconut husk waste as a carbon source to synthesize carbon material anchored with Nitrogen and Molybdenum disulfide, as a potential electrocatalyst for hydrogen evolution reaction (HER). Utilizing the combination of hydrothermal and pyrolysis methods, the synthesized Composite of N-AC-MOS_2 catalyst shows superior HER electrocatalytic performance in acidic solution, with an overpotential of 326 mV at 10 mA cm^2 and a Tafel slope of 157 mV dec^{-1}. This research shows N-AC-MOS_2 composite works very well and stable during HER in acidic condition.

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21

Understanding the Physical and Reactive extraction behavior of Malic Acid.

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Sustainable Engineering

Abstract

The recovery of organic acids from aqueous solutions is a crucial step in bioprocessing, as conventional separation techniques often involve high energy consumption and limited selectivity. This study will focus on the physical and reactive extraction of malic acid to identify efficient alternatives for acid recovery. Physical extraction will be conducted using various diluents to evaluate non-reactive solute transfer, while reactive extraction will employ a suitable extractant to enhance recovery through complex formation. The effects of extractant concentration, initial acid concentration, phase ratio, and pH on the distribution coefficient and extraction efficiency will be systematically investigated. Reactive extraction is expected to significantly improve malic acid transfer compared to physical extraction due to the formation of stable acid–extractant complexes. The study is expected to lay the groundwork for developing energy-efficient and selective solvent-based separation processes and to contribute to improving downstream recovery strategies for dicarboxylic acids produced through fermentation.

Keywords: Reactive extraction; Physical extraction; Malic acid; Distribution coefficient; Biochemical separation; Green separation process.

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32

Evaluating filtration efficiency of respiratory protective equipment against pesticide aerosol in agricultural environment.

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Abstract Category

Life cycle assessment

Abstract

Airborne pesticides, originating primarily from agricultural practices, pose significant environmental and human health risks. These pesticides enter the atmosphere primarily through volatilization, spray drift, and atmospheric transport. Their presence in the air can lead to increasing human exposure to harmful chemicals. Mitigation strategies recommend the use of respiratory protective equipment (RPE). There is limited research evidence on the pesticide filtration efficiency of RPE. The efficacy of commercially accessible RPE in the market requires investigation against these pesticides. The purpose of this study was to evaluate the pesticide filtering efficiency of several kinds of RPE, viz., surgical masks, cloth masks, kerchiefs, N95, N99, and half-facepiece respirators, against two commonly used organophosphate pesticides, chlorpyrifos and malathion, which are utilised by Indian farmers. The assessment was carried out using a simulated aerosol exposure setup, and pesticide concentrations were measured using UV-Vis spectrophotometry. Scanning Electron Microscopy (SEM) study demonstrated particle accumulation on mask fibres during exposure. The findings highlight the critical need for enhanced RPE selection and knowledge among farmers in order to reduce pesticide inhalation hazards

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33

Investigating S–O Interactions in MoS_2–MoO_3 on Ni-Co LDH for Bifunctional OER and HER

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Abstract Category

Catalysis For Energy

Abstract

Developing an efficient bifunctional catalyst for oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) is critical for advancing towards an era powered by Hydrogen. This study investigates the catalytic performance of MoS_2–MoO_3 composites supported on Ni-Co layered double hydroxides (LDH), synthesized via

hydrothermal and reflux methods followed by probe sonication-assisted exfoliation. The research focuses on elucidating the influence of Sulfur–Oxygen (S–O) interactions and vacancy engineering on electrochemical activity. Comprehensive characterization using XRD, SEM, and XPS reveals that creating ternary heterostructures yields significant synergistic effects, surpassing the performance of pristine counterpart.

Electrochemical evaluation identifies the ternary composites as superior bifunctional catalysts. Specifically, the composite with an equal MoS_2–MoO_3 ratio on LDH achieved maximum current densities of 55.63 mA/cm² for OER and -283.53 mA/cm² for HER. XPS analysis attributes this OER enhancement to a unique surface chemistry where the S–O interface stabilizes an exceptionally high concentration of Ni^{3+} species (~80.9%). Conversely, the MoS_2-rich ternary composite demonstrated the highest HER activity among the ternary samples (-309.54 mA/cm²) and robust OER activity (53.13 mA/cm²), driven by the modulation of the support to stabilize Co^{3+} active sites. These findings demonstrate that engineering complex S–O heterointerfaces is a powerful strategy for electronically modulating active sites to achieve high-efficiency overall water splitting.

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37

Poly (lactic acid)/ amine grafted mesoporous silica-based composite for food packaging application

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Abstract Category

Sustainable Engineering

Abstract

Poly (lactic acid)/ amine grafted mesoporous silica-based composite for food packaging application

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A B S T R A C T

The present study focuses on the development of environmentally friendly bio-composite films using poly(lactic acid) (PLA) as a biopolymer matrix. This is achieved by incorporating amine functionalized green mesoporous silica (GMS) and employing a solution casting method for film fabrication. The motivation behind the work is to improve the compatibility between PLA and green mesoporous silica sourced from rice husk by functionalizing GMS with APTES (3-Aminopropyltriethoxy silane). The primary objective is to explore how the inclusion of GMS influences both the physicochemical attributes and the efficacy of active food packaging in PLA. The introduction of GMS to the PLA matrix not only improves the flexibility of PLA/GMS composite films but also enhances their overall performance. The reinforcement of GMS in the PLA matrix has also significantly contributed towards the reduction in oxygen transmittance rate and provided an anti-bacterial effect towards pathogen i.e. *S. aureus and E. coli.* The PLA/GMS composite films exhibit antioxidant activity acting as potential scavengers with around 78 % efficacy against DPPH (2,2-diphenyl-1-picrylhydrazyl). Consequently, the PLA/GMS composite formulation proposed in this study shows promising outcomes in terms of strength, flexibility, antioxidant properties, and antibacterial

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42

Transition Metal-Loaded TiO2 Catalyst for Catalytic Thermoliquefaction of Municipal Solid Waste into Carbon-Rich Oil.

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Abstract Category

Catalysis For Energy

Abstract

The continued depletion of fossil fuels has intensified the search for sustainable, clean energy alternatives, with biomass emerging as a promising renewable resource. In this study, inexpensive transition-metal-loaded TiO_2 catalysts were explored for catalytic thermoliquefaction (mCTL) of biodegradable municipal solid waste to produce carbon-dense mCTL oil under mild reaction conditions. Various catalysts, including Cr/TiO_2, Ni/TiO_2, Fe/TiO_2, Co/TiO_2, and Cu/TiO_2, were synthesized from nitrate precursors and evaluated for mCTL performance. Among them, Co/TiO_2 exhibited superior activity, achieving biomass conversion (>68%) and mCTL oil yield (>58%) at 200°C without forming char or gaseous byproducts. Under optimized conditions (250°C, 60 min), biomass conversion and mCTL oil yield increased to >84% and >77%, respectively. Characterization studies confirmed uniform cobalt dispersion on TiO_2 with crystalline Co_2O_3 and Co_3O_4 phases. The catalyst exhibited a mesoporous structure with a surface area of 16.93 $m^2\ g^{-1}$ and pore diameters of 8–16 nm. The obtained mCTL oil was analyzed using elemental analysis, FTIR, GC-MS, and HPLC, revealing the presence of hydrocarbons, acids, esters, and alcohols. Recyclability studies demonstrated stable catalytic performance over five consecutive cycles. Sustainability assessment using E-factor, process mass intensity (PMI), and water and carbon footprints highlighted the environmental viability of the process. The superior performance of Co/TiO_2 is attributed to its balanced redox activity, hydrogenation capability, efficient C–O bond cleavage, and thermal stability.

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44

Catalytic Co-Liquefaction of Organic Biodegradable Fraction of Municipal Solid Waste and Sugarcane Bagasse

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Abstract Category

Catalysis For Energy

Abstract

Municipal solid waste (MSW) and sugarcane bagasse (SCB) are considered as promising feedstocks for energy and fuel production due to their abundant availability and high carbon content; however, efficient carbon accessibility remains a key challenge. This study presents a novel approach for synergistic co-liquefaction of MSW and sugarcane bagasse (SCB) using transition metal-dispersed TiO_2 catalysts under comparatively mild operating conditions. Proximate and ultimate analyses confirm the high carbohydrate and lignin content of the feedstocks, making them suitable for producing carbon-rich liquid fuels. A series of non-precious metal catalysts (Cr, Ni, Fe, Co, and Cu) supported on TiO_2 were synthesized and systematically evaluated; notably, Co-TiO_2 demonstrated superior catalytic performance, achieving high selectivity (>85%) and mCTL oil yield (>48%) with negligible char and gaseous byproduct formation, highlighting an efficient carbon retention pathway. The influence of operating parameters was systematically investigated. Under optimized conditions, the process achieved >70% biomass conversion, >65% Co-mCTL oil yield, and >80% selectivity, driven by a synergistic interaction between MSW and SCB that enhances depolymerization and stabilizes reactive intermediates. The Co-TiO_2 catalyst demonstrated excellent recyclability, with a carbon-based turnover number (TON) of 190.61 and turnover frequency (TOF) of $1.27 \times 10^2\ h^{-1}$. Product characterization using ATR-FTIR, elemental analysis, HPLC-RID, and total acid number (TAN) confirmed the formation of energy-dense liquid fuels. Furthermore, this study provides an integrated evaluation of process performance and environmental impact, demonstrating a scalable and eco-friendly pathway for simultaneous waste valorization and sustainable biofuel production.

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47

ONE-POT UPGRADING OF POLYETHLENE AND CO2 INTO AROMATIC CHEMICALS VIA TANDEM CATALYSIS

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

Plastic waste and increasing carbon dioxide (CO_2) emissions are major environmental challenges in modern society. This project presents an innovative approach for the one-pot upgrading of polyethylene (PE) and CO_2 into valuable aromatic compounds using a tandem catalytic system. Unlike conventional recycling methods, which often produce low-quality products and require high energy, this process converts waste materials into useful chemicals in a single reactor. The process involves the use of bifunctional catalysts where Zn/ZSM-5 catalyst helps in polyethylene depolymerization and aromatization, while Cu–Fe_3O_4 catalyst activates CO_2 through the reverse water–gas shift reaction. This integrated system enables the production of valuable aromatics such as benzene, toluene, and xylenes. This study demonstrates a sustainable and efficient method for converting plastic waste and greenhouse gases into high-value chemicals. The proposed approach supports the concept of a circular economy and offers a promising solution for future green chemical processes.

Keywords: Polyethylene upcycling; CO_2 activation; Tandem catalysis; Aromatics production; Circular carbon economy

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48

Pathways to Climate Positive Fuels: Experimental and Simulative Exploration of CO_2 Conversion

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

Atmospheric CO_2 levels are rising at an unprecedented rate, driven by fossil fuel combustion and industrial activity, and demand decisive mitigation strategies. Current approaches emphasize capture and storage, but sustainable progress requires active utilization of CO_2 as a resource.This study implements an electrochemical pathway to convert captured CO_2 into high-value liquid fuels using renewable electricity under controlled conditions. Key operating parameters and system configurations are systematically examined to establish a structured understanding of the conversion process. A parallel modelling-based techno-economic and energy assessment is conducted to evaluate feasibility, energy balance, and practical relevance. By integrating experimental validation with process-level analysis, this work

advances CO_2 utilization technologies in support of carbon-neutral and circular energy systems.

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49

Photocatalytic CO_2 Reduction for Sustainable Fuel Synthesis: Experimental and Simulation Approaches

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

Atmospheric carbon dioxide (CO_2) concentrations have increased significantly due to fossil fuel combustion, industrial activities, and deforestation, making CO_2 a major contributor to global climate change. The growing environmental impact of greenhouse gas emissions has created an urgent need for technologies that not only reduce carbon emissions but also convert CO_2 into valuable products. While carbon capture technologies have advanced considerably, storage alone does not fully utilize the potential of captured CO_2. Consequently, carbon capture and utilization (CCU) has emerged as a promising approach for transforming CO_2 into useful fuels and chemicals while supporting a circular carbon economy. This study investigates the photocatalytic conversion of captured CO_2 into sustainable fuels using advanced semiconductor-based heterojunction catalysts. The

research focuses on enhancing light absorption, charge separation, CO_2 activation, and product selectivity through catalyst design and optimization of reaction conditions. By utilizing solar energy as the driving force, photocatalysis offers a sustainable route for converting CO_2 into value-added products under mild operating conditions. Particular emphasis is placed on understanding the effects of catalyst properties and reaction environments on photocatalytic performance. To complement the experimental work, COMSOL Multiphysics simulations will be employed to model light distribution, charge carrier transport, mass transfer, and reaction kinetics within the photocatalytic system. The integration of experimental and computational approaches is expected to provide mechanistic insights, identify key parameters governing conversion efficiency, and assess the feasibility of scalable solar-driven CO_2 utilization technologies. The outcomes of this work aim to advance sustainable fuel production and support long-term carbon mitigation strategies.

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52

An Electrolytic Route to Sustainable Cotton Bleaching with In-situ Oxidant Regeneration

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Sustainable Engineering

Abstract

Conventional cotton bleaching uses hydrogen peroxide in strongly alkaline baths at near-boiling temperatures (95–98 °C), driving high water, energy, and auxiliary-chemical consumption and contributing to textile wet processing's roughly one-fifth share of global industrial water pollution. The undertaken study proposes an electrolytic bleaching concept

in which the active oxidant is electro-generated and continuously regenerated in situ at the electrode, reducing fresh-chemical demand and enabling lower-temperature operation, followed by a benign post-bleach conditioning step that removes residual species and supports bath reuse. Greige cotton is treated in a laboratory-scale cell using an aqueous alkaline medium and non-precious-metal electrodes, controlled on a Metrohm Autolab PGSTAT under galvanostatic and potentiostatic modes, with the oxidant state tracked by UV–Vis spectrophotometry. Treated fabric is assessed for CIE whiteness index, tensile-strength retention, and absorbency, benchmarked against a conventional peroxide baseline. The presented solution is expected to match conventional whiteness (reported optimised values ~135–140) while cutting water use and carbon-dioxide emissions, consistent with projected reductions of up to ~30% and ~40% respectively for next-generation bleaching, and to maintain fibre integrity through milder processing. The benign conditioning step manages residual deposition and enables a closed-loop, bath-reuse approach. This work therefore presents a greener, electrochemically regenerated bleaching route targeting conventional quality at substantially lower environmental footprint; detailed optimisation and life-cycle and techno-economic assessment are ongoing.

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56

AI-Driven Environmental Toxicity Prediction Platform for Sustainable Chemical Manufacturing: A Machine Learning Approach for Early Hazard Assessment of Industrial Chemicals

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Abstract Category

Sustainable Engineering

Abstract

The rapid growth of the chemical industry has led to the release of synthetic chemicals into aquatic ecosystems, creating challenges for environmental sustainability and regulatory compliance. Conventional toxicity assessment methods rely heavily on animal testing and extensive laboratory experimentation, making them costly, time-consuming, and unsuitable for high-throughput screening of emerging chemicals. The present study proposes an Artificial Intelligence driven Environmental Toxicity Risk Assessment framework capable of predicting the ecological toxicity of industrial chemicals before their large-scale production or discharge into water bodies.

A dataset containing physicochemical descriptors, molecular fingerprints, environmental persistence parameters, and experimentally reported ecotoxicity endpoints was compiled from publicly available environmental databases. Multiple machine learning algorithms were trained and validated to establish quantitative relationships between molecular structure and environmental toxicity. Model interpretability techniques such as Shapley Additive Explanations were employed to identify critical molecular features governing toxicity.

The developed framework generates a Sustainability Hazard Index that integrates predicted aquatic toxicity, bioaccumulation potential, persistence, and environmental mobility into a single decision-support parameter. Preliminary results demonstrate prediction accuracies exceeding 85% for major ecotoxicological endpoints while significantly reducing the need for experimental testing. Furthermore, the platform enables virtual screening of proposed industrial chemicals and identification of safer molecular alternatives during the design stage.

The present study is a step toward Sustainable Chemistry 5.0 by integrating artificial intelligence, green chemistry principles, and environmental chemistry into chemical manufacturing. The methodology can assist industries, regulatory agencies, and researchers in implementing proactive pollution prevention strategies, accelerating the transition toward safer chemicals and sustainable industrial development.

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57

Recoverability-Aware Industrial Operations: Quantifying Degradation Dynamics, Operational Observability, and Recovery Potential

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Abstract Category

Sustainable Engineering

Abstract

Industrial process and infrastructure systems are traditionally managed through monitoring, diagnostics, predictive maintenance, and control frameworks. While these approaches provide visibility into process behaviour and degradation, they do not explicitly quantify whether acceptable operating conditions can still be restored before significant operational, economic, or sustainability losses occur. This work introduces a conceptual and empirical foundation for recoverability, defined as the remaining ability of an operating system to return to an acceptable operating region before crossing an irreversible operational boundary.

A generalized energy-based operational modelling methodology was developed to characterize degradation dynamics and operational observability using multivariate industrial measurements. Validation was performed across sixteen experiments spanning synthetic degradation scenarios, NASA C-MAPSS turbofan engines, SKAB industrial water circulation systems, and causRCA industrial manufacturing systems, representing process operations, industrial infrastructure, rotating machinery, and manufacturing environments.

Results demonstrate consistent characterization of degradation progression across diverse industrial domains, achieving an average calibrated state-classification accuracy of approximately 73%, with controlled degradation scenarios approaching 100% accuracy. Strong monotonic relationships between operational instability and fault progression suggest that recovery potential may be inferred from degradation trajectories and operational state evolution, providing a practical basis for recoverability-aware decision making.

Recoverability is particularly relevant to sustainable industrial operations, where degradation-driven process upsets frequently result in increased energy consumption, material losses, reduced throughput, off-specification production, and unplanned downtime. The proposed perspective establishes a foundation for recoverability-aware engineering systems capable of assessing not only what is happening and why, but also whether operational continuity can still be preserved.

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61

A greener approach towards sustainable production of biodiesel from waste frying oil using biowaste-derived *Unio pictorum* shell-*Musa acuminata* peel ash nanocomposite catalyst

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

Sustainable biodiesel production from waste-derived feedstock utilizing an efficient, eco-friendly catalyst offers dual benefits of waste mitigation and renewable energy generation. In this work, an environmentally benign heterogeneous nanocomposite catalyst was synthesized from biowastes, including *Unio pictorum* shells and *Musa acuminata* peels, for the production of biodiesel from waste frying oil (WFO). Physicochemical characterizations revealed that the synthesized catalyst was predominantly composed of CaO and K_2CO_3 as active constituents responsible for the methanolysis of triglycerides. Numerous transesterification process parameters were optimized using Response Surface Methodology (RSM) within the Box-Behnken Design (BBD) model to maximize biodiesel conversion while minimizing resource utilization. An excellent biodiesel conversion of 98.2% and a yield of 97.5% were achieved under optimal reaction conditions. Additionally, the proposed catalyst demonstrated exceptional reusability over 7 catalytic cycles with minimal activity loss, indicating high conversion efficiency and structural stability throughout the reaction. Transesterification kinetics confirm the pseudo-first-order model, while thermodynamic studies indicate the reaction is non-spontaneous and endothermic. Achieving high turnover frequency and lower values of green metrics suggests that the subsequent transesterification process is clean, efficient, and environmentally friendly. Furthermore, several fuel characteristics, including calorific value, cetane number, kinematic viscosity, cloud point, and pour point, comply with ASTM D-6751 standards, rendering it suitable for diesel engines. This research showcases a clean and sustainable approach to producing biodiesel using biowaste-derived catalysts, aligning with green chemistry principles and promoting the circular economy

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66

Electrochemical Pathway for CO2 conversion into Ethanol

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Abstract Category

Sustainable Engineering

Abstract

The increasing concentration of carbon dioxide (CO_2) in the atmosphere, driven by the extensive use of non-renewable energy sources, has become a critical environmental concern. This has intensified the need for sustainable technologies capable of both mitigating CO_2 emissions and generating alternative fuels.

This study investigates a lab-scale electrochemical pathway for the conversion of carbon dioxide into value-added biofuels, specifically methanol and ethanol. The process utilizes a catalyst system based on copper (Cu), carbon, and nitrogen. Upon the application of an external electric potential, electrochemical reactions are initiated that facilitate the reduction of CO_2, effectively mimicking a reverse combustion pathway. Based on existing literature, the process can achieve yields of up to approximately 62% under optimized conditions.

The proposed approach offers a dual advantage by addressing carbon emissions while simultaneously producing useful and relatively cleaner fuels suitable for transportation and energy applications. This research focuses on evaluating the efficiency of CO_2-to-fuel

conversion at the laboratory scale, analyzing the role of Cu-based catalysts in enhancing selectivity toward methanol and ethanol, and assessing the feasibility of scaling such systems for practical, real-world implementation.

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68

Analytical Quality by Design optimization of dual RP-HPLC and ion chromatography methods for sustainable determination of edoxaban tosylate: Comparative validation and multi-metric greenness assessment

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Abstract Category

Sustainable Engineering

Abstract

We report the first dual-platform, AQbD-driven analytical strategy combining a green reversed-phase HPLC (RP-HPLC) and ion chromatography (IC) method for quality control of Edoxaban Tosylate Monohydrate (EDTM). Using Ishikawa risk assessment and Central Composite Design, a robust Method Operable Design Region (MODR) was established (R^2 > 0.87; prediction error <1%), providing ICH Q14-compliant regulatory flexibility. The ethanol-based RP-HPLC method (ZORBAX Eclipse XDB-C8; 0.1% acetic acid/ethanol, 80:20 v/v) was significantly more effective in reducing the acetonitrile compared to traditional methods while delivering better performance: linearity 5–150 µg/mL (r^2 = 0.9992), LOD 0.8 µg/mL, accuracy 100.4 ± 0.35%, precision RSD < 1.3%, and stability-indicating capability across all stress conditions (mass balance 98.5–100.3%). The orthogonal IC method (suppressed conductivity detection) provided increased sensitivity to ionic impurities (Cl^-, NO_3^-, SO_4^{2-}; LOD = 0.015–0.025 µg/mL). The orthogonal IC method has been validated as per the ICH Q2(R2) guidelines demonstrating excellent accuracy (100.2 ± 0.73%), and precision (RSD < 1.6%). Sustainability was measured by six complementary green metrics (Eco-Scale: 83/88; AGREE: 0.79/0.82 for HPLC/IC), exceptionally high quality of environmental profile. The dual-platform approach demonstrates that RP-HPLC optimally serves API assay and degradation profiling, whereas IC is indispensable for tosylate counter ion verification and trace ionic impurity monitoring together providing a sustainable, and ICH-compliant pharmaceutical QC framework.

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69

Effect of CaCO3 Concentration and Inoculum Size on Glucose Utilization by Aspergillus oryzae and Aspergillus wentii

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Abstract Category

Fermentation processes

Abstract

Organic acids are valuable platform chemicals with applications in the food, pharmaceutical, and chemical industries. Filamentous fungi have attracted considerable attention as microbial cell factories because of their ability to efficiently utilize carbohydrates under fermentation conditions. Process parameters such as buffering capacity and inoculum size play important roles in fungal metabolism and substrate utilization. This study investigated the effects of $CaCO_3$ concentration and inoculum size on the fermentation performance of *Aspergillus oryzae* and *Aspergillus wentii*. Batch fermentations were conducted in a glucose-based medium containing 100 g/L initial glucose using two inoculum sizes (5 and 10% v/v) and two $CaCO_3$ concentrations (60 and 90 g/L). Residual glucose concentration and pH were monitored over a 10-day fermentation period. Both fungal strains efficiently utilized glucose under all tested conditions. Increasing the inoculum size from 5 to 10% produced only marginal differences in glucose consumption, whereas $CaCO_3$ concentration significantly influenced fermentation performance. At 90 g/L $CaCO_3$, residual glucose decreased to approximately 16–21 g/L by day 8–10, corresponding to nearly 80% substrate utilization, whereas cultures containing 60 g/L $CaCO_3$ retained 37–51 g/L glucose after 10 days. The higher $CaCO_3$ concentration maintained the fermentation pH within 6.5–7.5, whereas cultures containing 60 g/L $CaCO_3$ exhibited a larger pH decline to 5.0–6.8. These findings indicate that enhanced buffering capacity coincided with improved glucose utilization and more stable fermentation conditions. The results provide a basis for optimizing fungal fermentation and guiding future metabolite characterization studies.

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71

Extraction of High-Grade Silica from Rice Husk Ash: A Sustainable Engineering Approach

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Abstract Category

Sustainable Engineering

Abstract

Rice husk ash (RHA) is an agricultural waste generated after the burning of rice husk and is often discarded without any proper use, causing environmental problems. However, RHA contains a large amount of silica, making it a valuable raw material for silica production. The present work focuses on the extraction of high-grade silica from rice husk ash using a simple and cost-effective chemical process.

In this study, rice husk ash was collected and treated to remove impurities. Further chemical treatment was carried out to extract silica, which was then washed, dried, and converted into high-grade silica powder. The extraction process is simple, economical, and environmentally friendly.

The study demonstrates that agricultural waste can be effectively utilized to produce a valuable material instead of being disposed of as waste. The extracted silica has potential applications in various industries, including glass, ceramics, rubber, cement, and other advanced materials.

This work promotes sustainable engineering by converting agricultural waste into a useful product while reducing environmental pollution. The findings highlight the importance of resource recovery and encourage the development of sustainable technologies for waste utilization.

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73

Sustainable synthesis of 3,4-dihydropyrimidinone scaffolds as potential antiviral agents

Disha Virnodkar[1,2], Shrinivas Joshi[3], Vidya Desai[1,2]

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Abstract Category

Atom economical catalysis

Abstract

Abstract:

In the recent past, viral diseases have been among the primary global health concerns and efforts are underway to design molecules with distinct antiviral properties. Additionally, the versatile biological activity of dihydropyrimidinone (DHPM) derivatives and their ability to combat viruses have made such compounds of profound medicinal interest in the development of antiviral agents. Synthesis of such bioactive compounds have been achieved by Biginelli synthesis via a multi-component strategy as a classical example demonstrating green and sustainable synthesis. Thus, in our green protocol, we synthesized a series of fifteen derivatives of 3,4-dihydropyrimidine-2(1H)-one via an atom-economical Biginelli reaction between dicarbonyl compounds, urea, or thiourea with heterocyclic/aromatic aldehydes under solvent-free conditions and evaluated their biological properties for possible drug leads against viral diseases. The structures of the compounds were established by ^{1}H NMR, ^{13}C NMR and mass spectral analysis. Molecular docking studies were performed to analyze the binding mode and interaction pattern of these compounds.

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74

Development and Characterization of "Oraalix":A Sustainable, Anhydrous Dentifrice Tablet

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Abstract Category

Sustainable Engineering

Abstract

'**Oraalix**' is a dentifrice tablet which creates an innovation in oral care industry. The Oraalix is a tablet which can replace the regular toothpaste by it's limitations and Disadvantages.

- The regular toothpaste contains harsh abusive and surfectants which are harmful for longer use in oral hygiene.
- The regular toothpaste tube contains different plastics, Aluminium foils and polymers hence, they are nearly impossible to recycle.
- The regular toothpaste has high amount of hydrus elements and pesticides and preservatives to prevent from microbial growth.

The Oraalix Tablet : Oraalix is an innovation over these issues:

- The Oraalix Contains no moisture contains hence, it is lighter easy to carry and preservative free.
- The Oraalix Tablet Contains very gentle abrasive and Surfectants which does not harm to the consumer.

- The Oraalix Tablet will reduce polution by using paper and recyclable material for packing.
- The Oraalix Tablet reduces water wastage and it decomposes it's materials in used water within 28 days.
- The Oraalix Tablets have very less transportation cost and manufacturing cost also, provides very high profit margins in the view of business. Hence, highly scalable.

Conclusion : Oraalix is a dentifrice tablet which is highly scalable and consumer friendly product while replacing toothpastes from day to day life.

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75

Analysis of Energy Consumption and CO_2 Emissions in India's Petrochemical Sector

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Abstract Category

Clean Energy

Abstract

India's petrochemical sector is undergoing rapid expansion due to rising demand for plastics, packaging materials, fertilisers, synthetic fibres, and downstream industrial products. However, petrochemical production is energy-intensive and is majorlydependent on fossil-based feedstocks and thermal energy systems, making the sector a major contributor to industrial CO_2 emissions.

A process-based energy-emissions model of India's petrochemical sector has been developed to quantify energy use and CO_2 emissions for petrochemical production. The research is focused on India's major upstream high-value chemicals and downstream polymers, which together dominate production in India's petrochemical industry.

The model follows a thermodynamically consistent bottom-up approach inspired by Neelis et al. (2007), in which petrochemical production routes are treated as black-box systems linking feedstocks, reaction energetics, utility consumption, and product outputs.

It has been identified that India's petrochemical energy demand remains highly thermal in nature, with fuel accounting for ~69% of total primary energy consumption, followed by steam (≈27%) and electricity (≈4%). Ethylene, ammonia, and propylene are the dominant contributors to both energy demand and CO_2 emissions because of their large production volumes and highly energy-intensive production pathways.

Overall, the findings indicate that India's petrochemical energy and emissions burden is concentrated in a limited number of high-volume production routes. The study highlights that the most effective decarbonisation strategies for the sector involve targeted improvements in thermally intensive processes such as steam cracking and ammonia synthesis through enhanced furnace efficiency, heat integration, waste-heat recovery, low-carbon hydrogen adoption, cleaner utility supply, and emerging electrification pathways.

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76

Synthesis of Fluorobased pyrazole scaffolds as sustainable design with antiflaviviral potential

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Abstract Category

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

Abstract

1. The increasing threat of flaviviral infections necessitates the development of potent antiviral agents. With increasing dengue cases at the state level, in the country as well as globally, and also the fact that the disease is non-curable, it remains a challenge to open a gateway towards new therapeutic to fight against dengue. The present study outlines the synthesis of novel lead compounds targeting dengue virus through a multi-step green synthetic approach. The hydrazones were efficiently synthesized using water as a solvent with sodium acetate, acetophenone, and arylhydrazine hydrochloride via a condensation reaction. The hydrazones were then converted to a pyrazole aldehyde through the Vilsmeier- Haack reaction. Subsequent aldol condensation yielded a chalcone, which was cyclized to an aminopyrimidine derivative and then further functionalized into a nucleoside analogue. All synthesized intermediates and final products (hydrazone, aldehyde, chalcone, pyrimidinone, and nucleoside) were characterized using NMR and mass spectroscopy. This synthetic pathway offers a promising route to generate potential anti-flavivirus lead compounds with varied functionalities. The intermediate and final compounds were then screened for possible activity. Encompassing the green

chemistry principles, the work fosters a sustainable approach towards medical, chemical, and drug discovery.

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1. Wang, Y.-T.; Shi, T.-Q.; Zhu, H.-L.; Liu, C.-H. Synthesis, Biological Evaluation and Molecular Docking of Benzimidazole Grafted Benzsulfamide-Containing Pyrazole Ring Derivatives as Novel Tubulin Polymerization Inhibitors. Bioorganic &Medicinal Chemistry, 2019, 27 (3), 502–515.

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77

Cyrene as a bio renewable resource towards synthesis of cyrenyl-quinolinyl chalcone hybrids having antimalarial potential.

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Abstract Category

Production of fine chemicals & chiral products

Abstract

The advent of green chemistry and its guiding principles have not just redefined the way we make chemicals, but it has also given a clean platform to make medicinally important compounds. Biomass valorisation is one of the key illustrations of how waste materials can be a useful resource. Biomass derived Cyrene, has been well demonstrated as a green solvent in important coupling reactions. With its interesting structural motif, there is enough scope to functionalize Cyrene into a promising alternative for existing drugs. Malaria is considered as a life-threatening vector borne disease, caused by plasmodium parasite and continues to be the global burden with increasing infection and death rate every year. Classified as tropical diseases as per the WHO, the mosquito infected menace affects millions of lives in the developing countries. Also, chloroquine and sulfadoxine-pyrimethamine have failed in treatment. Artemisinin, a naturally derived drug has shown resistance towards the plasmodium parasite hence increasing the need for an effective combination therapy or discovering new building blocks for the treatment towards the multidrug resistance strains.

With this review, we demonstrate herein a molecular hybridisation approach towards synthesis of Cyrenyl-Quinolinyl hybrids as leads for enhancing antimalarial activity. Series of chalcone have been screened for the mosquito larvicidal activity as preliminary antimalarial study.

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78

AI For Air pollution And monitoring Control

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Abstract Category

Sustainable Engineering

Abstract

Air pollution is one of the most serious environmental challenges faced by modern society. Rapid industrialization, urbanization, increasing vehicle emissions, burning of fossil fuels, and agricultural activities have significantly contributed to the deterioration of air quality worldwide. Poor air quality affects human health, ecosystems, climate, and overall quality of life. According to the World Health Organization, millions of premature deaths occur annually due to exposure to polluted air.

Traditional methods of air quality monitoring rely on fixed monitoring stations, which are often expensive to install and maintain. These stations also provide limited spatial coverage and cannot efficiently capture pollution variations across different locations. In this context, Artificial Intelligence (AI) has emerged as a powerful technology for monitoring, analyzing, predicting, and controlling air pollution.

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82

Microwave assisted intensification of n-octyl acetate synthesis over $H_5PW_{10}V_2O_{40}$/FAC catalyst: Kinetic Study

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Abstract Category

Cavitation

Abstract

The n-octyl acetate was synthesised in the microwave assisted batch reactor over $H_5PW_{10}V_2O_{40}$/FAC catalyst. The equilibrium conversion of 80% was obtained at the optimised process variables (acid to alcohol mole ratio 1:2, catalyst loading 5 % (w), and temperature 383 K) in the microwave assisted batch reactor. The reaction kinetic expressions were developed to determine the order of reaction with respect to reactants, overall order of reaction, and the reaction rate constants. Experimental data fit shows the reaction follows second order kinetics. The activation energy of the reaction was estimated for best fit kinetic equations. The thermodynamic parameters such as change in Gibbs free energy, change in entropy and change in enthalpy were also estimated. It has been seen that intensification using microwave an alternative energy source help to reduce the time of reaction considerably than that of the ultrasound and conventional batch reactor

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83

Design, Synthesis, Computational Evaluation, and Dual Cu^{2+}/Ag^{+} Sensing Studies of Alkyne-Functionalized Pyrimidine–Chalcone Hybrids

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Abstract Category

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

Abstract

The development of simple, selective and sensitive chemosensors for detecting biologically and environmentally significant metal ions, particularly Cu^{2+} and Ag^{+}, remains a critical challenge in environmental monitoring and medicinal chemistry. In this study, Novel alkyne functionalized pyrimidine-chalcone compounds have been designed, synthesised, and characterised by FTIR, ^{1}H NMR, ^{13}C NMR, and Mass spectrometry. The alkyne–functionalized pyrimidine–chalcone (5a) was tested for its metal-sensing ability by UV-Visible spectroscopy. A probe (5a) was found to be highly selective and sensitive towards the recognition of Cu^{2+} and Ag^{+} ions in methanol solution. Quantitative titration studies revealed low limits of detection (LOD) of 0.841×10^{-7} M for Cu^{2+} and 0.317×10^{-7} M for Ag^{+}, along with high association constants such as 1.233×10^{6} M^{-1} for Cu^{2+} and 4.077×10^{5} M^{-1} for Ag^{+} ions. The Density Functional Theory (DFT) calculations support the experimental sensing results; the HOMO-LUMO energy gap decreases dramatically when the metal is coordinated to the probe 5a (from 3.505 eV to ~1.6 eV), which also enhances electronic reactivity. In addition, the *in-silico* ADMET predictions and molecular docking analyses showed a favourable drug-likeness, oral bioavailability, and stable binding interactions with PDZ domain of Dishevelled-2 (PDB ID: 3CC0). These overall findings establish that the synthesised alkyne-pyrimidine-chalcone compounds are effective for transition metal ion sensing and can act as a promising candidate for medicinal chemistry applications.

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84

Hemp Fiber Inspired Iron Oxide synthesis and application as nanocatalyst fermentive biohydrogen production.

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Abstract Category

Clean Energy

Abstract

Hemp Fiber Inspired Iron Oxide Synthesis and Application as Nano catalyst Fermentative Biohydrogen Production

Abstract

Sustainable dark fermentative biohydrogen production from hemp fibre of *Cannabis sativa* as effective carbon source has been investigated in this study. Approach of sustainable fabrication of Iron oxide nano catalyst has been conducted from sol-gel method of using Cannabis fibre. Additionally, characterization investigation using different technical tools such as XRD, FT-IR, UV-Vis spectroscopy as well as SEM BET, and XPS have been analysed for identification of iron oxide nanomaterial. Newly synthesized nanomaterial applied as nano catalyst to boost dark fermentation process to produce biological hydrogen using newly isolated fermentative bacteria. Dumped sugarcane bagasse juice was used to isolate the desired fermentative bacteria for dark fermentative hydrogen production generation. Under optimized conditions, at 1 mg concentration of nano catalyst and 5 grams of hemp Fiber as carbon source ~2000 ml/L cumulative hydrogen was recorded at 32 degree Celsius and at pH 6.0 in 24h of incubation.

Keywords: Biohydrogen; *Cannabis sativa*; dark fermentation; nano catalyst; iron oxide nanomaterial

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85

Enhancing Bioactive Recovery from Pigeon Pea Seed Coat: A Comparative Evaluation of ultrasound assisted and Conventional Extraction

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Abstract Category

Cavitation

Abstract

Pigeon pea seed coat is an underutilized agro-industrial by product rich in phenolic acids and flavonoids with significant antioxidant potential[1]. Synthetic antioxidants are hazardous and raise safety concerns, therefore it is essential to switch to natural antioxidant derived from plant material[2]. This study compared conventional solvent extraction (CSE) and ultrasound- assisted extraction (USAE) for the recovery of bioactive compounds and optimized using response surface methodology (RSM) based on a Box-Behnken design (BBD).Extraction parameter evaluated for both techniques included temperature (30-60ºC), ethanol concentration (40-80% v/v) and extraction time. For CSE and USAE extraction time ranged from 4-8 h and 25-55min respectively. 2,2-Diphenyl-1-picrylhydrazyl (DPPH), Total flavonoid content (TFC) and Total phenolic content are preferred as response variables. USAE optimized condition were 40.88% ethanol concentration, 58.13ºC and 25 min whereas CSE was optimized at 47.23 % ethanol concentration, 59.23ºC and 4.25 hr. The response variable value at optimum condition for USAE was 126 mg GAE/g of DW, 318 mg QE/ g and 72 % DPPH radical scavenging activity. Similarly, best extraction value for CSE were 110 g GAE/g, 302 mg QE/g and 61 % DPPH radical scavenging activity. The improved extraction through USAE is due to cavitation process which enhances the mass transfer and solvent penetration.USAE is a rapid, efficient, and environmentally sustainable technique for extracting bioactive compounds from pigeon pea seed coat. The optimized process offers a promising approach for valorizing this agricultural by-product as a natural source of antioxidants for food and phytopharmaceutical applications.

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86

Visible-Light-Driven Reductive C–N Bond Formation of Renewable Aldehydes and Lignin Bio-Oil to Amines

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Abstract Category

Catalysis in biomass conversion

Abstract

Lignin is the most abundant renewable source of aromatic carbon, yet sustainable methods for converting lignin-derived molecules into nitrogen-containing chemicals remain limited. Herein, we report a visible-light-driven photocatalytic reductive amination strategy for transforming lignin-derived aromatic aldehydes into aromatic amines under mild and environmentally benign conditions. A Ru@CeO_2/ZrO_2 heterojunction photocatalyst enables efficient C–N bond formation in water at room temperature under low H_2 pressure (1.5 bar), thereby avoiding the use of stoichiometric reductants and harsh thermocatalytic conditions. The catalyst exhibits high activity and selectivity for a variety of lignin-derived aldehydes. The methodology was further extended to wheat-straw-derived lignin bio-oil through oxidative depolymerization-assisted amination, demonstrating compatibility with complex biomass streams relevant to biorefinery applications. CHEM21 green metrics revealed excellent material efficiency, with an atom economy of 90.6%, reaction mass efficiency of 82.2%, and low process mass intensity values (PMI = 1.4, reduced to 1.2 upon scale-up). Mechanistic studies suggest that visible-light irradiation promotes efficient charge separation within the Ru@CeO_2/ZrO_2 heterojunction, while Ru sites facilitate hydrogen activation for selective reductive amination. This work establishes a sustainable photocatalytic platform for nitrogen functionalization of lignin-derived feedstocks and highlights a mild, energy-efficient route for producing aromatic amines from renewable biomass.

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87

Photocatalytic Lignin Valorization through Selective Cleavage of C–O Linkages over Ru-Supported Holey g-C_3N_4 Nanosheets.

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Abstract Category

Catalysis in biomass conversion

Abstract

Lignin valorization into fuel-range hydrocarbons and value-added chemicals is hindered by its structurally complex network of C-O ether linkages, particularly the recalcitrant 4-O-5 bond with its high bond dissociation energy. Herein, Ru-decorated holey exfoliated carbon nitride nanosheets (Ru/ECNHS) were developed through a stepwise thermal exfoliation and Ru-decoration strategy for the selective photocatalytic hydrogenolysis of lignin-derived C-O bonds under visible light. Optoelectronic characterization revealed that exfoliation of bulk g-C_3N_4 significantly enhanced charge separation and prolonged the lifetime of photogenerated charge carriers, while Ru NPs acted as electron sinks and facilitated H_2 activation. The optimized Ru/ECNHS photocatalyst efficiently cleaved the challenging 4-O-5 linkage as well as α-O-4 and β-O-4 ether bonds, affording aromatic and cyclic hydrocarbons in 90–96% yields. The catalytic system also exhibited high activity toward lignin model compounds bearing representative –OH and $–CH_3$ functionalities. Control and radical-scavenging experiments confirmed the crucial involvement of photogenerated charge carriers and Ru-mediated H_2 activation in the hydrogenolysis pathway. Importantly, the developed photocatalyst successfully converted simulated lignin bio-oil and native lignin into arenes and hydrocarbons, demonstrating its applicability beyond simplified model substrates. Green chemistry metrics further indicated high atom efficiency and a low environmental footprint. These findings establish Ru/ECNHS as an efficient and reusable visible-light-responsive photocatalyst for the selective cleavage of diverse lignin C-O ether linkages, providing a promising strategy for sustainable lignin valorization.

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89

MOF-Incorporated Polymeric Membranes for CO2 Capture: A Comparative Literature Review

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Abstract Category

Sustainable Engineering

Abstract

Rising CO2 emissions from fossil fuel combustion have made carbon capture, utilization, and storage (CCUS) important for climate change mitigation. Among the available separation technologies, polymeric membranes offer a compact, energy efficient, and scalable alternative to conventional amine scrubbing and adsorption processes. However, pristine polymeric membranes suffer from a permeability-selectivity trade-off described by the Robeson upper bound. Mixed matrix membranes (MMMs), formed by dispersing porous fillers such as metal-organic frameworks (MOFs) within a polymer matrix, have emerged as a promising route to overcome this limitation by combining the polymers high surface area, tunable pore geometry, and CO2-philic character with the MOFs. This work presents a comparative survey of the literature on MOF-incorporated polymeric membranes for CO2 capture.

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90

Selective Hydrogenation of Furfural to 2-Methyltetrahydrofuran over Bimetallic Ru–Ni Nanoparticles Supported on Nanocrystalline CeO_2

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Abstract Category

Catalysis in biomass conversion

Abstract

Nanocrystalline ceria (CeO_2) with engineered surface defects provides a versatile platform for constructing catalytically active metal-oxide interfaces. Herein, we report a defect-rich nanocrystalline CeO_2-supported bimetallic Ru-Ni nanoparticles in which electronically coupled interfacial sites govern selective biomass upgrading. Structural and spectroscopic analyses (XRD, TEM, XPS, EPR, Raman, H_2-TPR/TPD, and NH_3-TPD) reveal strong metal-support interactions, abundant oxygen vacancies, and nanoscale Ru-Ni proximity, which promote interfacial electronic coupling without alloy formation. The optimized 3Ru-5Ni/CeO_2 catalyst achieves complete conversion of furfural (FAL) with 92% selectivity toward 2-methyltetrahydrofuran (2-MTHF) at 200 °C and 0.5 MPa H_2 in 2 h. Reaction optimization, substrate transformation studies, kinetic studies, and pyridine poisoning experiments establish a sequential pathway involving FAL hydrogenation to furfuryl alcohol (FOL) and its hydrodeoxygenation to 2-methylfuran (2-MF), and final ring hydrogenation to 2-MTHF. The enhanced performance originates from cooperative nanoscale interactions in which Ru facilitates H_2 dissociation, Ni promotes C-O bond activation, and vacancy-rich CeO_2 enables hydrogen spillover and intermediate stabilization. These findings demonstrate how defect engineering and bimetallic interface design in nanostructured oxide supports can precisely steer reaction pathways for sustainable upgrading of biomass-derived furans.

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91

Ni NPs decorated ZrO2 Phase-dependent activity for Furfural hydrogenation to yield THFA and CPO selectively

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Abstract Category

Catalysis in biomass conversion

Abstract

Biomass is an inexhaustible, renewable carbon source that can be converted into chemicals and fuels currently derived from fossil resources. In this context, biomass is first converted into highly reactive intermediate compounds, known as platform chemicals, which are subsequently converted into target products through processes such as hydrogenation and hydrodeoxygenation.In this work, we prepared a series of Ni-loaded ZrO_2 catalysts with three crystalline phases: tetragonal (t), monoclinic (m), and mixed (mix). These phases were synthesized with Ni loadings ranging from 5–15 wt.%, and the catalysts were designated as 5Ni/t-ZrO_2, 10Ni/t-ZrO_2, 15Ni/t-ZrO_2, 5Ni/m-ZrO_2, 10Ni/m-ZrO_2, 15Ni/m-ZrO_2, and 15Ni/mix-ZrO_2. The catalysts exhibited distinct activities in the hydrogenation of furfural (FFR), leading to the formation of tetrahydrofurfuryl alcohol (THFA) and cyclopentanone (CPO) via furfuryl alcohol (FAL) as an intermediate. Among them, 10Ni/t-ZrO_2 demonstrated excellent performance, achieving complete conversion with 92% selectivity toward THFA at 130 °C and 20 bar H_2 pressure, using water as the solvent, within 6 h. In contrast, 10Ni/m-ZrO_2 also achieved complete conversion but with 83% selectivity toward CPO under the same reaction conditions, in 4 h. Recyclability studies revealed that the catalyst maintained 100% furfural conversion and approximately 90% selectivity toward THFA over 4 consecutive cycles. The structure–activity relationship was established through detailed physicochemical characterization using XRD, BET, HR-TEM, XPS, NH_3-TPD, pyridine FT-IR, H_2-TPR, Raman spectroscopy, and EPR analysis. Finally, based on the catalytic activity data, literature reports, and physicochemical properties, a reaction mechanism has been proposed for product formation under identical reaction conditions for Ni-loaded ZrO2.

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93

Life Cycle Assessment of FDCA Production from Cellulose using Cradle to Gate Approach.

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Abstract Category

Life cycle assessment

Abstract

Global efforts toward sustainability demand greener alternatives to petrochemical-derived plastics. Polyethylene Furanoate (PEF), synthesized from Furan Dicarboxylic Acid (FDCA) and ethylene glycol, is a promising bio-based substitute for Polyethylene Terephthalate (PET), but its commercialization is hindered by unresolved production and separation challenges. FDCA, derived from lignocellulosic biomass, is fully biodegradable and holds significant market potential, yet most studies remain confined to lab and pilot scale. This work presents a cradle-to-gate Life Cycle Assessment (LCA) of FDCA production via crystallization-based separation, aimed at identifying environmental hotspots to guide sustainable large-scale process design.

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96

AI for Sustainability Evaluation of Waste-to-Value Technologies

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Abstract Category

Sustainable Engineering

Abstract

The growing emphasis on circular economy and sustainable engineering has accelerated the development of waste-to-value (WtV) technologies that transform industrial, agricultural and municipal waste into valuable products, chemicals and energy. Although numerous WtV technologies have demonstrated significant technical potential, evaluating their overall sustainability remains challenging due to the need to simultaneously consider environmental, technical, economic and implementation-related factors. Existing evaluation approaches are often fragmented and lack an integrated assessment perspective.

This study explores the potential of Artificial Intelligence (AI) in strengthening the sustainability evaluation of waste-to-value technologies through a structured multi-criteria assessment approach. The proposed methodology integrates key sustainability indicators, including resource efficiency, environmental impact, energy consumption, economic feasibility, technology readiness and scalability, to provide a holistic evaluation framework. AI-assisted analytical techniques are examined for their ability to process complex datasets, identify relationships among evaluation parameters and improve the consistency of sustainability assessments.

The study presents an illustrative framework demonstrating how AI can facilitate comparative evaluation and prioritization of representative waste-to-value technologies using published literature and sustainability criteria. The proposed approach aims to support researchers, industry practitioners and policymakers in selecting sustainable technological pathways while promoting resource efficiency and circular economy principles. The framework provides a foundation for future validation using industrial case studies and AI-based analytical models.

Keywords: Artificial Intelligence; Sustainability Evaluation; Waste-to-Value Technologies; Circular Economy; Sustainable Engineering.

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98

Nanofiller-Engineered Thin-Film Nanocomposite Membranes for Liquid and Gas Separation

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Abstract Category

Sustainable Engineering

Abstract

Thin-film nanocomposite (TFN) membranes have emerged as a promising class of separation materials by integrating functional nanomaterials into polyamide selective layers. The incorporation of nanofillers enhances membrane permeability, selectivity, mechanical stability, and fouling resistance through improved interfacial interactions and controlled molecular transport pathways. Furthermore, green fabrication techniques, such as vapor-phase interfacial polymerization (VP-IP), provide a sustainable alternative to conventional membrane preparation by eliminating hazardous organic solvents while enabling precise control over selective layer formation. Recent advances in nanofiller engineering and environmentally benign fabrication have significantly expanded the potential of TFN membranes for both liquid and gas separation applications, including water purification, wastewater treatment, carbon capture, and hydrogen purification. This work presents an overview of recent developments in nanocomposite membrane design, fabrication strategies, separation mechanisms, and emerging applications, highlighting current challenges and future opportunities for developing scalable, high-performance, and sustainable membrane technologies.

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100

Valorization of Lemon Peel Waste into Sustainable Biochar for Green Removal of Acidic Black 1 Dye from Wastewater: Insights from RSM and ANN Predictive Modelling

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Abstract Category

Sustainable Engineering

Abstract

Textile, dyeing, and leather industries discharge substantial volumes of acid dye-laden wastewater, with Acid Black 1 (AB1), a diazo acid dye, posing significant ecotoxicological and erythropoietic health risks due to its resistance to biodegradation. Conventional treatment methods remain costly and energy-intensive, motivating low-cost, renewable biosorbents. This study valorizes lemon peel waste, a citrus-processing residue generated at an estimated 1.9-2.1 million metric tons annually in India, into a chemically activated biochar for sustainable AB1 removal from wastewater. Lemon peel biochar (LPBC) was synthesized via pyrolysis at 500°C and functionalized with potassium hydroxide (KOH) at four biomass-to-activator ratios (1:1-1:4), yielding five adsorbent variants including a pristine control. Batch adsorption screening identified the 1:3 KOH-activated biochar (LPK3) as the most effective, achieving rapid visible decolorization within one hour. Kinetic studies conducted at 100, 200, and 300 ppm AB1 concentrations confirmed strong pH-dependence, with acidic conditions (pH 2.5-3.2) achieving 67-80% removal efficiency compared to only 8-36% under neutral and basic conditions, consistent with electrostatic attraction between protonated biochar surface groups and the dye's anionic sulfonate moieties. Ongoing isotherm experiments (120 data points across 8 concentrations and 5 biochar compositions) will generate a comprehensive dataset for Response Surface Methodology (RSM) and Artificial Neural Network (ANN) based predictive modelling of adsorption performance. This integrated experimental and computational approach aims to establish an optimized, scale-up-ready framework for sustainable dye wastewater remediation using a currently underutilized agricultural waste stream, supporting circular-economy principles in industrial water treatment.

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103

Unveiling the pore characteristics of Indian coal for geological CO_2 sequestration and natural gas recovery.

Shubham Kumar[1], Vikram Vishal[2], Ranjith Pathegama Gamage[3]

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Abstract Category

Clean Energy

Abstract

Interpreting pore characteristics in unconventional resources such as coal seams is vital for mitigating climate change and reducing anthropogenic carbon emissions. In this study, coal samples were collected from the gas-rich Jharia coalfield, Barakar Formation. The depth of the coal samples ranged from 73 to 653 m, and they were examined using the low-pressure CO_2-N_2 gas adsorption method. The results show that the total organic carbon (TOC) content in coal varies from 50.23 to 65.65%. In this context, the organic content shows a positive correlation with micropore attributes and aligns with the pathway for geological carbon sequestration. Additionally, samples SD-3 and SD-2 show positive correlations with higher clay mineral content. Interestingly, SD-4 and SD-5 contain higher amounts of siderite, which hinders the pore space in coal, thereby showing a negative correlation with CO_2 adsorption volume. Furthermore, the samples show a multimodal pore-size distribution, with SD-1 dominated in the micropore region and SD-3 in the mesopore region due to higher TOC and CM content. The micropore volume peaks at around 0.5 to 0.7 nm, while the mesopore volume peaks at > 20 nm. In addition, CO_2 volume adsorption is at least 10 times higher than that of N_2, indicating that the coal has significantly more micropore characteristics. Thus, the study plays a crucial role in gas exploration and storage in subsurface coal formations. Furthermore, the study findings can be applied to explore the gas adsorption capacity and storage in other Indian coal seams.

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106

A palladium bio-nanocomposite as an efficient heterogeneous catalyst for nitro reduction:a fungus mediated green and sustainable process

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Abstract Category

Biocatalysis

Abstract

Metallic nanocatalysts, particularly palladium nanoparticles (Pd-NPs), exhibit excellent catalytic properties due to their high surface-to-volume ratio, but their stability is often undermined by aggregation and metal leaching. This study introduces a sustainable biosynthetic method for creating bio-stabilized Pd-NPs using the fungal strain Aspergillus trinidadensis VM ST01 (OL587588) as a green reducing and capping agent, avoiding harmful chemicals and stabilizers. The effects of culture age (24–54 h), biomass loading (0.08–0.24 g mL^{-1}), and incubation time (8–24 h) on nanoparticle formation were comprehensively examined, resulting in uniform Pd-NPs averaging about 35 nm, stabilized within the fungal biomass. This bio-organic matrix minimizes aggregation and palladium leaching, heightening the catalyst's durability. Catalytic tests on the hydrogenation of nitrobenzene (NB) to aminobenzene (AB) under mild conditions (using NaBH4 at ambient temperature and pressure) showed that the optimized catalyst (0.16 g mL^{-1} biomass, 36 h culture age, and 24 h incubation) achieved full conversion in 30 minutes, demonstrating a turnover frequency (TOF) of 832 h^{-1} and a turnover number (TON) of 416. The kinetics of the reaction were analyzed, revealing the catalytic activity of the nanoparticles as a pseudo-first-order rate constant (kapp). The in situ bio-coating significantly limited palladium leaching to less than 1.5% ppm, improving storage stability and ensuring environmental compatibility, thus preserving both structural integrity and catalytic performance in relevant industrial settings.

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113

CO_2 Refinery: Catalytic Pathways for Conversion of Carbon Dioxide into Value-Added Chemicals

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

This presents the design, synthesis, characterisation, and evaluation of a novel KFeCoMn/ZrO_2 catalyst for the catalytic hydrogenation of carbon dioxide into value-added liquid oxygenates, with emphasis on ethanol production. The work includes catalyst synthesis via wet impregnation, catalyst screening, reaction studies, catalyst characterisation, data analysis, and interpretation of results. The initial screening included a fixed active KFeCoMn supported on various supports like ZrO_2, CeO_2, $ZrCeO_4$, Al_2O_3, and N-doped carbon. A systematic investigation revealed Zirconia as the most suitable catalyst due to its superior oxygenate selectivity. The influence of catalyst composition was further optimised by studying the Fe/Co ratio and potassium promoter loading, leading to the identification of an optimal Fe/Co ratio of 1.2 and a 3 wt.% potassium loading for enhanced oxygenate formation.

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116

Dry Reforming of Methane over Nickel-Based Catalysts: Mechanistic Understanding and Catalyst Design

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Abstract Category

Catalysis - Prospects & Perspectives

Abstract

Dry reforming of methane (DRM) offers a promising approach for simultaneously utilizing CH_4 and CO_2 to produce syngas while reducing greenhouse-gas emissions. In this study, **Ni–Fe/$MgAl_2O_4$ catalysts** were investigated for DRM, with emphasis on the influence of metal loading and reaction conditions on catalytic performance, stability, and carbon deposition. The catalysts were characterized using **XRD, SEM, TEM, BET, TGA, and TPD** to establish relationships between their physicochemical properties and catalytic behaviour. The effects of reaction temperature, Ni–Fe loading, and CH_4/CO_2 feed ratio were systematically evaluated. The optimized catalyst exhibited improved CH_4 and CO_2 conversion at elevated temperature, with the $MgAl_2O_4$ support contributing to enhanced Ni dispersion and CO_2 activation. The catalytic behaviour was further evaluated in terms of stability and resistance to carbon deposition. Although Fe incorporation influenced the catalytic performance, **direct evidence for Ni–Fe alloy formation was not obtained from the present characterization**, and its contribution is therefore interpreted cautiously. The results demonstrate the potential of Ni–Fe/$MgAl_2O_4$ catalysts as cost-effective materials for efficient DRM and syngas production.

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117

Sustainable Conversion of Biomass to Deoxygenated Bio-Oils via Catalytic Hydrothermal Liquefaction

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Abstract Category

Catalysis in biomass conversion

Abstract

Achieving net-zero greenhouse gas (GHG) emissions by 2050, as outlined in the Paris Agreement (2015), has intensified the global pursuit of sustainable alternatives to fossil fuels. Biomass, a renewable and abundant resource, has emerged as a viable feedstock for producing fuels, chemicals, and advanced materials. The transformation of biomass into hydrocarbon fuels centres on two primary strategies: the substantial reduction of the feedstock's inherent oxygen content to increase energy density, and the formation of carbon–carbon bonds to raise the molecular weight of the final products. This study explored hydrothermal liquefaction (HTL) as a one-pot process to achieve hydrogenation and hydrodeoxygenation of biomass, using water and ethanol as solvents. A bifunctional 10 wt. % Ni/Al-SBA-15 catalyst, incorporating highly active metal and acidic sites, was synthesized and evaluated for its performance in this reaction system. The product characterization was done using GC-MS. The process parameters, including catalyst type, hydrogen concentration, operating pressure, and temperature, were systematically optimized to maximize bio-oil yield. Various heterogeneous catalysts were investigated for their ability to facilitate the conversion of biomass into oligomeric intermediates and, subsequently, into deoxygenated fuel-range compounds. All experiments were conducted in a batch-mode autoclave reactor setup. Catalyst characterisation was done using XRD, BET, FTIR, SEM-EDAX, NH_3-TPD, and TGA-DSC.

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119

Development of a Bio-based Polymeric Surfactant from Epoxidized Mahua Oil and Hydroxyethyl Cellulose

Pravin Tadkar[1], Yogeshwar Ingale[2], Sfurti Kaduskar[2], Virendra Rathod[3]

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Abstract Category

Sustainable Engineering

Abstract

The use of renewable, inedible vegetable oils as substitute raw materials has been prompted by the growing need for environmentally friendly and sustainable surfactants. In the current study, hydroxyethyl cellulose (HEC) and Mahua oil (Madhuca indica) were combined to create a bio-based polymeric surfactant using a series of epoxidation, grafting, alkaline hydrolysis, and neutralisation procedures. Hydrogen peroxide and acetic acid were used to epoxidise Mahua oil in the presence of sulphuric acid. Epoxidised Mahua oil (EMO) was then reacted with HEC via epoxide-ring-opening grafting. After that, sodium hydroxide was used to hydrolyse the resultant EMO–HEC compound, and hydrochloric acid was used to neutralise it. The structural alterations that occurred during the synthesis were examined using FTIR spectroscopy.

The epoxidation of Mahua oil was supported by the FTIR spectra of EMO, which had distinctive aliphatic C–H stretching bands at 2921.82 and 2852.61 cm^{-1}, an ester carbonyl band at 1741.76 cm^{-1}, and an epoxide-associated band at 869.90 cm^{-1}. O–H, aliphatic C–H, and C–O-containing absorptions were seen in the grafted product, which is consistent with EMO and HEC interacting through epoxide ring opening. Important O–H and C–O-containing functions were preserved in the final hydrolysed product. The produced material showed detectable foam formation, a surface tension of around 37.7 mN/m, and a conductivity of

2.8 mS/cm. These findings show how Mahua oil can be used as a sustainable feedstock to create bio-based polymeric surfactants with surface-active qualities.

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38

Regeneration of High-Quality NMC cathode from Spent Lithium-Ion Batteries

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Abstract Category

Sustainable Engineering

Abstract

In recent years, lithium-ion batteries (LIBs) have become the leading technology for energy storage applications, leading to a rapid increase in the number of end-of-life batteries requiring proper recycling and reuse. This study presents a sustainable and cost-effective strategy for regenerating Li-NMC cathode active materials from spent lithium-ion batteries. The degraded cathode collected from used NMC batteries was directly utilized as a source of valuable transition metals, reducing the need for fresh raw materials. By carefully adjusting the elemental composition, different NMC variants, including NMC111 and the Ni-rich NMC622, were successfully synthesized with high phase purity. Detailed structural, elemental, and morphological investigations confirmed that the regenerated materials possessed excellent crystallinity and showed negligible cation mixing, comparable to commercially available NMC cathodes. Unlike conventional pyrometallurgical and hydrometallurgical recycling techniques, which often recover metals in the form of alloys or separate salts, this direct regeneration approach preserves the cathode structure and minimizes processing complexity. The findings demonstrate that spent NMC batteries can be transformed into high-quality cathode materials with excellent structural integrity, providing an environmentally friendly and economically viable pathway for battery recycling while promoting the sustainable recovery and reuse of critical metals.

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59

Sustainable Adsorbent Development: Activated Carbon from Kigelia Africana Fruit Shells for Acid Blue (AB158) Dye Removal

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Abstract Category

Sustainable Engineering

Abstract

This project focuses on the synthesis of activated carbon using Kigelia Africana fruit shells as a precursor. These fruit shells, available as waste in the Western Ghats region, contribute to environmental and water pollution. Kigelia Africana is a poisonous fruit, abundantly available in nature, rich in cellulose and carbon, and has low ash content, making it an ideal precursor for producing low-cost activated carbon. The project explores the potential of converting Kigelia Africana fruit shell waste into value-added chemicals like activated carbon adsorbents, which can be used in industrial effluents and wastewater treatment. Activated carbon is synthesized using chemical activation with various chemicals such as KOH, NaOH, H_3PO_4, and $ZnCl_2$, respectively. The project optimizes several parameters, including impregnation ratios of 1:1, 1:2, 1:3, activation time (120 min), Temperature (400-500^{O}C). The surface properties of the final adsorbent are characterized using FT-IR and BET surface area analysis. Batch adsorption studies have been conducted to remove Acid Blue 158 dye using various combinations of synthetic dye solution concentrations (50-1000 mg/L), adsorbent dosage (10-90 mg/L), contact time (10-310 min), and pH (2-12). The highest adsorption removal efficiency of 93.07% was achieved with the synthetic AB 158 dye solution. The experimental data validate with theoretical models like isotherm and kinetic models, respectively.

Keywords: Adsorption; Kigelia Africana fruit shells; Acid Blue (AB158) Dye; Batch Study; Wastewater treatment.

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72

An exploratory attempt on integrating anaerobic digestion fundamentals with machine learning concepts in Indian and European Chemical Engineering Academic Classrooms

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Abstract Category

Clean Energy

Abstract

Chemical Engineering Education needs to respond to current major transitions in process industries owing to digitalization and a shift towards sustainable energy sources. There is a great need to integrate data-driven modelling tools in addressing achievement of sustainable development goals since complex, variable, and uncertain process conditions demand adaptive , data informed optimization beyond traditional models. Within this context, the authors recognize the need to enrich students' ability to apply machine learning (ML) in real process systems scenarios particularly addressing sustainability.

Following the 2024 Digital Green Talents Award conferred by the German Federal Ministry of Education and Research (BMBF) to the principal author (PS), this work was advanced through participation in the ERASMUS+ InnoLAB (Innovative Learning Across Borders) framework. Within this framework, a case study-based chemical engineering education module was designed to integrate anaerobic digestion fundamentals with ML modelling of biogas systems. The module focused on predicting CO_2 content using correlation analysis

and Random Forest regression. The delivery of the education module was explored during classroom interactions at IIT Ropar (India) and TU Dresden (Germany). A mixed-method pre-post academic evaluation conducted with 40 international participants revealed improved understanding of regression modelling and increased confidence in ML-based process analysis.

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94

Valorisation of waste biomass and industrial by-products for various applications

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Abstract Category

Catalytic reactions in which wastes are converted to useful products

Abstract

Esters are a significant class of functional groups that are found in both natural products and pharmacological scaffolds. A caesium-doped graphitic carbon nitride (Cs/g-C_3N_4) catalyst is developed and applied for the esterification of palmitic acid with methanol to produce methyl palmitate. The present work demonstrates the effectiveness of Cs-modified g-C_3N_4 as a thermally driven heterogeneous catalyst for long-chain fatty acid esterification. Esterification of oleic acid with methanol exhibited optimal catalytic performance at a 10 wt.% V_2O_5 loading on Wet copper slag, which showed 92.4% yield.

The growing demand for sustainable technologies and the transition toward a circular economy has accelerated research on the valorisation of biomass and waste materials. Agricultural residues, forestry waste, food waste, industrial by-products, and other renewable resources represent abundant feedstocks for producing value-added chemicals, fuels, functional materials, and catalysts. Through environmentally benign chemical, thermochemical, biological, and catalytic processes, these low-value waste streams can be transformed into high-value products, reducing environmental pollution while conserving natural resources. The research is devoted to the conversion of biomass-derived polyols into important drug intermediates. The Ni/HAp catalyst shows a higher yield of 2-deoxyribose. In addition, value addition of industrial copper smelting byproducts by converting them into catalysts for the synthesis of various industrially important flavours, fragrances, and biofuel.

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102

Sustainable Bio-derived P-CSG Nanocoatings for Fire-Safe PU Foams and Cotton Fabrics

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Abstract Category

Sustainable Engineering

Abstract

Polyurethane (PU) foam is lightweight and flexible but highly flammable, limiting its safe use. In this work, a sustainable bio-based flame-retardant coating, phosphorus-modified chitosan/sodium alginate/graphene oxide (P-CSG), was prepared from chitosan, sodium alginate, and graphene oxide. The coating was applied to PU foam and cotton fabric using a simple dip-and-dry process. The coated materials were characterized by XPS, FTIR, SEM-EDX, elemental mapping, and TGA, while flame-retardant performance was evaluated using cone calorimetry, LOI, UL-94, vertical flame test, and flame exposure tests.

The P-CSG-coated PU foam exhibited improved flame-retardant performance, including rapid self-extinguishing behavior, a UL-94 V-0 rating, reduced heat release, and carbon monoxide emissions below the detection limit under the test conditions. The coating also showed a temperature-dependent electrical response. For cotton fabric, the coating increased the LOI from 18.16% to 32.50% and produced a residual char length of 11 cm in the vertical flame test. These results demonstrate that the P-CSG coating enhances the flame-retardant performance of both PU foam and cotton fabric using a sustainable bio-based approach.

Keyword:

Polyurethane foam; Chitosan; Sodium alginate; Graphene oxide; Flame retardancy; Cotton fabric.

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110

An Adaptive Palladium Single-Atom Catalyst Enabling Reactivity Switching between Borylation and C–C Coupling

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Abstract Category

New catalytic routes And processes

Abstract

The development of single-atom catalysts (SACs) with site-specific and tunable catalytic functionalities remains a highly desirable yet challenging goal in catalysis. In this study, we report a SAC featuring anisotropic coordination cavities synthesized via a one-step polymerization of 2,6-diaminopyridine and cyanuric chloride. These cavities provide a robust framework for anchoring isolated Pd single atoms with exceptional stability. The unique broken symmetry of the catalyst's local structure enables precise control over reaction pathways, allowing reactivity to be switched between distinct catalytic outcomes. Specifically, under tailored reaction conditions, the catalyst can either halt at the borylation step or proceed seamlessly to Suzuki coupling in a self-cascade process. Mechanistic studies unveil the pivotal role of Pd single atoms in driving key steps, including oxidative addition, base exchange, and reductive elimination. Furthermore, green metrics demonstrate the process's sustainability, with minimized waste generation and reduced reliance on hazardous reagents in the self-cascade transformation. This work establishes an innovative benchmark in the field of single-atom catalysis: by enabling complex, multistep transformations via strategic activation of multiple functional groups, this catalyst exemplifies the potential of self-cascade processes to revolutionize synthetic chemistry via catalysis engineering.

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