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SusChemE 2023 in Honour of Professor G. D. Yadav, celebrating his excellence in Chemical Engineering & Research

> **THEME: CATALYZING RESEARCH & TECHNOVATION FOR A SUSTAINABLE FUTURE**

# **ABSTRACT BOOK**

#### AM+

Emerging Applications of Additive Manufacturing in Chemical Sciences and Engineering Dist. Prof. Suresh K. Bhargava, AM

# (Member of Order of Australia, Queen's Honours 2022)

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#### Abstract:

Additive Manufacturing is one of the key enabling technologies for the fourth industrial revolution (4IR). While the automotive, aerospace engineering, mechanical engineering and biomedical industries have hastily adopted AM technologies for associated benefits, the chemical industries have been lagging in the uptake due to the lack of agility and adaptability in industrial chemical processes.

Application of AM to chemical sciences and engineering engenders benefits such as complete design freedom, capability to manufacture sophisticated geometries, improved material utilization, tool-less fabrication, and shortened lead times.1 Thus, AM has tremendous potential in facilitating wide-scale upgradation, improvisation, and miniaturization of chemical processing equipment and manufacturing plants in line with the ethics of Industry 4.0. Future chemical reactors will be complex tailor-made devices with design optimized for fluid and particle flow, heat and mass transport, and reaction thermodynamics. This will lead to improved efficiencies of existing chemical processing technologies, improved process economics, environmental compatibility, reduced carbon footprint, and reduction in wastes and emissions. This talk will focus on the concept of AM+ i.e. promising avenues which take additive manufacturing to the next level. Some examples of emerging applications of additive manufacturing in chemical sciences and engineering such as in clean energy, sustainable critical mineral processing, carbon dioxide capture and

utilization, 3D microfluidics, advanced microreactors and sensors will be discussed.

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# Nanostructured Materials – The New Generation Heterogeneous Catalysts: Applications in Bioprocessing, Energy, and Environmental Technology PARASURAMAN SELVAM Indian Institute of Technology-Madras, Chennai 600 036, India

The discovery and development of periodic porous materials of well-defined pore geometry with precise and easily controllable pore shape and size are of great importance in many areas of modern science and technology. Mesoporous and hierarchical molecular sieves, including metal-organic frameworks resembling zeolites, represent the latest class of organized porous materials characterized by extensive surface area, sizable pore entrances, and substantial pore volumes. On the one hand, the unique flexibility of these materials, in terms of synthetic conditions, pore size tuning, large internal hydroxyl groups, framework substitution, etc., has created new avenues not only in catalysis but also in the areas of advanced energy materials and environmental pollution control strategies. Furthermore, preparing and characterizing high-quality materials with well-defined pore characteristics are paramount for many applications in nanomaterials, catalysis, adsorption, and separation. In designing such materials, several characteristics of pore structure may be addressed, which include their shape, size, pore interconnectivity, etc. Likewise, traditional preparation methods of supported catalyst systems are neither efficient in generating/dispersing uniform-sized clusters nor chemically

inert toward the guest molecules. Nevertheless, the confinement of nanoclusters/nanofilaments/enzymes cavities/voids/pores in the of nanostructured matrices is attracting much attention as a way to stabilize highly dispersed materials in the form of atoms, clusters, colloids, or filaments, and prevent their coalescence into to larger, ill-defined aggregates. In this self-assembly context. the of nanoparticles into ordered pore structures, i.e., encapsulation of the



nanosized materials in zeolitic pores, is a promising option. Therefore, this presentation will discuss the recent progress in the development of numerous nanoscale materials and their applications in the areas of Bioprocessing, Energy, and Environmental Technology.

**Dr. Parasuraman Selvam** is currently Head, National Centre for Catalysis Research, and Professor in the Department of Chemistry, IIT-Madras, Chennai; Visiting Professor at Kumamoto University, Kumamoto, Japan. Earlier, Prof. Selvam was a Faculty at IIT-Bombay, Mumbai, and Tohoku University, Sendai, Japan. He has also held several Visiting/Adjunct Faculty positions in various Universities/Institutes including the University of Delaware, Newark, USA, The University of Manchester; the University of Surrey; Queen's University Belfast, UK; The University of Queensland, Brisbane; Western Sydney University, Penrith, Australia; Institute of Chemical Technology, Mumbai. Prof. Selvam has been bestowed with several national and international honors including the Young Scientist Awards in Catalysis and Solid State Chemistry; the Elected Fellow of the Royal Society of Chemistry. Prof. Selvam's research work involves mainly the

development of novel synthetic routes for the preparation of crystalline porous materials including conventional-, nano-, and hierarchical-zeolites as well as metal-organic frameworks; size- and shape-controlled nanomaterials. Prof.Selvam has published over 350 original research papers and is a co-inventor of about 30 patents.

# Catalytic Non-Thermal Plasma for Environmental and Energy Applications Dr. C.Subrahmanyam Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi-502284, India csubbu@iith.ac.in

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The potential of Nonthermal plasma (NTP) for the removal of air pollutants removal will be discussed. Volatile organic compounds (VOCs) are typical industrial emissions that have a negative impact on the environment. For the abatement of dilute VOCs, conventional techniques like thermal and thermocatalytic techniques are not energetically favorable. Among the alternatives, NTP generated under ambient conditions is an energy saving approach. The specific advantage of NTP is selective formation of high energetic electrons (with energy up to 10 eV), whereas, the back ground gas remains close to room temperature. The selectivity to total oxidation (CO2 and H2O) can be improved in the catalytic plasma technique, where a heterogeneous catalyst will be integrated with the plasma. Catalytic plasma incinerator not only improves the removal efficiency, but also enhances the complete oxidation of the VOCs. The effect of ozone, gas flow rates and VOC input concentrations, the applied voltage and the physico-chemical changes on integration of the catalyst will be discussed. The efficiency of VOC removal at a large scale was tested to handle high flow rates.

Mitigation of CO2, one of the most important greenhouse gases, is one of the important issues. Several methods focus on the capture the CO2, but not on the utilization. In this context, NTP assisted CO2 reforming of methane for the production of value added products would be advantageous. CO2 reforming of methane is being considered as a potential method for conversion of methane and carbon dioxide into value added products. The potential of NTP technologies for the utilization of CO2 will be also discussed in this presentation.

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# Synthesis of Carbon Nanotubes Supported Catalysts for Light Olefins via Fischer-Tropsch synthesis Ajay K. Dalai and Arash Yahyazadeh Catalysis and Chemical Reaction Engineering Laboratories (CCREL), Department of Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, S7N 5A9, Canada

## Abstract

Light olefins as one the most important building blocks in chemical industry can be produced via thermal or catalytic cracking of petroleum-derived hydrocarbons. However, environmental and economic concerns are urging exploration of alternative routes for light olefin production. Applying biomass-derived syngas, light olefins can be obtained through high temperature Fischer-Tropsch synthesis (FTS) over iron catalyst. In this study, we report the synthesis of iron catalyst supported on CNTs for olefin-rich liquid hydrocarbons through FTS. This way, monometallic (iron) catalyst supported on calcium carbonate was used for the synthesis of carbon nanotubes (CNTs) via catalytic chemical vapor deposition method (CCVD). Optimization on the formation of CNTs by acetylene decomposition over Fe/CaCO3 catalyst was performed using a central composite design in response surface methodology to study the effects of deposition temperature, growing time, and iron loading. The synthesized CNTs was thoroughly characterized. 20Fe/CNTs-synthesized, 20Fe/CNTscommercial, and 20Fe/Al2O3 were analyzed in terms of physio-chemical properties and FTS catalytic performance. 20Fe/CNTs exhibited a lower rate of water-gas-shift (WGS) reaction compared with 20Fe/CNTs-commercial, with C2-C4 selectivity of 23.6%. Considering promoted iron catalyst, a twolevel full factorial design was applied for K and/or Mo-promoted Fe/CNTs catalyst to investigate the effects of synthesis conditions including Mo/K mass ratio, ultrasonic time, and iron loading on light olefins' yield. Compared with the un-promoted Fe/CNTs catalysts, addition of molybdenum as a promoter increased light olefins' selectivity by 33.4%, while potassium led to an increase in CO conversion by 96.3%. The optimum formulation (0.5K5Mo10Fe/CNTs) obtained olefins' yield of 35.5%.

#### SusChemE 2023

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September 14-16, 2023, Institute of Chemical Technology, Mumbai Catalyst Options for Downstream Processing of Furan to Fuel Additives Chandrashekhar. V. Rode\* *Chemical Engineering and Process Development Division, CSIR-NCL, Dr. Homi Bhabha Road, Pashan, Pune-411008, India cv.rode@ncl.res.in; cvrode8@gmail.com* 

# 1. Introduction:

High functionality in biomass derived molecules, demands design of appropriate catalytic strategies for efficientlycarrying out the cascade type reactions in a single pot. Another interesting feature of bio-derived substrates is that these are multi product reactions (MPR). Furfural (FFR) obtained from arabinose and xylose of natural resources was selectively hydrogenated in a single pot process to give 2-methyltetrahydrofurfuran (2-MeTHF), which is identified as a second generation P-series fuel [1]. Furan derivative 5-(hydroxymethyl)furfural (HMF) obtained from C6 sugars (hexoses) can be processed under the cascade reductive etherification conditions to give 5- (ethoxymethyl)furfural (EMF) which can be used directly as fuel or fuel additive (due to its high cetane number and high energy density). For etherification reactions of 5-HMF, Zr based solid catalysts with a combination of acid and base properties were developed [2,3]. This presentation will cover highlights of our recent work on various heterogeneous catalyst systems for directing hydrogenation of furfural to give selectively the desired product among a variety of products such as furfuryl alcohol (FAL),

tetrahydrofurfuryl alcohol (THFAL), 2-methylfuran (2-MF) and 2-methyl tetrahydrofuran (2-MTHF), cyclopentanone, pentanediols etc. All these products have extensive applications as green solvents, fuel additives and as monomers for a variety of polymeric products. The underlying basic aspect of structure-activity relation required for catalyst design will be discussed.

# 2. Material and Methods:

Furfural, furfuryl alcohol, tetrahydrofurfuryl alcohol, 2-methylfuran, 2-methyltetrahydrofuran, pentanediols as

well as all noble metal precursors [PdCl2. anhy, RuCl3.xH2O, IrCl3.xH2O, H2PtCl6] were purchased from Sigma Aldrich, Bangalore, India. Activated Charcaol (Sr no 70710, EC no- 264-846-4) and Alumina (Al2O3) support was purchased from Riedel-de Haen, Germany. All nitrate precursors of Ni, Co, Cu, NaOH and NaBH4 were purchased from Thomas Baker, India. Hydrogen gas (99.9% purity) was obtained from Vadilal Chemicals Pvt. Ltd., India. 5 g activated charcoal was dispersed in 100 mL 10% sulphuric acid solution and stirred for 6 h at 65 oC. The solid was filtered and washed successively with DI water till neutrality. This cake was and used for preparation of catalysts.

# 3. Significant Results and Discussion

4%Ir-4%Ni/C catalyst showed excellent activity in terms of FFR conversion with maximum selectivity of 74% to 2- MeTHF suppressing the formation of side chain as well as ring opening products. The catalytic activity was found to be mainly affected by catalyst preparation methods, metal loadings, surface composition, temperature, pressure and catalyst loading. Different phases of Ir were found to be responsible for FFR to 2-MF conversion while, Nio and NiO were responsible for further hydrogenation to 2-MeTHF. Synergic effect between Ir and Ni was established through XPS, H2-TPR analysis.

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In another example, synthesis of 2,5-bis(alkoxymethyl)furan was successfully achieved through a cascade sequence involving etherification, transfer hydrogenation and re-etherification over a combination of acidic catalyst (Zr- Mont) and CTH catalyst [ZrO(OH)2]. Acidic character of Zr-Mont facilitates the etherification of HMF while, acidbase characteristic of ZrO(OH)2 facilitates transfer hydrogenation of reaction intermediates (aldehyde).

# 4. Conclusions:

The significance of our work lies in developing an approach involving mutifunctional catalyst and cascade

pathways for selective transformation of biomass derived platform molecules to high value products of commercial importance.

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## Biomass to Chemicals and Polymers – Opportunities & Challenges Kannan Srinivasan Inorganic Materials and Catalysis Division, CSIR-Central Salt and Marine Chemicals Research Institute, Council of Scientific and Industrial Research, GB Marg, Bhavnagar 364002, India Email: skannan@csmcri.res.in

#### Abstract:

The world's energy and chemical requirements are largely met through fossil resources like petroleum, coal, and natural gas. The demand for energy and quality of life is continuously growing, making the world look for alternate solutions. Biomass is the only renewable source with useful carbon atoms that could fervently be explored with significant potential for producing chemicals that include polymers. This is de facto an attractive option considering the balance between the availability and consumption patterns. The approach also has the intrinsic advantage of reducing the indispensability of fossil fuels to an extent besides reducing CO2 emission, thereby positively contributing to climate change. Researchers across the world have made considerable advancements in biomass value addition for producing chemicals. India, with its strong roots in agriculture, diverse availability of enormous forest/agro resources, and vast coastline for marine macro/microalgae, is likely to generate non-edible/waste biomass which can potentially be explored for the production of chemicals sustainably in the years to come. A strong research impetus is being made in India, including at CSIR-CSMCRI, on the valorization of biomass and their derived products to make value-added chemicals. This lecture will address a few of the ongoing work in the domain of biomass to chemicals and polymers carried out at this institute with an emphasis on 2-valerolactone, levulinic acid derived plasticizers, 2,5-furandicarboxylic acid (FDCA) and furanic polymers that have the impending opportunity (at the same time with challenges) in establishing a new chain of industries.

# Studies on the catalytic systems for valorization of biomass-derived platform molecules to valueadded chemicals and fuels

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The research interest in sustainable chemistry is growing intensely due to the fast depletion of fossil reserves worldwide. Lignocellulose biomass showed its potential to stand out as a renewable carbon source for the production of important platform chemicals like 5-Hydroxymethylfurfural (5-HMF), furfural (FA) and levulinic acid (LA), etc. via acid-catalyzed reactions. These platform molecules transformed into fine chemicals and biofuels such as ethyl levulinate (EL), gamma-valerolactone (GVL), furfurylamine (FAM), dimethylfuran, etc. over acidic/basic heterogeneous catalysts [1]. Heteropoly acid catalysts and metal-organic framework (MOF) -derived N-doped carbon catalysts could be effectively used for biomass conversion with suitable Lewis/Bronsted acidity and metallic character at moderate reaction conditions. We have explored modified heteropoly acid (HPA) catalysts for catalytic conversion of biomass to value-added chemicals like EL, EMF, FAL, etc. The heteropoly acid-based catalysts were synthesized by exchanging protons of HPA's with transition metals like Nb, Zn, Ti, Al to generate Lewis acidity in HPA system. Furthermore, we also studied MOF-based metal-embedded N-doped carbon catalysts where metals like Ni, Cu, Co and Fe were investigated for the hydrogenation and reductive amination of biomass-derived substrates [2-3]. All synthesized catalysts are characterized through various characterization techniques like XRD, XPS, FE-SEM, Raman, HR-TEM, FT-IR, NH3-TPD, CO2-TPD, H2-TPD to derive their physiochemical properties. The catalytic systems were developed for the conversion of platform compounds into HMF, EMF, FAM and GVL. The activities of the catalysts were explained on the basis of their surfacestructural properties, presence of sufficient Lewis/Bronsted acidity, and metallic character of the catalysts.

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# Catalytic and other Materials for Diesel Exhaust Emission Control & Chemical Looping Applications Nitin Labhsetwar

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Cleaner and sustainable energy as well as environmental issues are among the most important challenges world is facing today and therefore attracting a lot of R&D attention in recent years. Although electric and hydrogen mobility has been pitched as a future of automobiles, the energy mix outlook, clearly suggests significant use of fossil fuels in the transport and energy sectors for another two decades or so. Looking at the air pollution scenario, especially in urban settlements, there is no assimilative capacity left for any additional pollution loads. Carbon dioxide (CO<sub>2</sub>) and particulate matter are among the most important pollutants of environmental and health concerns and demand further R&D efforts to address cost related and other challenges. Materials including catalysts, adsorbents play key role in advancing emission control and energy technologies.

There is a renewed interest in perovskites, mixed oxides, intermetallic and other low cost, non-noble metal-based catalysts and materials mainly due to lowering of sulphur content in fuel, as well as due to the higher cost of noble metals. Introduction of blended and new fuels present another opportunity for new generation of automobile catalysts including those required for control of methane slip in CNG fueled automobiles. We have been working on substituted perovskites, other mixed oxides for diesel soot oxidation with some of the catalysts evaluated as full-scale DOC (Diesel oxidation catalyst) and Diesel Particulate Filter (DPF) prototypes using real diesel engine exhaust. We have also explored development of mixed oxides and other compositions as potential oxygen carriers for their applications in Chemical Looping Combustion for CO<sub>2</sub> capture, Chemical Looping Hydrogen generation as well as CO<sub>2</sub> reforming.

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#### Importance of by-products valorization in renewable energy generation

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In the present times a lot of emphasize is given on the use of renewable energy in place of conventional energy such as fossil based (coal, crude oil etc.). This is because it is required to mitigate the problems arisen due to global warming, pollution etc. which are linked to increasing use of fossil feedstocks. For considering the use of renewable sources for energy generation, several options are available such as, wind, solar, tidal, geo-thermal, biomass etc. In all one of the most conventional energy source is biomass, in which it is burnt to get the energy. In later stage, manure, a kind of biomass was used to generate bio-gas, which again was used for cooking and several other purposes. Considering this, there is a long history on extracting energy from biomass sources. However, in recent times, biomass utilization for gas generation and liquid fuel generation is looked up on as a major pathway.

Due to ongoing activities on the generation of bio-ethanol from 2G resource, the limelight has again come back on biomass. It is suggested that oil companies will put several bio-ethanol plants based on 2G source such as crop waste (rice straw, wheat straw, bagasse etc). It is known that these crop wastes are made up of cellulose, hemicellulose and lignin. It is possible to convert cellulose and hemicellulose into bio-ethanol however, the by-product generated in this is lignin. It is estimated that while getting 1 L of bio-ethanol, almost 1-2 kg of lignin is generated depending on the efficiencies of the processes. Lignin is a phenolic polymer and in itself can be used for burning purposes to generate heat due to its high calorific value compared to total biomass. However, there are discussions that to make the 2G bio-ethanol process economically viable, lignin needs to be converted into other value added chemicals. Thus, it becomes essential to find ways/methodologies to convert this by-product into value-added chemicals. During the presentation, various pathways for doing so will be discussed.

Additionally, synthesis of bio-diesel from oils is known and in this process too, glycerol is generated as a major by-product. Again it becomes essential to value-add glycerol by synthesizing various chemicals. Briefly this topic also would be discussed during the presentation.

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# Catalytic C-H functionalization of Triazole: Synthetic tool for preparation of triazolophenanthridines and quinolines Pravin R Likhar Department of Catalysis and Fine Chemicals CSIR- Indian Institute of Chemical Technology, Hyderabad Email: plikhar@iict.res.in

Incorporating one or more heteroatoms within the core ring make them different from their allcarbon analogs and thus exhibiting special properties in biology. They are fundamental to all fields of chemistry and, therefore, their synthesis and modification has attracted a great deal of attention in recent years. Transition metals have played a crucial role and the methodology recognised as synthetic tools for generating new heterocyclic compounds. The triazole ring, a privileged heterocycle, is found in several pharmaceutical, electronic materials, and agrochemicals owing to its unique chemical and structural properties. This talk will discuss the palladium catalyzed domino reaction of 1,4- disubstituted triazoles via double C-H functionalization to produce one- spot synthesis of triazolo[1,5-f] phenanthridines. The domino coupling involves the formation of biaryl and bi(hetero)aryl bonds through five membered carbopalladacycle intermediate. In the second part of the talk, the palladium catalyzed coupling reaction followed by dual annulation for the synthesis of various triazolo/pyrrolo fused benzofuro-quinolines will be discussed. The developed protocol proceeds through palladium catalyzed Sonogashira coupling, benzannulation followed by C-H activation triggered second annulation reaction cascades in a single pot. In particular, the polycyclic compound formed by this method consists of three different heterocyclic structures: benzofuran, quinoline, and triazole/pyrrole and thus provides simple access to obtain the range of fused benzofurotriazalo/pyrrolo-quinolines.

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# Design and Synthesis of Heterogeneous Catalysts for Production of Renewable Fuels for 21st Century: Wealth Creation from Waste

# <sup>1</sup>Ganesh More, <sup>1</sup>Arjun Manal,<sup>1</sup> Ashish Kumar Kar, <sup>1</sup> Abhinav Kumar,<sup>1</sup> <u>Rajendra Srivastava<sup>1</sup>\*</u> <sup>1</sup> Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab E-mail: rajendra@iitrpr.ac.in

Lignocellulosic biomass obtained from the sources such as agricultural wastes, forestry, or energy crops is renewable and has been focused on obtaining fuel and chemicals. Lignocellulosic biomass comprises 35-50 % cellulose, 20-35% hemicellulose, and 10-25% lignin.<sup>1</sup> Cellulose/ hemicellulose provides a wide range of furans, diols, and linear alkanes, Lignin has a polymeric structure composed of aromatic units. These aromatic units have phenolics, hydroxy, alkoxy, alkene, and aldehydic units, which can be valorized to obtain several important phenolics such as vanillin, eugenol, guaiacol, and phenol, which further can be converted into various platform chemicals and fuels thus providing renewable energy route.<sup>2</sup> Similarly, plastics which are polymeric compounds, utilize fossil-based feedstocks, more specifically, petroleum-based monomers. Broadly plastics can be categorized into two main classes: thermoplastics and thermoset plastics. Thermoplastics, in general are recyclable and majority of its waste is recycled but the polystyrene plastics waste, for example, expanded polystyrene (EPS), which is most widely used, is lightweight which makes it challenging to collect andtransport economically, due to which they are mainly incinerated or dumped in landfill sites. In the case of thermoset plastics, polyurethanes are most widely used, which are mostly discarded in landfilling or incineration sites. Polystyrene waste is mainly generated through EPS packaging material, food-grade cups and plates, and several polystyrene-based household and industrial containers. The source of polyurethane waste is mainly from used mattresses, cushions, automobile seats, shoes, and rigid foams. Polystyrene and polyurethane waste which faces significant challenges in recycling (as mentioned earlier) can be converted into fuels and value-added chemicals through catalytic solvolysis, hydrogenolysis, and hydrogenation.<sup>3,4</sup> The traditional biomass and plastic waste treatment methods such as landfills and incineration emit toxic and harmful gases and substances, which contribute to global warming. The global warming mitigation action and increasing energy demand worldwide motivated me to fulfill the need for environmental protection and provide partial fulfillment of the demands of chemicals and fuels required for the 21<sup>st</sup> century by utilizing plastic waste and readily available biomass resources.<sup>5.6</sup> So far, the chemical waste treatment method, especially catalytic hydrogenation/hydrogenolysis, is the most efficient and beneficial method, which aims to transform biomass and plastic waste into high-value chemicals and fuels.<sup>7</sup> In this presentation, I shall discuss the selective reduction/hydrogenolysis of lignocellulose model-compounds to valuable chemicals and

fuels.<sup>8,9</sup> I will also discuss the selective production of jet-fuel range chemicals by the selective hydrogenolysis of bisphenol A plastic waste.<sup>10</sup>



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# Zeolite Catalytic Technologies for Green Chemical Production

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Zeolites due to their high crystallinity, varied surface functionalities, molecular sized pore dimensions and high thermal and hydrothermal stability provide a very strong portfolio of heterogenous industrial catalysts for chemical industry. Zeolites have been conventionally been used as catalysts in a wide variety of industrial processes, especially in oil refining and petrochemistry. Its application has extended to fine chemicals and even in biomass conversion to value added products in recent times. Present talk will briefly discuss industrial catalytic application of zeolites.

Talk will discuss in detail about zeolite based REL-ORCAT technology developed and commercialized at Aromatic plant of Reliance Industries Limited. Aromatics produced from platformer invariably contains trace amounts of olefins, styrene and heavy aromatics contaminants. Olefins in reformate are undesirable because of their oligomerization tendency and formation of subsequent species which adversely affect the activity of high value catalysts and adsorbents in downstream processes. The current practice for removing olefins contaminants involves clay treating process using acid treated clays such as, activated bentonite. Clay treating process has following operational issues observed existing aromatics plants:

- Shorter cycle life, 3-6 months
- P Frequent clay change overs
- Disposal of huge quantity of spent clay, which is serious problem for environment.
- Loss of C8 Aromatics yield
- D Spikes in outlet bromine index of single clay treater during clay change-over.

To resolve above issues, RIL has developed REL-ORCAT Technology. The performance provided by the REL-ORCAT technology leads to significant reduction in operating cost as well as provide debottleneck opportunities with following advantages:

• Novel REL-ORCAT catalyst is a highly potential catalyst for diverse acid catalyzed transformations

• Catalyst specially designed for liquid phase operation to have optimum activity, stability with high geometric surface area

- Long operating cycles that reduce the solid waste significantly Eco-friendly process
- Reduce the number of shutdowns that happen in clay treaters during clay change-over
- Capital savings: retrofit
- No benzene production and no loss of C8 aromatics
- Shorter dry-out period.

8.5 MT of REL-ORCAT catalyst was manufactured and commissioned at one of the aromatics plants of Reliance Industries Ltd on 7 June 2021 and is running smoothly since then. Since SOR, the performance of the catalyst is maintained at > 95 % of olefins reduction without any side products, C8A loss with no sign of deactivation. This is truly a Game-Changer and novel technology developed at RIL and has potential to make clay catalyst in aromatics plant a history.

# Bio-inspired Strategies to Assemble and Stabilize Polyoxometalate Clusters as Heterogeneous Catalyst

R. Chilivery, V. Chaitanya, J. Nayak, S. Seth, <u>R. K. Rana</u>,\* *ACS Sustainable Chem. Eng.*, 2022, *10*, 6925–6933.

# Abstract:

Bio-inspired synthesis has shown great potential for developing nanostructured materials. The integration of inorganic and organic phases that biology achieves in mineralized matrices across scales and its link to properties are the key factors for developing functionalities in these materials. In this context, our approach has been to use polypeptides and related polyamines, which are known to be responsible for the biosilicification process, for assembling functional materials under environmentally benign conditions. It involves a tandem two-step process, in which cationic polyamines form supramolecular aggregates with multivalent anions via ionic crosslinking, and negatively-charged nanoparticles assemble around these aggregates to form a multilayer-thick shell. The method allows assembly of various nano-components other than silica to form hierarchical nanostructured materials. In this talk, a bio-inspired method rendering control on the morphology during the assembly of polyoxometalate (POM) clusters and their application in catalysis will be discussed. Effective heterogenization of the water-soluble Keggin units is demonstrated to aid in not only catalyzing oxidation of alcohols, but also in encapsulation of enzyme to design nanozyme-enzyme systems.

# **Representative References:**

- R. Chilivery, V. Chaitanya, J. Nayak, S. Seth, <u>R. K. Rana</u>,\* ACS Sustainable Chem. Eng., **2022**, 10, 6925–6933.
- G.Begum, P.Swathi, A.K.Bandarapu, J. Nayak, <u>R.K.Rana</u>, \**ACS Appl. Mater. Interfaces***2020**, *12*, 45476–45484.
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#### **Industry Academia Collaboration**

#### "Catalyst for Optimizing the Sustainable Growth Story of the Chemical Sector"

Name: Dr. Kumar Samir Singh Designation: Vice President-R&D Affiliation: Jubilant Ingrevia Limited Email: DrSamir.singh@jubl.com

#### Abstract

Chemicals industry in India having a growth rate of 1.2-1.5 times the GDP is highly diversified & covering more than 80,000 commercial products. India is the 6th largest producer of Chemicals in the world and 3rd in Asia.

To make India a global center of research & innovation in 'Amrit kaal' "India is going ahead with the PM Modi mantra of 'Jai Jawan, Jai Kisan, Jai Vigyan and Jai Anusandhan". To boost Research & Innovation in India, PM Modi in June'23 approved the introduction of the National Research Foundation (NRF) Bill in the Parliament to provide strategic direction for research & innovation. Further, Indian government may announce a Research-linked incentive (RLI) scheme for the Indian pharmaceutical/Chemical industry to raise contribution to research and development.

Many countries in the world are encouraging "Innovation Orchards" in the form of Government-Industry-Academia partnership to facilitate the incubation of new technology enterprises. Keeping in mind this practice our Indian government is also very keen to work on creating an ecosystem for Research & innovation in India through "Industry Academia Partnership".

Industry & Academia both can bring distinct perspectives, researchers are motivated by science, whereas industry is motivated by the market. Knowledge exchange and cooperation between academia and industry, can help industries leverage the tremendous advancements made by scientific groups.

"Industry Academia Partnership" will work as a catalyst in the sustainable growth of Indian Chemical sector to knock sound in among top three in world.

#### Biomass Based Biorefinery Event: SusChemE 2.0 at ICT, Mumbai-14.09.2023 Dr. Sangeeta Srivastava, Godavari Biorefineries Limited (GBL)

Sustainability and Circularity are becoming key drivers for the industry growth today. As the recent COP27 Summit outcomes reveal, sustainability is no longer an option for the world – it is imperative. Hence organizations need to renew the focus on leveraging innovation to provide sustainable products or services that facilitate a reduction in their overall carbon footprint.

All around the world many steps are being taken to move from today's fossil based economy to a more sustainable economy based on use of renewable resources. The transition to a bio-based economy has multiple drivers: the global issue of climate change and the desire to reduce the emission of greenhouse gases, an over dependency of many countries on fossil fuel imports, the need for countries to diversify their energy sources, and the need to stimulate regional and rural development.

A key factor in the deployment of a successful bio-based economy will be the development of biorefinery systems allowing highly efficient and cost effective processing of biological feedstocks into a range of bio-based products, and successful integration into existing infrastructure.

An integrated biorefinery approach producing both bio-based products and secondary energy carriers (fuels, power, heat), in analogy with oil refineries, is probably a more efficient approach for the sustainable valorisation of biomass resources in a future bio based economy.

Sustainability has been at the heart of what we do at GBL and how we operate since our incorporation in 1939 and that sets us apart from other organizations. Our business principles reflect who we are as a company, emphasizing the need of striking a balance between financial success, environmental stewardship, and social responsibility. We have begun our journey to produce increased and shared value for all our stakeholders by focusing on a sustainable future, or the Green Future as we call it. We collaborate with our clients and communities to make the world a better place.

We aspire for long-term growth through creating high-quality sugar, biofuel, bio based chemicals and green energy. Bagasse is converted into clean power and molasses is processed into ethanol, a green fuel. We work on fermentation of sugar to chemicals. Our productivity continue to increase as we commercialize renewable assets as a raw material for chemicals which plays a significant role in long-term value creation for a variety of industries. As a result, our product has a low environmental impact.

Our strategy is to add value to biomass processed. To increase the value of our feedstock such as sugarcane, ethanol, molasses, bagasse, or any other crop, through bio refining is converted into a useful product, such as fuel, energy, chemicals, intermediates, etc.

We as a company want and will take our responsibility for sustainable future by developing biobased products using renewable resources and bring them as a part of the mainstream products for a better tomorrow. To sustain a long-lasting and successful business in these changing times, it is imperative for chemical companies to integrate sustainability values in their long-term business strategies, business policies, operational processes and procedures. This will shape and prepare companies to address the changing behaviour and expectations of the internal and external stakeholders, and at the same times, improve competition and profitability. Green Catalytic Delignification Process for Microcrystalline Cellulose from Sugarcane bagasse

Ankit Maharshi, M. K. Dongare, Shubhangi B. Umbarkar\*

Catalysis Division, CSIR-National Chemical Laboratory, Pune-411008, India, Contact: <u>sb.umbarkar@ncl.res.in</u> Ph. 020-25902009/9423577812

#### Abstract

India is second largest producer of sugarcane in the world after Brazil producing around 18% of the world production. Bagasse is a large volume byproduct of the sugar industry which is presently used only for energy generation in boilers. For every 10 ton sugarcane crushed, 3 ton wet (~50% moisture content) bagasse is generated. In 2017-18 and 2018-19 around 3500 lakh tons of sugarcane was produced in India. [Sugarcane and sugar industry, Final report of the Task Force published by NITI Aayog March 2020] Hence if all sugarcane is crushed, 1050 lakh tons wet bagasse (500 lakh tons dry bagasse) will be available. The bagasse is presently used as fuel for burning in boiler, for power generation or as pulp after delignification in Paper& Pulp Industries. For conversion of bagasse into fermentable sugars, pretreatment is essential for removal of lignin and breaking lignocellulosic structure. The typically followed thermochemical methods involve steam explosion, alkali pretreatment, acid pretreatment, ammonia fiber expansion and organosolv. Steam explosion and ammonia fiber expansion involve high temperature high pressure whereas the NaOH and H<sub>2</sub>SO<sub>4</sub> are used in alkaline/acid pretreatment and needs neutralisation after the treatment. Organosolve process needs organic solvent at high temperature. Hence delignification process under milder conditions without using acid/base is desired.

Lignin is the most abundant aromatic biopolymer obtained from renewable resources after delignification process. Bagasse contains around 20-24% lignin. If all generated bagasse (500 lakh tons dry bagasse) is not used for burning then in principal 100 lakh tons of lignin can be available if promising technology is developed for its valorisation to chemicals/fuels.

Cellulose is also a major constituent in most of the biomass waste. It is a ubiquitous biopolymer with an estimated annual production of  $7.5 \times 10^{10}$  tons. Sugarcane bagasse is one of the major lignocellulosic biomass abundantly available in India. Microcrystalline cellulose and nano-cellulose are very high value and low volume products which finds application in large variety of sectors.

Typically Kraft process is used for separating cellulose from lignocellulosic materials which is highly energy intensive due to use of high temperature and high pressure along with use of large excess of alkali and sulphur compounds which generates large amount of effluent. Though this is existing commercial process, the more environmental friendly process is highly desired.

**CSIR-NCL** has developed catalytic process for delignification of sugarcane bagasse under very mild conditions without generating any effluent. The end product of the delignification process is microcrystalline cellulose (MCC) which is a high value product with applications in various sectors. Microcrystalline cellulose (MCC) is a pure partially depolymerized cellulose synthesized from  $\alpha$ -cellulose precursor is used as a texturizer, an anti-caking agent, a fat substitute, an emulsifier, an extender, and a bulking agent in food production. The most common form is used in vitamin supplements or tablets. It is also used in plaque assays for counting viruses, as an alternative to carboxymethylcellulose. The MCC can be synthesized by different processes such as reactive extrusion, enzyme mediated, mechanical grinding, ultrasonication, steam explosion and acid hydrolysis. The later process can be done using mineral acids such as H<sub>2</sub>SO<sub>4</sub>, HCl and HBr as well as

ionic liquids. The role of these reagents is to destroy the amorphous regions leaving the crystalline domains.

Some of the pictures of the microcrystalline cellulose prepared from bagasse are given below:



The process developed by NCL have following advantages:

- □ Hydrogen peroxide as oxidant
- □ Homogeneous catalyst
- □ No NaOH/Na<sub>2</sub>S required as in Kraft process
- □ No harsh reaction conditions needed
- □ Low cost catalyst
- □ No acid/base, hence no special MOC for reactor
- □ Water used in the process can be recovered & reused
- **D** Experiment on 1 kg bagasse scale carried out
- □ No effluent generated ZLD process

#### Summary:

Green, environmental friendly catalytic process for microcrystalline cellulose from bagasse and other agricultural residue has been developed by CSIR-NCL.

#### Sustainable Aviation Fuel- Challenges and Opportunities

#### Chiranjeevi Thota

#### Corporate R&D Centre, Bharat Petroleum Corporation Limited, Plot 2A, Udyog Kendra, Greater Noida-201306,

GHG emissions by various sectors such as road transport, industries, aviation, marine etc are a major area of concern worldwide. The aviation industry is critical to the country's economic development. According to the International Air Transport Association (IATA), the worldwide aviation sector produces around 2-3 % of global CO2 emissions. CORSIA (Carbon Offsetting and Reduction Scheme for International Aviation) norms obligate airlines to use Bio-ATF/SAF and it will be mandatory in India from 2027 onwards. Sustainable aviation fuel is produced from sustainable feedstocks and is very similar in its chemistry to traditional fossil jet fuel. SAF gives a reduction of up to 80% in carbon emissions over the lifecycle of the fuel compared to the traditional jet fuel it replaces, depending on the sustainable feedstock used, production method and the supply chain to the airport.

Commercially bio-ATF produced through different production routes and Hydroprocessed Esters and Fatty Acids (HEFA) has reached highest FRL (fuel readiness level) of 9 and Bio-ATF produced through this route can provide 50% blending in conventional fossil ATF. Worldwide HEFA route is contributing the highest percentage of bio-ATF since many refineries in the western world have converted to biorefinery and processing locally available vegetable oils in the refinery hydroprocessing units. Alcohol to Jet (ATJ) route also catching up where ethanol is widely available. However, since ethanol is currently blended with gasoline in many parts of the world because of government policy, the availability of ethanol as a feedstock for bio-ATF production in the short to medium term is uncertain in India.

In the current communication, the importance of SAF in the aviation sector, different methods of making SAF, challenges, and opportunities in implementation on a commercial scale will be analyzed.

# Compositional and interface engineering of perovskite absorbers to enhance the stability and efficiency of perovskite solar cells and modules

#### Bin Ding, Yong Ding and Mohammad Khaja Nazeeruddin\*

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#### Abstract:

Perovskite solar cells (PSCs) have gained significant attention due to their high efficiency, 26% and low-cost potential. Deposing two-dimensional perovskite (2D) layers between the perovskite absorber and hole-transporting layer is considered an essential strategy for reducing defects in state-of-the-art PSCs. This strategy, however, suffers from the inevitable formation of in-plane-favoured 2D perovskite layers with impaired charge transport, especially under thermal conditions, impeding photovoltaic performance and device scale-up. Therefore, to overcome this limitation, we designed and investigated various cations that form 2D perovskite layers on top of the 3-dimensional perovskite layer. The ensuing PSCs achieve an efficiency of over 25.5% with long-term operational stability (over 1000 hours). Notably, a record efficiency of 23% for the perovskite module with an active area of 27 cm2 was achieved using compositionally engineered perovskite. This talk will present strategies to enhance PSC's power conversion efficiency and stability by compositional and interface.

# Fundamental Role of Interfaces in Electrocatalytic Enhancement: Case Studies of Oxide/Oxide Interfaces

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In the context of increasing energy demand and concern over environmental pollution, fuel cells (FCs) are considered as promising source of alternative clean energy because FCs exhibit high efficiency and negligible noxious emissions. Proton exchange membrane fuel cell (PEMFC) has been actively developed among various types of FCs. The catalyst coating at the cathode in PEMFCs is a major limiting factor for the energy conversion efficiency of the devices. Although Pt or its alloy is regarded as the most effective oxygen reduction reaction (ORR) electrocatalysts, the high cost and the scarcity of the precious metal restrain the mass production and viable commercialization of FCs. Nanostructuring and interface tuning has become a crucial methodology to enfold the challenges associated with creating highly active materials for advanced electrocatalytic processes. In recent years, interfacial catalysis has been widely emerging in the field of electrochemistry to achieve the adequate kinetics of electrode reactions. To design and develop high performance electrode catalyst, interfacial mechanism has attained considerably superior characteristics to replace noble metal-based ECs. Accordingly, oxide/oxide interfaces in multi-metal oxides play pivotal role in oxygen electrochemistry. Thus, this presentation will focus on the creation of oxide/oxide interfaces in  $Co_3O_4/CeO_2$  and  $MnOx/CeO_2$  as representative examples and their role toward oxygen electrode reactions.

#### Reference

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- [2] S. Patowary, R. Chetry, C. Goswami, B. Chutia, P. Bharali, *ChemCatChem* 14, e202101472 (2022).
- [3] K.K. Hazarika, B. Chutia, RR. Changmai, PK Boruah, MR Das, P Bharali, *ChemElectroChem* 9, e202200867 (2022).
- [4] C. Goswami, K.K. Hazarika, Y. Yamada, P. Bharali, *Energy Fuels*, 35, 13370–13381 (2021).

# Catalytic perspective towards energy and environment: Case study of CO<sub>2</sub> reduction, and Dioxin and Furan Mineralization

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The concepts of green and sustainable chemistry have gained significant attention around the world. One of the greenest approaches is reduction of CO<sub>2</sub> in atmosphere using solar energy and moisture. Likewise, polychlorinated p-dibenzo dioxins/furans (D&F), comprising of 210 congeners (among them 17 are highly toxic, A1-carcinogens), generated during combustion of solid municipal/bio-medical waste, also need urgent attention. Our group is engaged in development of photocatalytic materials for CO<sub>2</sub> reduction and degradation of organic pollutants. A few typical examples are Cu-doped TiO<sub>2</sub> and TiO<sub>2</sub> nano tubes which were used as photocatalyst for reduction of CO<sub>2</sub> to CH<sub>4</sub>. Cu-doped TiO<sub>2</sub> photocatalyst was shown to produce CH<sub>4</sub> with 100 % selectivity, under ambient conditions using sunlight and moisture, without using any hydrogen. The role of structural parameters like oxidation state, particle size, band gap *etc.* with a propensity for electron-rich centres of surface (Cu<sup>1+</sup> species). The V<sub>2</sub>O<sub>5</sub>-WO<sub>3</sub>-TiO<sub>2</sub> catalyst along with V<sub>2</sub>O<sub>5</sub>-TiO<sub>2</sub> and WO<sub>3</sub>-TiO<sub>2</sub> are shown to mineralize o-DCB (a representative molecule for Dioxin and Furan) at 150 °C and the reaction mechanism is established. Detailed mechanistic understanding for ethylene and methane degradation were performed using vanadium dopes titania. Some of these results will be discussed.

#### Many Dimensions of that Vexing Question of Sustainability Ashutosh Sharma Institute Chair Professor Indian Institute of Technology Kanpur & President, Indian National Science Academy

While sustainability is a holistic concept, the many fundamental dimensions of sustainability and their interplays are mostly not discussed and appreciated in scientific and technology conferences. Thus, it is also not generally well understood that new, more efficient technologies, while certainly desirable, are not sufficient for sustainable development. In my talk I will also briefly discuss some of the major foundational aspects of a sustainable earth's ecosystem:

(00) S&T based products with nexus and lifecycle; (0) efficient procedures and processes for S&T to work; (1) Sustainability of knowledge by balancing inventions with relevance, direction and purpose with innovations that consume that knowledge to create new socio-economic opportunities, especially at the grass-roots; (2) Socio- psychological- cultural dimensions of sustainability; (3) cultural determinants of Aatamnirbhata in the triad of Aatam- Viswas, Samman, Chintan; (4) Diversity, inclusion and equity; (5) policy and regulatory dimensions as basic enablers; (6) structure and processes of a seamless integration of invention and innovation ecosystems; (7) overarching technosocietal challenges of the future and the new mind required to meet them; (8) the balance and deployment of the triad of Dhandha (business as usual)- Juggad- Panga (disruptive) for problem solving; (9) compelling roles of humanities and social sciences; (10) connect of S&T with society; (11) replacing *for-profit* ecosystem with *for- benefit* ecosystem; from extractive economy to LiFE economy (Lifestyle for Environment); (12) from ownership to trusteeship; (13) lifestyle choices; (14) strong global cooperation in the spirit of one earth, one family, one future; (15) remastering of Maslow's hierarchy of needs by balancing of the outer and inner engineering.

I will illustrate the Policy Dimension with a recent example of the DST, Gol policy on Liberalization and Democratization of Surveying, Mapping and Geospatial Data which among other things is driving high resolution digital mapping of India at 10 cm resolution. The SVAMITVA Scheme launched by Hon'ble Prime Minister of India on National Panchayat Day (24th April 2020) will now allow digital land ownership certificates for rural India through drone and land-based surveys. This is an unprecedented instrument of rural empowerment allowing bank loans (rather than local moneylender loans!) and resolution of infinite litigations!

#### Net Zero Transition: Potential Implications for Catalysis

#### **Bala Subramaniam**

# Dan F. Servey Distinguished Professor of Chemical and Petroleum Engineering Director, Center for Environmentally Beneficial Catalysis (CEBC) University of Kansas, Lawrence, KS 66047

#### Abstract

This talk will discuss some of the potential implications of the net zero energy transition from fossilbased energy to renewable energy on the supply/demand dynamics of critical metals as well as the supply of traditional petrochemical feedstocks. Some of these changes, such as the displacement of gasoline and diesel-powered passenger cars by electric vehicles, are already occurring and expected to steadily increase during this decade and beyond. Consequently, petroleum refining output and thereby petrochemical feedstocks, are likely to encounter disruptions. Common assumptions about the abundance of catalytic metals may no longer hold and unexpected opportunities may arise for alternate feedstocks such as biomass and recycled carbon to make the products of everyday life. This talk will emphasize why the catalysis community should consider such changes and seize appropriate opportunities as it develops R&D strategies to deliver a well-guided transition towards industrial decarbonization and sustainability. It will also feature examples of technologies developed at the CEBC for the decarbonization of industrial chemical processes for making and recycling plastics, and the use of emerging feedstocks including biomass and carbon dioxide for making chemicals, guided by quantitative sustainability assessment.

## Biswajit Chowdhury\*<sup>1</sup>, Anirudhha Singha<sup>1</sup>

## <sup>1</sup>Department of Chemistry and Chemical Biology; Indian Institute of Technology (ISM), Dhanbad, P.O 826004; Jharkhand; INDIA

#### 1. Introduction:

In the catalytic chemistry, biomass conversion to fine chemicals and fuels as well as CO<sub>2</sub> mitigation reactions have drawn significant attention for extensive research. Recent development of carbonbased catalyst has opened a new horizon where doping of higher valent metals, mixing with silica etc. resulted very useful for these reactions. In our works surfactant modified carbon catalyst for glycerol acetalization reaction [1], metal free carbon-silica catalyst for glycerol carbonylation reaction as well as glycerol esterification reaction [2] have been developed. For CO<sub>2</sub> mitigation pathway several reactions have been identified in the literature through thermo-catalytic pathway [3]. We have explored formation of cyclic carbonate by fixation of CO<sub>2</sub> in several epoxides using N, S doped hollow sphere carbon catalyst.

#### 2. Material and Methods:

The preparation of the catalysts is well described in the literature [1-3]. The catalysts were characterized by several techniques e.g. XRD,  $N_2$  physisorption study, FTIR etc.

#### 3. Significant Results and Discussion

A surfactant modified carbon catalyst was prepared by eco-friendly solid state grinding method. The catalyst was highly selective towards production of solketal from glycerol with five regeneration cycles [1]. Another metal free high surface area carbon-silica catalyst was prepared by rotary evaporation-based technique which was active for glycerol carbonylation and glycerol esterification reaction. [2]. The synthesis of cyclic carbonate from epoxide and CO<sub>2</sub> using homogeneous and heterogeneous catalysts have been studied extensively in our group. For CO<sub>2</sub> fixation most exciting material was the N,S doped hollow sphere carbon catalyst synthesized by template free method for epoxide substrate with high conversions and selectivity. The reaction conditions were ambient (1 atm pressure) and 343K temperature. At higher pressure (5 bar) biobased trans-mixture of limonene oxide gives (1,2 limonene carbonate) which is a useful biorenewable monomer.

#### 4. Conclusions:

A series of carbon-based catalysts were developed by tuning physicochemical property for biomass conversion and  $CO_2$  fixation as well as  $CO_2$  utilization reactions. The further study for generation of hydrogen from biomass and production of cyclic urea derivatives by  $CO_2$  are in progress.

#### **References:**

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- 3. Prof. B. Chowdhury, et, al Green Chem., 2022 (24) 1673-1692

En-Lightening C-H functionalization

# Debabrata Maiti IIT Bombay dmaiti@iitb.ac.in

#### Abstract:

The scientific community has long sought to emulate nature's mechanisms, particularly in understanding how enzymes achieve chemical transformations with precision. Through extensive research, we have gained a thorough understanding of how enzymes catalyze the functionalization of inert C-H bonds in a regio- and stereoselective manner, utilizing metal-active sites. Taking inspiration from these natural processes, we have successfully developed catalytic methods for the functionalization of carbon–hydrogen (C–H) bonds. The Fujiwara–Moritani reaction is one of such reaction which made significant impact on the development of modern C-H activation methodologies. Despite the traditional approach's widespread applicability in various fields, issues related to reactivity and regioselectivity have limited its effectiveness. To revive this remarkable reaction, it is necessary to establish a mechanistic framework that allows simultaneous control over both reactivity and regioselectivity. The conventional high-temperature conditions required for olefination often lead to undesired multiple functionalizations at different sites. In our work, we have successfully established a photoredox catalytic system by merging a palladium catalyst with an organo-photocatalyst (PC). This innovative system enables selective oxidative olefination of diverse arenes and heteroarenes in a highly regioselective manner. The utilization of visible light plays a crucial role in driving these "regioresolved" Fujiwara–Moritani reactions, eliminating the need for silver salts and high thermal energy. Our catalytic system also exhibits compatibility with both proximal and distal olefination, facilitated by the appropriate directing groups (DGs). This versatility allows us to engage the entire spectrum of C(sp2)-H olefination. The broad scope of this protocol allows for the synthesis of diverse compounds, including natural products, chiral molecules, and drugs. The established mechanistic insights further enhance our understanding of this reaction, enabling future advancements in this field. Importantly, this method offer significant advantages over traditional synthetic approaches, both in terms of economic feasibility and environmental impact.

#### **Recent Refernces:**

J. Am. Chem. Soc. **2022**, 144, 4; Science, **2021**, 372, 701; Nat. Commun. **2021**, 12, 1393; Angew. Chem. Int. Ed. **2021**, 60, 14030; J. Am. Chem. Soc., **2020**, 142, 12453; J. Am. Chem. Soc., **2020**, 142, 3762

#### **Presenter Details:**

Prof. Debabrata Maiti received his PhD from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies.

#### Currently he is an Associate Editor of Journal of Organic Chemistry.

## Reductive Catalytic Fractionation (RCF) - A Novel Approach for Value addition of Lignocellulosic Biomass

#### Thallada Bhaskar

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Lignocellulosic biomass valorization has become one of the most intensive areas of research due to the continuous depletion of fossil resources. Presently, the use of lignocellulosic biomass is mainly focused on creating pulp, paper, sugars and bioethanol from the holocellulose component, leaving behind lignin to be discarded or burned as waste despite of its highest aromatic carbon and energy content (22-29 KJ/g). During the pulping process, lignin undergoes significant structural changes to yield technical lignin. For a circular bioeconomy, there is an urgent need to enhance the use of native lignin for generating more valuable products and reduce the environmental/carbon foot print. Over the last few years, a new method called 'lignin-first', or 'reductive catalytic fractionation' (RCF), has been devised to achieve selective phenolic monomers under milder reaction conditions. This involves extraction and depolymerization of lignin and stabilization of obtained phenolic monomers before capitalizing on carbohydrates. Through reductive catalytic fractionation, the underutilized lignin component can find its potential for the production of bio-chemicals and the left-over pulp residue containing carbohydrates can be utilized for bioethanol production. The strategic design of novel catalysts is the key for the fractionation and value addition of lignocellulosic biomass/polymers.

#### Science–Engineering–Technology Synergy Needed for Sustainable Future Indranil MANNA Vice Chancellor, Birla Institute of Technology Mesra, Ranchi Professor, Metall. & Mater. Engg. Dept., IIT Kharagpur President, Indian National Academy of Engineering imanna@metal.iitkgp.ac.in; vc@bitmesra.ac.in; www.imanna.in; www.inae.in

#### Abstract

Science or scientific intervention has made a huge impact on the society throughout the ages. In the present era of knowledge-based society, science is no longer only a curiosity-driven act but is considered an intrinsic necessity and urge to translate knowledge into societal benefit through engineering invention and technological innovation. If science is driven by the primary desire to learn about the nature and origin of certain truths or phenomena, engineering or technology utilizes that fundamental knowledge to convert it into a viable and useful product or process and offer a tangible benefit to society or humanity at large. In simple words, if science is 'know-why' and engineering is 'know-how', then technology is 'know-what-sells'.

In the present talk, I intend to begin by referring to the early system of pursuing knowledge in India through 'gurukul' and defining the present status of our society in the context of population, economic status, opportunities, urges, and targets. I shall borrow from the experience of a national initiative of the Government of India called IMPacting Research INnovation and Technology (IMPRINT) aimed to act as the vehicle for engineering innovation and technological progress through academic institutions with the motto: million challenges, billion minds. IMPRINT was all about pursuing the goal of translational research through collaboration between academia and industry under ten representative technology domains. Though the program is over, the lessons learned remain relevant in all such pursuits for innovation-driven sustainability.

At the end, I shall present a few engineering projects oriented towards developing innovative products and processes conducted at CSIR-CGCRI, Kolkata, and also, discuss selected examples of research endeavors concerning engineering materials from our own research group at IIT Kharagpur aimed at a fundamental understanding of novel scientific properties. In summary, the main objective of this discourse will be to illustrate how research efforts based on scientific principles can lead to engineering inventions and innovations for sustainability.

#### Design of Novel Electro-Catalysts For the Cost-Effective Generation of Hydrogen Kandalam V. Ramanujachary Department of Chemistry and Biochemistry 201 Mullica Hill Road Rowan University Glassboro, NJ, 08028 chary@rowan.edu

#### Abstract:

Rapid depletion of non-renewable fossil resources is posing an imminent threat to the energy and supply of fine chemicals that are vital to the global economy. Currently, efforts are being undertaken at an accelerated pace to develop technologies that would help us deal with the disastrous consequences. We have been working in the areas of bio-mass conversion to renewable fuels/chemicals as well as the production of hydrogen through electrocatalytic splitting of water using non-noble metals. In both of these areas, there is a dire need to develop cost-effective materials to increase the efficiency of the processes. We have been exploring the use of anionically modified molybdenum oxides and phosphides for efficient splitting of water in both acidic and alkaline conditions. The presentation will summarize our findings and the opportunities for exploring inorganic materials for the production of value added chemicals and fuels

# MXene: A Sustainable Materials for Energy and Environmental Application Kulamani Parida, Centre for Nanoscience and nanotechnology, Siksha 'O' Anusandhan, Deemed to be University, Bhubaneswar-751030

## Abstract:

Two-dimensional transition metal carbides, nitrides and carbonitrides named "MXenes", have grabbed considerable attention in various research areas owing to their intriguing physico-chemical properties and intrinsic multilayer structure. In this context, MXene-based and MXene-derived nanomaterials deliver motivation for fabrication of sustainable materials with optimum activity, and long-term stability. Especially, titanium carbide Ti3C2 is the most studied layered 2D MXene displaying remarkable potential in photocatalysis for sustainable development in the sector of energy and environment for its fascinating characters. In our investigations, Ti3C2 has shown huge potential as a co-catalyst in the photocatalystic H2 evolution, H2O2 production, and pharmaceutical antibiotic degradation. Particularly, Ti3C2 MXene combining with other semiconducting materials such as N, S doped TiO2 and g-C3N4 participate as a co-catalyst to form an interfacial Schottky heterojunction to accelerate the separation of charge carrier pairs in the hybrid heterostructure for sustainable H2 evolution. Also our latest advances proved that metallic MXene layers acts as the solid-state electron mediator to develop a high-flux electron-shuttling route between multiphase heterojunction such as TiO2@MXene/B-g-C3N4 and TiO2@Ti3C2/MgIn2S4 to fascinate the charge carrier separation for enhancing the photocatalytic H2O2 production, H2 evolution and Ciprofloxacin degradation. Overall, this work will provide a useful scaffold for the rational design of an efficient and stable MXenes-based photocatalysts for energy and environmental applications.

# New Surfactants : Gemini and Microbial type Sunil S Bhagwat Department of Chemical Engineering Institute of Chemical Technology Matunga, Mumbai 400019, INDIA and Indian Institute of Science Education and Research, Pune 411008, INDIA

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## September 5, 2023

Some of the new surface active molecules synthesized and characterized in our recent work are presented here. Lauramidopropyl glyceryl dimethyl ammonium chloride or LGDMAC is a quaternary ammonium surfactant where glycerol contributes towards the hydrophilic part of the molecule. The CMC is comparable to conventional quaternary ammonium compounds while the C20 is lower. Owing to the quaternary ammonium nature, this molecule has antimicrobial activity as well. Sophorose is a sugar which can work as a polar headgroup.

Sophorolipids were prepared microbially by using fatty alcohols instead of usual fatty acids and as a result, the molecule remains nonionic. Cationic gemini surfactants were synthesized from fatty acids via amidoamine derivative and these molecules show low CMC and good antimicrobial activity. Anionic biphosphodiester gemini surfactants and ardanol sulfonate gemini surfactants of various alkyl chain lengths were synthesized and these molecules show a low CMC, slow dynamics and consequently low foamability.

#### **Bi-Functional MOFs and Catalysis**

#### Srinivasan Natarajan

Framework Solids Laboratory, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India, E-mail: <u>snatarajan@iisc.ac.in</u>; <u>rajan1960@gmail.com</u>

The synthesis of framework structures with channels and pores are important for their many uses in the areas of catalysis, sorption and separation. The metal-organic framework (MOF) compounds with their well characterized pore and channel structures provide an important alternative for the well established framework compounds of aluminosilicate and the aluminophosphates. Thus, many MOFs have been prepared and investigated over the years in inorganic materials chemistry. The rapid growth and expansion in the study of such compounds have been due to the possibility of synthesizing compounds with periodic pore structure, creating coordinatively unsaturated metal sites within the framework and good flexibility in the structure. Currently, the MOFs have been explored for many different heterogeneous catalytic reactions. In this presentation, the usefulness of MOFs especially bifunctional ones towards heterogeneous catalysis would be discussed: (a) the Lewis-acid catalysis, (b) Lewis-base catalysis, (c) Tandem catalysis, (d) MOFs as catalytic support for transition elements for catalysts.

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## **Case studies in Catalysis and Process Development**

for the Manufacture of Fine Chemicals Sanjay Mahajani Department of Chemical Engineering Indian Institute of technology Bombay, Mumbai 400 076

Green products and green processes are the important elements of sustainable development. Heterogeneous catalysis and process intensification play a crucial role in developing such processes and products. Use of heterogeneous catalyst makes the process clean, environment-friendly, and sometimes reduces raw material requirement and energy consumption. In this talk, I will present three case studies.

The first one deals with manufacture of methyl pentanone, a perfumery intermediate produced by the reaction of acetaldehyde and methyl ethyl ketone in the presence of acid catalyst. A step-by-step procedure including identifying the right catalyst, understanding the reaction mechanism, developing kinetic model, detailed study on catalyst deactivation and the design and demonstration of an appropriate continuous reactor will be described in detail. The overall costing and environment load will be compared with the conventional process that uses homogeneous catalyst.

The second case study involves use of multifunctional reactor for the production of another perfumery intermediate, phenyl ethyl acetate, synthesized by esterification of phenyl ethyl alcohol. The use of reactive distillation or reactive chromatography has a potential to improve the existing process considerably.

The third case study deals with process development for a green solvent produced from furfural, a biological feedstock, in multiple steps. The reaction is accompanied by the formation of heavy products involving both furan (reactant) and the product. I will present the ongoing work, that involves identification of catalyst, suitable reaction conditions and the contacting pattern to achieve maximum yield and good catalyst life.

# Regenerative, nature-inspired mining operations to produce critical metals for society's electric future

# Prof. Vikramaditya G. Yadav Department of Chemical & Biological Engineering The University of British Columbia

Society needs unprecedented quantities of metals to transition to net-zero. What if we could produce them without ever having to build new mines?

Tailings represent the material left over after desirable metal fractions have been extracted from mined ore. Since tailings are easier to transport as a slurry, they are typically stored in water in large ponds known as tailings ponds. The unique environment within the tailings pond accelerates natural biogeochemical processes that culminate in the accumulation of heavy metals in the water. Tailings ponds are frequently toxic and acidic, and the water in some ponds is also radioactive. Worse, tailings ponds are susceptible to catastrophic breaches that cause permanent environmental damage, representing long-term health impacts without additional economic activity. There are over 9,000 tailings ponds across the globe that cumulatively contain over 200 trillion liters of contaminated water. Mines also produce a more concentrated and acidic liquid waste stream called Acid Rock Drainage (ARD), which is the leading contributor to the global mining sector's environmental impacts and attached liabilities. Moreover, over \$20 billion worth of metals are lost in ARD annually in North America alone. These critical and technology metals are vital for the modern economy and national defense. No economical solutions exist to treat this large body of waste. Current solutions to manage tailings – not treat, mind you – incur steep costs, and none are capable of recovering even a small fraction of the metals in the ponds.

Traditional mining extracts valuable metals from ores and leaves behind tailings. What if the next generation of mining operations treated tailings as ore? In this scenario, one could extract the metals from the ore and leave behind clean water. We have successfully developed a continuous and scalable tailings water treatment technology that combines metal recovery, water treatment, and carbon abatement into a single process. It is a two-stage, continuous process. The first stage comprises a stack of flow-based microbial fuel cells (MFCs) that selectively recover metals from the tailings. The water is further processed in the second stage using microbial carbonate precipitation (MCP) and conditioned to a state that meets environmental regulations for discharge and recycle. Our process has been shown to successfully recover over 90% of base metals such as copper and over 80% of precious metals such as gold, silver, platinum and iridium. The process also successfully eliminates over 90% of toxicants such as arsenic and selenium. The technology is currently being commercialized by Tersa Earth Innovations, a mining biotechnology company, which is building pilot units for field testing. The field units have shown that they are readily deployed at scale and significantly reduce carbon emissions in comparison to conventional processes for management of tailings. When the process realizes its attainable market, it could improve productivity of the mining sector by 10% and reduce its GHG emissions by 15%. We are leveraging mining waste as a resource and contributing to humanity's shift to a zero-waste economy.
## Hot Electrons in Black Gold as Green Catalyst Vivek Polshettiwar\* Department of Chemical Sciences, Tata Institute of Fundamental Research (TIFR), Mumbai, India. Email: <u>vivekpol@tifr.res.in</u>, Web: www.nanocat.co.in

# Abstract:

The urgent challenge of capturing and converting CO<sub>2</sub> into valuable chemicals and fuels, essential for promoting the principles of the Circular Economy, remains a critical endeavor. In this context, our research efforts have led to the discovery of a unique nanomaterial called Dendritic Fibrous Nano-Silica (DFNS),<sup>1,2</sup> which has gained worldwide attention and adoption in over 150 research groups for various applications. Our group has pioneered several nano-catalytic processes in the field of environmentally friendly catalysis and CO<sub>2</sub> capture-conversion,<sup>3-10</sup> achieving significant breakthroughs like "Black Gold," "Defective Catalysts," "Solid Acids," "Lithium Silicate Nanosheets," and "Magnesium-CO<sub>2</sub>." These innovations are all aimed at addressing the complex challenges posed by climate change.

During this presentation, I will explain our recent achievement in harnessing the synergy between solar energy collection and CO<sub>2</sub> utilization, exemplified by the concept of using "Black Gold as an Artificial Tree." Our innovative approach involves transforming regular gold nanoparticles into a unique "black gold" form by precisely adjusting the size and spacing of the nanoparticles, taking advantage of the supportive structure provided by DFNS. This material exhibits outstanding light-absorbing properties that cover a wide range of the solar spectrum, including visible and near-infrared regions. Building on this foundation, we have developed black gold catalysts loaded with nickel, which display an exceptionally high rate of photocatalytic CO production along with an impressive 95% selectivity. This outstanding catalyst maintains its stability for an extended period of at least 100 hours. Furthermore, the versatility of Black Gold-Ni is demonstrated in its effectiveness across various catalytic reactions, including H<sub>2</sub> activation, C-Cl bond activation, and the hydrogenation of propene and acetylene, all conducted under visible light at room temperature, highlighting its significance in the realm of eco-friendly catalysis.

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## Rapid Catalyst screening tool for Fischer-Tropsch reaction

Karthikeyan Sathrugnan1, Ichi Watanabe<sup>2</sup>

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#### **Abstract Category**

Catalytic preparation & characterization

#### Abstract

The Fischer-Tropsch (FT) process (converting CO and H2 to liquid fuels) has been the subject of considerable study for many years. R&D efforts are on-going attempt to develop new catalysts to increase the product yield and selectivity of the FT process..[1] Evaluation of newly developed catalysts using conventional reactor experiments is time consuming and expensive since such reactors use large amounts of catalyst in the bed. In this study, we present the details of a single micro reactor system which can be coupled to GCMS and evaluate the catalyst performance rapidly through online reaction monitoring. The system configuration of the RSR-GC/MS using a Single  $\mu$ -Reactor (Rx-3050SR) is shown in Fig. 1. Ru (5%)-alumina (Aldrich 381152, 194 mg) was packed in a quartz catalyst tube (i.d., 3 mm) with a catalyst bed length of 30 mm The catalyst tube was placed in the reactor and the reactor at a rate of 18 mL/min. The reaction products were transferred to GC separation column with the help He carrier gas, and separated compounds were detected by MS detector

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#### Conversion of Jatropha press cake to BTEX using Tandem micro-Reactor GC/MS system

Anusha Kadimisetti

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## **Abstract Category**

Catalytic reaction engineering & scale up

## Abstract

Conversion of Jatropha press cake to BTEX using Tandem micro-Reactor GC/MS system The conversion of the press cake to useful chemicals is of interest. In this study we present a two-step process which converts a common feedstock to high-value compounds. First, the Jatropha press cake is pyrolyzed using the Tandem  $\mu$ -Reactor (Rx-3050TR) and the pyrolyzates are then converted to hydrocarbons (BTEX) via a catalytic reaction using a zeolite catalyst. The Tandem reactor µ-Reactor (Rx-3050TR) comprises of two reactors a pyrolysis furnace in which Jatropha press cake Ca. 0.55 mg of finely powered was pyrolyzed in the 1st Reactor (550°C) is shown in Fig. 1. and a catalytic reactor, the 2nd Reactor (550°C) which contains a zeolite catalyst ZSM-5 (38 mg). The Tandem  $\mu$ -Reactor (Rx-3050TR) can be directly mounted on a gas chromatograph mass spectrometer (GC/MS) to observe realtime changes of the products formed by the gas-phase catalytic reaction between the sample and the catalyst. The catalytically converted products were temporarily cryo-focused at the head of the separation column using a Micro Jet Cryo-Trap (MJT-1035E) before starting the GC/MS analysis is shown in Fig. 1. The reaction products were transferred to GC separation column with the help of He carrier gas, and separated compounds were detected by MS detector. By Flash Pyrolysis we observed that major constituents were C16 and C18 linear chain fatty acids. As the pyrolyzates flow to the 2nd Reactor (550°C) which contains a zeolite catalyst, they are transformed to highvalue, monocyclic hydrocarbons

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Dopamine functionalized, red carbon quantum dots for in vivo bioimaging, cancer therapeutics, and neuronal differentiation

Pankaj Yadav

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**Abstract Category** 

Nano Technology

## Abstract

One of the crucial requirements of quantum dots for biological applications is their surface modifications for very specific and enhanced biological recognition and uptake. Toward this, we present the green synthesis of bright, red-emitting carbon quantum dots derived from mango leaf extract (mQDs). These mQDs are conjugated electrostatically with dopamine to form mQDs-dopamine (mQDs: DOPA) bioconjugates. Bright red fluorescence of mQDs was used for bioimaging and uptake in multiple cell lines, tissues, and in vivo models like zebrafish. mQDs exhibited the highest uptake in brain tissue as compared to others. mQD:DOPA conjugate induced cellular toxicity only in cancer cells while showing increased uptake in epithelial cells and zebrafish. Additionally, the mQDs: DOPA promoted neuronal differentiation of SH-SY5Y cells to complete neurons. Both mQDs and mQDs: DOPA exhibited potential for higher collective cell migrations implicating their future potential as next-generation tools for advanced biological and biomedical applications.

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#### LIFE CYCLE ASSESSMENT OF SOLAR DRYERS FOR SUSTAINABLE AGRICULTURAL PRACTICES

Amardeep Khaire, Sachin Jadhav, Bhaskar Thorat

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#### **Abstract Category**

Life cycle assessment

#### Abstract

Solar energy drying is an ideal method for environmental sustainability and global solar energy utilization. In this context, the environmental impacts of Solar Cabinet Dryer (CD), Corrugated Solar Conduction Dryer (CSCD) & Heat Pump Dryer (HPD) are compared through Life Cycle Analysis (LCA). The "Cradle-to-grave" assessment of dryers is performed using openLCA software to analyse the environmental impacts caused due to the fabrication, recycling, and operation of selected solar dryers. The present study involved the calculation of impact assessment values using the ReCiPe 2016 Midpoint(H) & ReCiPe 2016 Endpoint(H) Life cycle Impact assessment(LCIA) model. The endpoint assessment reveals that the Solar Cabinet dryer has a 61.37% higher impact on human health (DALY) and a 72.5% higher impact on the ecosystem (species.yr) compared to the Corrugated Solar Conduction dryer. Similarly, the Heat Pump Dryer shows a 47.7% higher impact on human health and a 54.62% higher impact on the ecosystem than the Corrugated Solar Conduction dryer. Furthermore, when considering the operation phase, all indicators of the Solar Cabinet dryer and the Heat Pump Dryer have greater environmental impacts. These findings highlight the significant reduction in environmental impacts associated with the CSCD, indicating its superior sustainability compared to the CD and HPD. Consequently, this study offers valuable insights into the adoption of solar food dryers that harness renewable energy sources. Keywords: Solar Energy, Agriculture, Environmental Preservation, Sustainability, Renewable Energy, Life Cycle Analysis

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# Chemical Upcycling of Polycarbonate Plastic Waste: Revealing the Structure-Activity Relationship by Alloying Ni with Ru Supported H-Beta Catalyst.

Arjun Manal, Rajendra Srivastava

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#### **Abstract Category**

Catalytic reactions in which wastes are converted to useful products

#### Abstract

The upcycling of waste plastic into renewable chemicals is recognized as a crucial endeavor for environmental preservation and the circular economy of plastic waste. However, the quest for sustainable catalysts and energy-efficient mild reaction conditions remains a formidable challenge. Bimetallic bi-functional catalysts offer the potential for eliminating oxygen functionalities through liquid-phase hydrodeoxygenation (HDO), leading to the production of liquid fuels and value-added chemicals. In this study, we demonstrate the efficacy of the Ru-Ni/H-Beta bi-functional catalyst in the HDO of bisphenol A (BPA), a typical monomer of polycarbonate (PC), and polycarbonate plastic waste under mild reaction conditions. The catalyst achieves a remarkable ~ 99 % conversion and > 90 % selectivity of propane-2,2-diyldicyclohexane, a JET fuel range C15 cycloalkane. The catalysts exhibit highest TOFs of 204 h-1, reusability, and adaptability to various substrates. The performance of Ru-Ni/H-Beta catalysts hinges on the synergy between Ru and Ni, with the optimal performance observed at the Ni/Ru atomic ratio of 0.5. Kinetic results and DRIFT studies reveal the efficient adsorption of substrate on the 1Ru0.5Ni/H-Beta interface, leading to highly selective conversion of BPA to bicycloalkane. However, higher Ni/Ru ratios > 0.5 yield larger Ni species domains, significantly influencing product selectivity and promoting the formation of low-range hydrocarbons through C-C bond cleavage. The process was scaled up to 5 g of plastic waste. The bimetallic Ru-Ni catalytic strategy and mechanistic insights presented in this work offer promising prospects for catalyst design and may find application in other chemical transformations necessitating efficient hydrodeoxygenation catalysts.

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# Metal-Free N-Doped Carbon Catalyst Derived from Chitosan for Aqueous Formic Acid-Mediated Selective Reductive Formylation of Quinoline and Nitroarenes

Arzoo Chauhan, Rajendra Srivastava

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## **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

#### Abstract

The work presents the demonstration of a metal-free, chitosan-derived N-doped carbon catalyst for the one-pot reductive N-formylation of quinoline and nitroarene in an aqueous environment using formic acid as both a hydrogenation and formylating source. Chitosan, a semisynthetic fiber sourced from chitin shells of crustaceans such as crabs and shrimps, serves as a vital carbonaceous material for heterogeneous catalysis due to its inherent nitrogen content and cost-effectiveness as a biowaste. The 8% nitrogen content, primarily derived from amino groups, proves to be a suitable precursor for synthesizing N-doped carbons, providing favorable basic sites for substrate and formic acid adsorption, as well as substrate activation. The catalyst's synthesis involves a simple carbonization process, leading to high yields of reductive formylation products under mild reaction conditions. Notably, the carbonized catalyst prepared at 700°C exhibits superior activity, resulting in a 92% yield of N-formyl-tetrahydroquinoline after 14 hours and a >99% yield of N-formyl anilide after 12 hours at 160°C. The exceptional catalytic activity is attributed to the specific "N" species present and the catalyst's inherent basicity. Density functional theory calculations reveal a waterassisted formic acid decomposition pathway involving deprotonation and dehydroxylation, leading to the generation of surface-adsorbed -H and -HCOO species, crucial for the formation of Nformylated products. Overall, this study provides valuable insights into the development of a sustainable and efficient chitosan-derived N-doped carbon catalyst for reductive N-formylation, facilitating the utilization of biomass-derived resources in catalytic applications.

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Catalytic interplay of metal ions (Cu<sup>2+</sup>, Ni<sup>2+</sup>, and Fe<sup>2+</sup>) in MFe<sub>2</sub>O<sub>4</sub> inverse spinel catalysts for enhancing the activity and selectivity during selective transfer hydrogenation of furfural into 2-methylfuran

Ganesh More, Rajendra Srivastava

Indian Institute of Technology Ropar, Ropar, India

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

2-Methylfuran obtained via the hydrogenation of furfural is an important biomass-derived liquid fuel. However, the large-scale production of 2-methylfuran from furfural requires cost-effective, active, and selective heterogeneous catalysts. Herein, we have performed experimental and DFT investigations on MFe<sub>2</sub>O<sub>4</sub> (M =  $Cu^{2+}$ , Ni<sup>2+</sup>, and Fe<sup>2+</sup>) inverse spinel catalysts to selectively hydrogenate furfural into 2-methylfuran via transfer hydrogenation, and to determine the nature of active sites. CuFe<sub>2</sub>O<sub>4</sub> afforded 99.4% furfural conversion and 97.6% 2-methylfuran selectivity at 200 °C in 1.5 h. In contrast, NiFe<sub>2</sub>O<sub>4</sub> and Fe<sub>3</sub>O<sub>4</sub> catalysts afforded furfuryl alcohol as a major product. The comprehensive characterization of the catalysts revealed that the acidity of these inverse spinel catalysts originates from the Lewis acid sites which influences the catalytic activity. DFT calculations revealed the energetically favorable interactions of furfural and furfural alcohol with the Fe<sup>3+</sup> sites of  $Fe_3O_4$  and  $Fe_3O_4$  and  $Fe_2O_4$  and  $NiFe_2O_4$  catalysts, whereas  $Cu^{2+}$  and  $Ni^{2+}$  sites present in CuFe<sub>2</sub>O<sub>4</sub> and NiFe<sub>2</sub>O<sub>4</sub> catalysts have stronger interactions with the isopropanol molecule. Hence, it is proposed that the Fe3+ sites present in CuFe<sub>2</sub>O<sub>4</sub> are the active Lewis acid centers to selectively convert furfural into 2-methylfuran via transfer hydrogenation. The present findings on the elucidation of the active sites of cost-effective, recyclable mixed metal oxide catalysts for the selective transfer hydrogenation of furfural into 2-methylfuran using isopropanol are attractive from the green chemistry perspective, and therefore extremely important for the academic catalysis community and to industrialists.

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# Unravelling the Synergistic Participation of Ni-Sn in Nanostructured NiO/SnO<sub>2</sub> for the Catalytic Transfer Hydrogenolysis of Lignin Model Compounds

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#### **Abstract Category**

Catalysis in biomass conversion

#### Abstract

The selective transfer hydrogenolysis of lignin-derived aromatic ethers without aromatic ring hydrogenation is essential for mono-aromatic production. Achieving high activity and selectivity with non-noble metal-based catalysts in this process remains challenging. Here, we present a simple nanostructured NiO(x%)/SnO<sub>2</sub> catalyst based on non-noble metals for the catalytic transfer hydrogenolysis of lignin model compounds. The catalyst achieved over 95% conversion and 100% selectivity in forming aromatic compounds using 2-propanol as the hydrogen source. Raman, FT-IR spectroscopy, and XPS analysis investigated the oxygen vacancy, while temperature-programmed desorption and pyridine adsorbed FT-IR analyzed acidity. The participation of NiO and SnO<sub>2</sub> nanoparticles, their reducing ability, and the formation of an interface in NiO/SnO<sub>2</sub> were confirmed through temperature-programmed reduction and multiple physicochemical characterizations. The physicochemical techniques confirmed the crucial role of an optimal NiO loading (only 10 wt%) in controlling aromatic selectivity and highlighted the catalyst's recyclability. The study also involved comprehensive analyses of the catalyst's chemical composition and catalytic activity by performing controlled experiments. This eco-friendly and cost-effective process using non-noble catalysts and 2propanol as a hydrogen source for converting lignin-derived aromatic ethers to selective aromatic platform chemicals would attract significant attention from both researchers and industrialists in the catalysis field.

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Photocatalytic selective conversion of furfural to γ-butyrolactone through tetrahydrofurfuryl alcohol intermediates over Pd NP decorated g-C3N4

Rajat Ghalta, Rajendra Srivastava

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#### **Abstract Category**

Catalysis in biomass conversion

#### Abstract

The increasing demand for renewable chemicals and fuels has led to extensive research into efficient and sustainable methodologies for converting biomass-derived platform chemicals. This study employed a photocatalytic selective reduction strategy to synthesize tetrahydro furfuryl alcohol (THFA) from furfural (FAL) using 2 bar H2 and a 150 W LED/sunlight at ambient temperature. An efficient light-absorbing g-C3N4 was synthesized to facilitate the reactions, and different loadings of Pd nanoparticles (Pd NPs) were incorporated into g-C3N4 to enhance catalytic transformations. Remarkably, 3 wt% Pd NP-decorated g-C3N4 exhibited exceptional performance, achieving nearly 100% FAL conversion and 100% THFA selectivity within 5.5 hours under a 150 W white LED. Subsequently, THFA was transformed into y-butyrolactone (GBL) with almost 100% selectivity under ambient conditions in O2 (1 bar) after 8 hours of photocatalysis using a 150 W white LED or sunlight. Physicochemical characterization, optoelectronic measurements, control reactions, and scavenging studies confirmed the catalyst's efficiency, with the incorporation of Pd NPs significantly enhancing the photoactivity and photoelectrochemical properties of g-C3N4. Additionally, the catalyst demonstrated excellent recyclability and photostability during repetitive use, providing a simple, eco-friendly, reproducible, and cost-effective approach for the photocatalytic valorization of FAL to THFA and THFA to GBL. This pioneering work paves the way for developing similar catalysts to produce other valuable renewable chemicals, thus contributing to a sustainable and green future.

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# Reaction Kinetics of Propane Deep Oxidation over Commercial Pd/Pt Bimetallic Supported Catalyst Hanmant Gurav1, Suchita Itgekar2, Uttam Maity1, Sharad Lande3, Kiran Patil2, Rakshvir Jasra1

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# Abstract

Due to growing concerns about the environment, the catalytic propane (C3H8) deep oxidation is becoming more and more significant for residual from the exhaust gases of LPG-fueled engines and the operation of refineries. However, being a non-polar molecule having saturated C-H bonds, low temperature propane oxidation is challenging. The most common catalysts used for deep propane oxidation are Pt, Pd, Au, Ru and Rh supported mixed metal oxide catalyst and bimetallic catalyst. However, very limited literature found that on the detailed kinetic study of industrial commercial catalyst for same work. Considering this fact, we studied deep propane oxidation over commercial Pd/Pt bimetallic supported catalyst with process conditions like effect of GHSV, temperatures, propane and oxygen concentration and catalyst stability study. It was found that the propane conversion increased with temperature and highest propane conversion was observed at 350°C. The catalyst stability was studied for 35 h TOS study, without any major impact on the catalytic activity. We explored the relationship between the reaction rate and various oxygen concentrations in reaction kinetics and observed that at high oxygen concentrations, the oxidation rate basically becomes independent of the oxygen concentration and the estimated apparent activation energy was 32.47 KJ/mol. Several kinetic models have been tested. Best fit was obtained with the Mars-van Krevelen kinetic model.

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# A Bio-waste derived Sustainable Heterogenous Catalyst for Classical Biginelli Reaction

Vikas Patil1, Amrut Patil<sup>2</sup>, Vinayak Chaudhari<sup>2</sup>, Gokul Borse<sup>2</sup>, Sharad Patil<sup>3</sup>

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# **Abstract Category**

Biocatalysis

# Abstract

This study is targeted at agricultural waste-derived heterogeneous catalysts, which have been effectively employed for Biginelli reaction. The application of cotton waste (Gossypium) derived lignin as a heterogeneous catalyst for C-C bond formation via one pot multicomponent Biginelli reaction. Here we hypothesize that the preparation of bio-waste derived catalyst by high temperature pyrolysis method under anaerobic conditions. The bio-waste derived heterogeneous catalyst (BDC) was well characterized by using different analytical techniques such as BET, SEM, TEM, XRD, DSC, TGA, ICP. The acidity of the catalyst was determined by a Hammett indicator test and titration method. An excellent yield of 6-methyl-2-oxo/thio-4-phenyl substituted-1,2,3,4-tetrahydropyrimidine-5-ethyl carboxylate derivatives was obtained in shorter reaction time (>80% yield in 15-30 minutes). The catalyst used in these studies has the advantage of being a waste material. Consequently, it is a low-cost, easily prepared, recyclable and environmentally benign. In

addition, the use of a biogenic renewable catalyst, its atom economy, and room temperature and solvent-free reaction conditions and the avoidance of column chromatography make the protocol highly significant from green and sustainable chemistry perspectives. The synthesized compounds were characterized by modern analytical techniques like NMR, MS, FT-IR, CHNS analysis. The experimental parameters like % mole of catalyst, mole ratio, temperature and time for reaction completion were also optimized to achieve maximum yield and purity. The surface interaction between BDC and reactant was also studied.

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# Exploring an Eco-Friendly Green Route to Synthesize Mono and Diesters using Zirconium Amino Phosphonic Acid Catalyst

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# **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

# Abstract

In conventional esterification reactions, liquid acids have been commonly used as catalysts. However, these liquid acid catalysts are known to be environmentally unfriendly. In alignment with global trends toward sustainability, the current study focuses on replacing these conventional homogeneous liquid acid catalysts with more environmentally benign heterogeneous solid acid catalysts. In this study, a novel hybrid catalytic material belonging to the class of tetravalent metal acid (TMA) salts has been synthesized through the sol-gel method. The process involves the reaction between zirconium oxychloride and an organic phosphonic acid, specifically amino tris methylenephosphonic acid (ATMP), under carefully optimized conditions, as previously reported. The resulting hybrid material, termed ZrATMP, exhibits proton donating properties, making it an intriguing candidate for use as a solid acid catalyst in catalyzed esterification reactions, enabling the synthesis of both monoesters and diesters. The findings of this research clearly demonstrate the potential of ZrATMP as an effective solid acid catalyst for various organic transformations, in addition to its application in catalyzed esterification reactions.

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# Effect of surface hydration on acidic and catalytic properties of silica functionalized with propylsulfonic acid

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# **Abstract Category**

Micro- And meso-porous catalysts

## Abstract

The silica functionalized with propylsulfonic acid (SFS) was synthesied by grafting of 3mercaptopropyltrimethoxysilane followed by oxidation using hydrogen peroxide and sulfuric acid. The as-synthesized SFS contained strongly bound water molecules with sulfonic acid ( $-SO_3H$ ) groups, which greatly lowered the strength of Brønsted acidic sites (of  $-SO_3H$  groups) and exhibited reduced catalytic activity. These bound water molecules could be removed by heating the SFS at a high temperature (225°C), which strengthened the acidity of -SO3H groups and enhanced the activity. The catalytic activity of SFS has been investigated for the isomerization of longifolene to isolongifolene as a model reaction. The SFS being a metal free solid acid catalyst can provide a costeffective and environmentally benign process for the synthesis of iso-longifolene.

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# Synthesis of biofuel additives from bio platform molecules over 12-tungstophosphoric acid anchored to zeolite HY

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

The current consumption of fossil fuels has prompted the legal obligation to swiftly adopt renewable energy sources. From this viewpoint, biomass acts as a pillar that improves the current circumstances. The development of polyoxometalate-based catalysts is a new area of research that has led to an enormous revolution in the biomass conversion. In the current study, a novel catalyst made up of 12-tungstophosphoric acid zeolite HY was synthesized. The catalyst has been thoroughly described using a variety of physicochemical techniques, and its efficacy in catalyzing the esterification of two of the most prominent bio platform molecules—levulinic acid and succinic acid, was assessed in order to produce fuel additives. Both the reactions were gone through a complete optimization study to achieve the significant conversions, 88% and 92% of levulinic acid and succinic acid with high TON of 3400 and 1777 respectively. The order of the reaction and activation energy for both reactions was determined in the kinetic study. The sustainable nature of the catalyst was confirmed via regeneration and viability towards other bio-based molecules which enhances its industrial importance.

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# Hydrotreating of a Lignin Derived Phenolic Compound, over Group VIII metal loaded Large Pore Zeolite

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#### **Abstract Category**

Catalysis in biomass conversion

## Abstract

Large-pore zeolites are exceptionally noted for hosting bulky biomass model compounds and their conversion. Large pore zeolite was synthesized through the dry gel method. The Group VIII metal species were incorporated through an incipient wet impregnation method. Brunauer-Emmett-Teller (BET) surface area and  $N_2$  adsorption-desorption of the samples were determined by an automatic micropore physisorption analyzer (Micromeritics ASAP 2020, USA). The hydodeoxygenation of mcresol was carried out using 4 mmol of substrate in liquid phase at varying temperatures and hydrogen pressures (Solvent: Isopropanol Catalyst: 0.05 g). Large-pore zeolite with a high surface area of 690 m<sup>2</sup> g<sup>-1</sup> was synthesized. The group VIII metal at various concentrations was introduced on large pore zeolite and investigated for hydrodeoxygenation of m-cresol to methyl cyclohexane at 170 °C and under 10 MPa of hydrogen for 8 hours. The surface area of the 5 wt% group VIII metalloaded sample was 613 m<sup>2</sup> g<sup>-1</sup>, which is slightly less than the parent sample and indicates the uniform distribution of metallic species on the zeolite surface. The spent catalyst showed a slight decrease in surface area compared to the fresh catalyst, which is due to the carbonaceous deposition during the reaction. The recyclability demonstrated that the catalyst could convert completely for several catalytic cycles. Calcination could regenerate the catalyst and return it to its initial activity. The hydrotreating activity of several substrates over group VIII metal loaded zeolite produced significant conversion (81% for eugenol, 100% for guaicol, phenol, etc.).

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# Hydrotreating using ITQ-2 Metal Oxy-hydroxide Composite

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

The development of multilayer or 2-D zeolites with substantial surface areas expanded the possibilities for bulk molecule and biomass model component conversions. A recent advance is the development of base-metal-containing zeolite for biomass processing. The current study concentrates on the production of a base metal oxy-hydroxide-ITQ-2 composite and its catalytic study for biomass model components. The MCM-22 precursor was prepared using the hydrothermal method. It was further delaminated to obtain metal ITQ-2 composite. The powder XRD patterns of material exhibited a disappearance of the peak at  $2\theta = 6.6$  (002) and broadening of the (100), (220), and (310) planes that confirmed the delamination and formation of randomly oriented layers. The material exhibits a type-IV isotherm, which is characteristic of microporous materials that contain slit-like mesopores. The developed catalyst was used for hydrotreating m-cresol in a batch reactor under the pressure of H2 at different temperatures for several hours. The result showed that methyl cyclohexane was obtained as the major product (100 % conversion).

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## Hetero element doped Strontium ferrite: Synthesis strategies and Application

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#### **Abstract Category**

#### **Catalysis in biomass conversion**

#### Abstract

Perovskite is a fascinating class of mixed metal oxides with the general formula ABO3 that have immense potential as piezoelectric, ferroelectric, superconducting, magnetic, and catalytic materials. Strontium ferrite (SrFeO3- $\delta$ ) is a well-studied perovskite oxide with chemical compatibility due to B site substitution, enhanced oxygen-ion transport, electrochemical and chemical properties, and several uses. The current project aims to dope various transition elements (such as molybdenum. nickel, and copper) on SrFeO3-δ and investigate its catalytic activities in the conversion of biomass model components to value added products. The different hetero element doped SrFeO3-δ (SrFe1xBxO3-δ; B= Mo, Ni, and Cu) and a series of copper doped SrFeO3-δ (SrFe1-xCuxO3-δ, x=0-0.45, SFCx) were prepared by the combustion method. The X-ray diffraction of copper-doped samples clearly indicates the formation of single phase perovskites with cubic structures in the copper concentration range of x = 0.3. The copper-doped series was systematically evaluated for catalytic hydroxylation of anisole using hydrogen peroxide as an oxidant and acetonitrile as a solvent. The catalytic reactions were optimized with catalyst concentration, H2O2/substrate molar ratio, solvent, reaction temperature, and time. A maximum anisole conversion of 76.9 with 62.5% guaiacol selectivity was observed in the presence of the SFC0.45 catalysts under optimum reaction conditions. The catalytic reaction proposed to proceed through the hydroxyl radical mechanism via the redox mechanism is well supported by electron paramagnetic resonance (EPR) studies.

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# Guanylation of NH<sub>2</sub>-MIL-125 under green condition to strengthen basic sites for enhanced base catalysis

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## **Abstract Category**

Micro- And meso-porous catalysts

## Abstract

The Guanylation of NH<sub>2</sub>-MIL-125 by the treatment of an aqueous solution of cyanamide at room temperature (30°C) converts few amine functionality (-NH<sub>2</sub>) into guanidyl group (~16 % modification) without affecting the framework structure. Guanidyl group provides stronger basic sites which was observed in CO<sub>2</sub>-TPD analysis as a desorption peak appeared at higher temperature (268 °C). The guanidyl group in the resulted material exhibits enhanced catalytic activity in Claisen-Schmidt condensation reaction of benzaldehyde and acetophenone under solvent free condition to synthesize chalocone. This study indicates that guanidyl-modified form of NH<sub>2</sub>-MIL-125 hold promise as solid base catalysts. The developed protocol for guanylation could also be useful for the modification of amine functionalized materials under green and benign condition to strengthen their surface basic sites for enhanced catalytic performance of industrial purpose.

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# Efficient Aqueous Phase Oxidation of Crude 5-Hydroxymethyl Furfural (HMF) to 2,5-Furandicarboxylic Acid (FDCA) for Industrial Applications

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

Efficient valorization of cellulose, hemicellulose, and lignin into industrial chemicals is vital for sustainability goals. Researchers focus on synthesizing 2,5-furandicarboxylic acid (FDCA) from 5-hydroxymethyl furfural (HMF) for its potential in PEF synthesis, but challenges in HMF synthesis, storage, and isolation persist due to its instability. Utilizing crude HMF for FDCA synthesis becomes essential, given the cost sensitivity in purifying HMF according to techno-economic studies.

In this study, we showcase the oxidation of laboratory-synthesized crude HMF into FDCA using nonprecious-based mixed metal oxides in an aqueous medium with oxygen/air. Among the catalysts explored the Cu-Mn catalyst achieved a significant 90% FDCA yield at 120°C under oxygen pressure (10 bar) within 8 hours, closely rivaling the performance of the well-established Ru/C (5wt%) catalyst, which attained a 93% yield. Additionally, we systematically investigate the influence of HMF purity, air as an oxidant, and the role of temperature, pressure, and reaction time on the oxidation process. Our findings indicate that FDCA formation follows HMFCA and FFCA intermediates.The success of the process is validated through the isolation of FDCA and its purity (>99%), confirmed using various analytical techniques such as NMR, IR, and HRMS. This study provides valuable insights into the efficient synthesis of FDCA from crude HMF, contributing to the advancement of sustainable chemical production and aligning with environmental goals. The application of these findings may have far-reaching implications in the field of green chemistry, supporting the transition towards a more sustainable and eco-friendly industrial landscape.

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# Visible-light-driven catalysis of AuPd plasmonic nanostructured materials

Priyanka Verma1, Robert Raja<sup>2</sup>, Hiromi Yamashita<sup>3</sup>

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# **Abstract Category**

**Catalysis For Energy** 

# Abstract

The influence of surface functionalization and hierarchical porosity on the activity enhancement of PdAu-based plasmonic catalyst in the Suzuki-Miyaura coupling reaction under visible light irradiation has been investigated. The presence of amines in the nanostructured catalyst enhanced the turnover number (TON) by 4.12 times under light irradiation conditions in comparison to dark conditions. The existence of active metal nanoparticles and the formation of electron-enriched species were found to be the main factors contributing to achieving superior product yields under light irradiation conditions.

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# Development of Novel Microsphere Structured - Calcium Tungstate as Efficacious Electrocatalyst for the Detection of Antibiotic Drug Nitrofurantoin

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## **Abstract Category**

Sustainable Engineering

## Abstract

In this report, a synthetic and nitro groups containing antibiotic drug nitrofurantoin (NFT) was electrochemically quantified under amended conditions using constructed novel calcium tungstate microspheres modified on glassy carbon electrode (CTMs/GCE). The calcium tungstate microspheres was synthesized by facile sonochemical method and characterizations was done by various techniques such as X-ray diffraction spectrometry (XRD), Fourier transform infrared spectroscopy (FTIR), Raman, field emission scanning electron microscopy (FE-SEM), x-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). Ahead to this, electrochemical investigations are demonstrated using electrochemical impedance spectroscopy (EIS) cyclic voltammetry (CV), amperometry and linear sweep voltammetry (LSV). The well distributed microspheres arises more active metal sites regarding to remarkable electrocatalytic activity towards NFT detection with excellent sensitivity (0.724  $\mu$ A  $\mu$ M-1 cm-2) and low detection limit (21 nM) with wide linear range 10-140  $\mu$ M. The practical feasibility of the developed CTMs/GC electrode was elucidate using distinct real sample river tap water and clinical sample (NFT capsule) and thus modified electrode manifested acceptable recovery results.

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# Role of materials engineering to develop thin-film nanocomposite membranes for liquid and gas separation and purification

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# **Abstract Category**

Sustainable Engineering

#### Abstract

The increasing demand for efficient and sustainable separation and purification processes has driven the development of advanced membrane technologies. Among them, thin-film nanocomposite (TFN) membranes have emerged as a promising solution due to their superior selectivity, permeability, and stability. This current work explores the crucial role of materials engineering in designing and fabricating TFN membranes for liquid and gas separation and purification. Here we developed TFN membranes for the separation of heavy metal ions for the purification of water. Also, the TFN membranes were used for the gas separation; here, we presented the CO2 and CH4 separation results. In conclusion, materials engineering plays a central role in advancing the field of thin-film nanocomposite membranes for liquid and gas separation and purification. By incorporating innovative nanomaterials, optimizing fabrication techniques, and understanding the influence of material properties, we developed TFN membranes with improved performance, reliability, and sustainability, paving the way for future more efficient and eco-friendly separation technologies.

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# Unraveling of Tectona grandis reduced palladium nanoparticles decorated on Mg-Al layered double hydroxide for efficient Hiyama and denitrogenative cross-coupling reactions

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## **Abstract Category**

**Catalysis - Prospects & Perspectives** 

## Abstract

A promising approach for creating environmentally benign nanocatalysts is encapsulating active noble metal nanoparticles onto inert support materials. Despite various claims, progress is being made in the search for supported nanocatalysts that use sustainable and contained methods. This work provides a brief explanation for a biogenic protocol for fabricating palladium nanoparticles (Pd NPs) onto Mg-Al layered double hydroxide using Tectona grandis leaves extract as a capping and reducing agent has been implemented to develop Mg-Al-LDH@TGLE Pd nanocatalyst. The characterization of the synthesized nanocatalyst by different analytical tools such as FT-IR, p-XRD, FE-SEM, EDS, UV-Vis, ICP-OES, TG-DTA, HR-TEM, and XPS confirmed its chemical composition, crystal structure, and thermal stability. Owing to the significance of Pd NPs in cross-coupling reactions, the Mg-Al-LDH@TGLE Pd nanocatalyst was examined for its catalytic performance in the Hiyama and denitrogenative cross-coupling reactions in the formation of biaryls. The Mg-Al-LDH@TGLE Pd nanocatalyst gave pronounced results with good stability and selectivity in both reactions with recyclability up to four cycles. This study presents a greener approach to avoiding complicated methodologies for support materials and their advances in catalytic reactions. Keywords: Palladium nanoparticles; Mg-Al layered double hydroxide; Tectona grandis; Hiyama cross-coupling; Denitrogenative cross-coupling.

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# Efficient vapor-phase catalytic hydrogenation of benzaldehyde to benzyl alcohol over Coppersupported Magnesium-Zirconium catalyst

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

The increasing concern about the excessive usage of fossil fuels and the increase in global warming has led to an impact on the industrial sector. Lignocellulosic biomass is one of the best carbon sources and its derivatives are scaffolds for various applications and bio-fuels. [1-3] The vapour-phase catalytic hydrogen transfer of benzaldehyde to benzyl alcohol using a copper-supported magnesium-zirconium (CMZ) as a catalyst was synthesized with different methods. The effect of different parameters such as copper loading, feed flow, reaction temperature and reduction temperature was studied for the catalytic performance. The developed catalyst was analysed by different analytical techniques to study the physiochemical properties. Better results were obtained for the 12.5 wt% Cu-impregnated magnesiumzirconium catalyst with a conversion of 60% for benzaldehyde and selectivity of 98.53% for benzyl alcohol. The literature revealed that the most dispersed Cu metal on the support surface with CuO /Cu+ sites is responsible for the higher catalytic activity of the optimized catalyst. [4,5]

**KEYWORDS:** Copper, Magnesium, Zirconium, CMZ, Benzaldehyde, Benzyl alcohol, catalytic hydrogen transfer.

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An Electrochemical Cascade Process: Synthesis of 3-Selenylindoles From 2-Alkynylanilines with Diselenides

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# **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

## Abstract

The substituted organoselenium compounds are crucial structural motifs in pharmaceutical molecules. Herein, we report a metal, oxidant, and base-free electrochemical approach to access 3-selenylindoles through an oxidative cyclization of 2-alkynylanilines with diselenides. This environmentally friendly approach demonstrates a wide range of substrate scope under benevolent reaction conditions in an electrochemical undivided cell setup.

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# One-Pot Catalytic Conversion of Sucrose to 1,2-Propanediol over Titania Supported Ni-Ce Metal Catalyst Under Milder Reaction Conditions.

Sreejith Sreekantan1<sup>,2</sup>, Sarath Sreedharan<sup>3</sup>, Arun Arunima Balachandran Kirali<sup>1,2</sup>, Parmeshwar Yadav<sup>1,2</sup>, Banu Marimuthu<sup>1,2</sup>

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# **Abstract Category**

Catalysis in biomass conversion

# Abstract

Researchers are seeking renewable and sustainable alternatives to fossil fuels for clean energy production. Sucrose, with its high solubility and limited reactivity, shows promise as a candidate for catalytic energy chemical production. Converting surplus sucrose to propane-1,2-diol (1,2-PDO) is particularly attractive due to its various applications and market demand. However, there are limited studies on sucrose conversion to 1,2-PDO, and commercial methods involve propylene oxide which is a non-green route. In this work we have synthesized Ni-Ce bimetallic catalysts supported on titania for selective 1,2-PDO production. Titania's stability and interaction with metals enable lower reaction temperatures and pressures. After careful optimization of the reaction conditions, the 5%Ni-15%Ce/TiO<sub>2</sub> catalyst achieved approximately 74% yield of 1,2-PDO from 2wt% sucrose under mild conditions(180°C, 30 bar H2, 3h , 200 mg catalyst). Characterization revealed the catalyst's

synergistic effect between Ni and Ce, contributing to enhanced selectivity. A multifunctional catalyst capable of hydrolysis(acid sites –  $TiO_2$ ), retro aldol condensation (Ce-sites) and hydrogenation (Nisites) was crucial for superior activity. Further research should focus on enhancing reusability to make sucrose conversion to 1,2-PDO a sustainable and efficient pathway for valuable chemical production.

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# Sucrose Conversion to Value-Added Products Using Metal-Supported Graphitic Carbon Nitride Surfaces

Arun Arunima Balachandran Kirali1, Hariprasad Narayanan<sup>2,3</sup>, Balasubramaniam Viswanathan<sup>2</sup>, Banu Marimuthu<sup>1</sup>

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Catalysis in biomass conversion

# Abstract

1,2-propanediol (1,2-PD) is an important polyol widely used for pharmaceuticals, polyester resins, paints, cosmetics, antifreeze, etc. Sucrose has emerged as a promising feedstock to produce 1,2-propanediol (1,2-PD), as indicated by recent research findings. Graphitic carbon nitride (g-C3N4/g-CN) supported Ni–Mo catalysts were synthesized via wet-impregnation for sucrose hydrogenolysis. Catalysts with varying Ni (x = 0-8 wt%) and Mo (y = 0-15 wt%) contents were characterized using XRD, BET, XPS, FE-SEM, and HR-TEM. The catalyst containing 8% Ni and 10% Mo on g-C3N4 exhibited the best performance, achieving complete sucrose conversion with a 63% yield of 1,2-propanediol (1,2-PD) under mild temperature (180 °C) and pressure (28 bar) conditions for 6 hours. Synergistic effects were observed when both Ni and Mo were present. XPS analysis confirmed the presence of multiple oxidation states of Ni and Mo, indicating their involvement in the catalytic reactions. Ni facilitated hydrogenation, while Mo's acid sites promoted the isomerization of glucose and fructose, followed by retro-aldol condensation, leading to increased 1,2-PD production. The layered g-CN support facilitated high metal dispersion and selective 1,2-PD formation due to its high thermal stability and electronic properties, preventing the catalyst deactivation caused by particle aggregation or sintering. In summary, the synthesized g-CN supported Ni–Mo catalysts demonstrated excellent performance for sucrose hydrogenolysis, with the optimized composition yielding high conversion and 1,2-PD selectivity.

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## N-heterocyclic Based New Molecule as a Hole Transporting Material

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#### **Abstract Category**

**Clean Energy** 

#### Abstract

Due to the increase in demand of energy and emission of carbon dioxide gas, it is necessary to develop renewable source of energy. Among many renewable source of energy, perovskite solar cells (PSCs) have drawn a global attention due to its affordability and comparable efficiency to conventional silicon-based solar cell. For the practical application of perovskite solar cells (PSC), it is desirable to have high efficiency and long-term stability and low manufacturing cost. Therefore, it is required to develop inexpensive, and well-performing hole-transporting materials (HTMs). In this study we synthesized compound based on N-heterocyclic system termed as DJ01.2-Acetylthiophene, N-ethylcarbazole-3-Carboxyaldehyde was dissolved in 1,4-dioxane. Next, ammonium acetate and ethyl cyanoacetate were added while stirring and were reflux for 24 hours at 80 °C. DJ01 compound showed absorption band in the region of 393 nm and an emission band in the region of 457 nm. Finally, its cyclic voltammetry measurement revealed that the HOMO lies at -5.67 eV and LUMO at -2.79 eV with a band gap of 2.88 eV. Thermal gravimetric analysis (TGA) was measured which shows thermal stability (Td) at 260 °C. . This is easily synthesized by one step with the commercially available compounds which is of low cost. Energy band gap of DJ01 was calculated to be 2.88 eV. As a whole, the obtained preliminary results suggest that the compound can be used further utilized as optoelectronic material.

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# Graphitic carbon nitride enriched phytochemicals-based integrated membranes for perilous Chromium (VI) ion removal

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## **Abstract Category**

Bioprocess engineering aspects, e.g. membrane bioreactors

## Abstract

The current study signifies a competent method for the fabrication of BLE@g-C3N4 using plant leaves extract as a source of phytochemicals. Which acts as an efficient agent to enhance the functionality of g-C3N4. BLE@g-C3N4 was further used as a novel composite to construct polysulphone composite membranes for heavy metal removal as a function of pH. The as synthesised nanomaterial was characterised using various analytical techniques to confirm the structural and functional properties. The incorporation of the nano additive into the membrane ensures structural changes in the membrane matrix which was confirmed by FESEM, AFM, water uptake, porosity etc. The separation capacity of the membrane was assessed using chromium feed solution at different operating pressure at various pH condition. The membrane containing 5 wt% additives showed a Cr rejection up to >99% with a flux of 73.23 LMH at 5 bar pressure in acidic pH. The same membrane showed a rejection of 79.26±0.76% and 90+0.55% at basic and neutral pH respectively. Further on evaluating the antifouling behaviour of the composite membrane using Bovine Serum Albumin (BSA) as the feed solution at a pressure 5 bar over a time span of 45 hours it was found that M2 membrane (0.5 wt%) showed high antifouling ability with a flux recovery aspect as high as 91.13%. The fabricated membranes were thereby confirmed to be well poised as far as trade-off between productivity and selectivity is concerned and also found to be a promising material in removal of chromium (VI) ion at different pH.

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# Green synthesis of palladium nanoparticles supported on boron carbon nitride for the catalytic reduction of nitroarenes

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# **Abstract Category**

Catalytic preparation & characterization

# Abstract

# Abstract

Heterogeneous catalysts, on an industrial level, are favored over homogeneous catalysts considering their ease of handling and simple work-up procedure. In line with this, we report the synthesis, characterization and catalytic activity of the heterogeneous nanocatalyst: palladium nanoparticles decorated on boron carbon nitride (BCN@Pd-NPs) for reduction of nitroarenes. The BCN@Pd-NPs nanocatalyst was synthesized in a facile three-step route by biogenically assisted formation, stabilization and immobilization of the palladium nanoparticles onto the support material. Successively, the BCN@Pd-NPs nanocatalyst was characterized by several analytical techniques to confirm its composition, structure, morphology, and stability. The catalytic aptitude of the BCN@Pd-NPs nanocatalyst towards reduction of nitroarenes is being explored. Further, the functional group tolerance and recyclability of the BCN@Pd-NPs nanocatalyst substantiates its heterogeneous nature.

Keywords: Boron carbon nitride; Biogenic; Palladium nanoparticles; Nanocatalyst; Reduction of nitroarenes

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## Carbazole based Electron Blocking Materials for Perovskite Solar Cells

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## **Abstract Category**

**Clean Energy** 

## Abstract

Replacement of non-fossil energy is in demand due to rapid development of social economy and energy crises. Solar cells are the best alternatives for renewable, sustainable, and clean energy, which can convert solar energy directly into electricity for practical purposes. In particular, Perovskite solar cells are very promising for practical applications owing to their rapid rise in power conversion efficiency and low cost of solution-based processing. The use of hole transporting materials remains indispensable in perovskite solar cells. Perovskite can conduct holes, they are present at the valance band, and for effective hole extraction the hole transporting material (HTM) is a prerequisite. Herein we designed a carbazole based HTM (CyCz and PyCz), the synthesis route is facile consisting of one step, from inexpensive commercially available materials.

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# Ti-promoted erythritol C—O hydrogenolysis activity of Pt/W/Ti-SBA-15 catalysts

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

Biomass conversion over heterogeneous catalysts is a research area of high priority as biomass is a potential renewable source for energy and chemicals replacing fossils. Hydrodeoxygenation (HDO)/hydrogenolysis of biomass-derived polyhydroxy compounds into terminal diols is one of the important transformations as those diols find huge applications in the polymeric industry. Erythritol is a C4 sugar alcohol (C4-polyol) sourced from fruits and fermented food. Amongst those C4 products of erythritol hydrogenolysis, 1,4-butanediol (1,4-BDO) is the targeted product. HDO of erythritol to 1,4-BDO is quite challenging as a variety of products are co-formed in the chemical transformation. Thus, there is a need for engineering catalysts for high yield of the terminal diols. Pt/WOx supported on neutral silica are quite selective to terminal diol formation. In this study, the application of Pt/WOx catalysts supported on Ti-SBA-15 is explored for the HDO of polyols. Accordingly, a series of Pt/W/Ti-SBA-15 catalysts (4 wt% Pt; 1 wt% W; Si/Ti molar ratio = 50, 33, 20, and 10) was prepared, and characterized. Ti-incorporation into the silica framework improved the support-metal interactions and altered the catalytic performance.

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# Selective hydrogenation of furfural over Ni exchange supported 12-tungstophosphoric acid on neutral alumina

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# **Abstract Category**

Catalysis in biomass conversion

# Abstract

For the sustainable future and developing the new techniques for conversion of naturally occured biomass to value added products required the suitable catalyst. Alkyl levulinates (ALs) which is widely utilized as a fuel additive and it were obtained from furfural (FA) by various route. Furfural (FA) is a low-cost aldehyde and the most prevalent industrial chemical derived from the decomposition of hemicellulose and recognized as one of the most important platform molecules. Conventional method and catalyst show the hydrogenation of FA by applying external hydrogen source and not exhibit any desirable selectivity for Als. In contrast, the present study shows the designing of a new bifunctional heterogenous catalyst comprising Nickel exchanged 12-tungstophosphoric acid supported on neutral alumina. The detailed characterization was carried out via a variety of physicochemical techniques. The efficiency of the catalyst was evaluated by in the selective hydrogenation of furfural with 2-propanol to alkyl levulinates without using any external H2 source.

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# Application of Microkinetic modelling using Nickel catalyst for methane cracking

Sharon K Thomas, Rahul Kumar, Koustuv Ray

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## **Abstract Category**

Computational catalysis

#### Abstract

Catalytic methane cracking is often considered to be a promising process for the generation of blue hydrogen and valuable solid carbon. The primary focus is to design a supported Nickel catalyst combining results from first-principles-based Microkinetic modeling (MKM) and catalytic fixed-bed reactor experiments. However, the active sites of the Nickel catalyst suffer from carbon deposits leading to catalyst deactivation. We are aiming to use the MKM technique initially to validate experimental results by varying reaction parameters such as contact time (0.2 - 0.6 g-h. mol-1) and temperature (723 – 923 K) and later to develop a robust kinetic model considering deactivation effects into MKM. In the present study, one fixed bed (plug flow) reactor with a series of zerodimensional reactors was modelled to theoretically calculate the conversion and turnover frequency of methane by considering the surface coverage of intermediate species of elementary reactions. The results indicate that methane dissociation and carbon deposition rates are faster at higher temperatures. A lower conversion was preferred over a higher conversion for methane to reduce carbon deposition on the catalyst surface and thereby reducing the deactivation. A decrease in turnover frequency with temperature indicates deactivation at higher temperatures. Our initial MKM results will be validated by comparing the turnover frequency of methane and H<sub>2</sub> yield using a 15wt.% Ni/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst over a fixed bed catalytic reactor with a similar contact time regime.

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# Transformation of Levulinic acid into Ethyl levulinate using Keggin type heteropolyacid

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# **Abstract Category**

Catalysis in biomass conversion

## Abstract

Ethyl levulinate (EL) is a potential biofuel with properties comparable to gasoline and diesel which renders it a promising alternative to traditional fossil fuels. Heteropolyacids are efficient green solid acid materials with diverse applications in various domains such as catalysis, energy storage, fuel cells, etc. Herein, we demonstrate the efficient conversion of levulinic acid to ethyl levulinate catalysed by phosphovanadotungstic acid under mild conditions.

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# A DFT study of Fe based bimetallic catalysts for thermocatalytic decomposition of methane

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#### **Abstract Category**

Computational catalysis

#### Abstract

Thermocatalytic decomposition of methane over Fe catalysts is an economic route to produce hydrogen without any emission of carbon oxides. The side product is carbon nanotubes which have commercial value. First dehydrogenation step of methane is the rate determining step. In this work, Density Functional Theory calculations were used to model Fe3M(111) single atom alloy catalysts with M=Co, Cu, Ni. The choice of these transition metals has shown to influence the stability and activity of the catalysts. Phyisorption of methane was found to be less influenced by the use of bimetallic Fe3M catalysts over monometallic Fe. We have found that activity is influenced significantly, with Fe3Co exhibiting lowest activation barrier and Fe3Cu relatively inactive. The adsorption and dissociation of CH4 is modelled on these SAA catalysts. The reaction energy and activation energy of CH4 dissociation were calculated for the first C-H bond breaking in CH4. It is observed that the reaction energy and the activation energy are linearly correlated on Fe-based SAA catalysts and thus follows Bronsted Evans Polanyi relationship. Therefore it is proposed reaction energy can be used as descriptor for screening large number of Fe-based SAA catalysts for thermocatalytic decomposition of methane.

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# Pt/W@UiO-66 promoted selective C—O hydrogenolysis of glycerol in aqueous medium

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# **Abstract Category**

Catalysis in biomass conversion

## Abstract

Sustainable routes for chemicals production from renewable feedstock have gained immense interest both in the academia and industries in order to lighten the shortage of the fossil fuels. In this context, glycerol, the by-product of biodiesel production, is an attractive, inexpensive renewable feedstock towards production of commodity C3 chemicals. Herein, we prepared a series of Pt and WOx embedded UiO-66 catalysts and efficiently utilized them in the hydrogenolysis of glycerol to value-added diols and mono alcohols. Suitably tuned Brönsted acidity, dispersed Pt in association with WOx and electronic contact are some features enabled the high activity and selectivity of these Pt/W@UiO-66 catalysts. The synergistic effect between Pt and the WOx played a significant role to promote the C-O hydrogenolysis and selective formation of 1,3-PDO over Pt/W@UiO-66 catalyst.

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# Next-Generation Catalysis: Unveiling the Astonishing Efficiency of Hetero Calixarene-Encapsulated Nano-Palladium Catalyst

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# **Abstract Category**

New catalysis routes

## Abstract

In this study, we used mesomodified hydroxycalix(4)pyrrole derivatives to synthesize Calix[4]pyrrolepalladium nanoparticles (PdNPs). OHCP-PdNPs have shown remarkable performance as a Nano catalyst in C–C coupling reactions. Our study focused on the effect of pH and stability on fine PdNPs. The electron-rich hydrazide functional group and the presence of four pyrrole units in the OHCP ligand facilitated the reduction and encapsulation of metal ions. Compared with common hydrazine, CP hydrazide exhibited stronger retraction properties, resulting in a web-like coating effect around palladium at the edge of Pd-NPs. In addition, OHCP-PdNPs showed excellent stability in water and air, leading to the cost-effective production of stable PdNPs. Encapsulation in OHCP enhanced the activity and selectivity of PdNPs, opening a wide range of exciting applications for efficient catalysis. Overall, our study highlights the remarkable potential of OHCP-encapsulated PdNPs as a highly efficient and stable nanocatalyst for various catalytic processes.

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# Palladium nanoparticles grafted on phytochemical functionalized biochar: A sustainable nanozyme for colorimetric sensing of glucose

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## **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

# Abstract

#### Abstract

The numerous drawbacks of natural enzymes, such as their high cost, lack of stability, difficulties in storage, and difficulty in retrieval, have stimulated the creation and development of numerous enzyme mimics (artificial enzymes) [1, 2]. In this work, we introduce BC-AHE@Pd as a novel nanozyme to mimic the peroxidase-like activity en route for the quick detection and colorimetric sensing of H<sub>2</sub>O<sub>2</sub> using o-phenylenediamine as a substrate. The sustainable BC-AHE@Pd nanocatalyst was prepared using green solvents under green reaction conditions by functionalizing biochar (carbonized biomass) obtained from *Artocarpus Heterophyllus* (Jackfruit) seed powder after extraction of phytochemicals. The BC-AHE@Pd nanocatalyst was characterized using various analytical techniques and investigated for its peroxidase-like activity in H<sub>2</sub>O<sub>2</sub> sensing. Furthermore, the potential of the nanocatalyst in the detection and quantification of glucose was explored. The reliable performance of the BC-AHE@Pd nanocatalyst in sensing exhibits a promising future for its fabrication as a nanosensor for real-time applications.

*Keywords:* Artocarpus Heterophyllus, Biochar, Nanozyme, H<sub>2</sub>O<sub>2</sub> sensing, Glucose.

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# Tetraalkylammonium halide promoted CO<sub>2</sub> and CH<sub>4</sub> semi-clathrate hydrate: Quality of phase equilibrium modeling with different cubic equation of state

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## **Abstract Category**

Sustainable Engineering

## Abstract

Semi-clathrate hydrates using TBAB and TBAF present a promising option as a potential remedy for gas sequestration, transportation, and storage. In this study, the extended Chen-Guo model is employed to conduct modeling research on the formation of  $CO_2$  and  $CH_4$  hydrates using TBAB and TBAF as the key components. Three equations of state were employed to compute the fugacity of the gas phase. At the outset, a comparison is conducted for distinct equations of state (EoS) at a 5wt% concentration. The equation of state that demonstrates the least average absolute deviation (AAD%) is selected further and a comparison over the two quaternary ammonium salts (QASs) is contemplated. These findings significantly enhance our comprehension and predictive capabilities within the field of semi-clathrate hydrate systems.

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## UNIQUAC-ext-PDH\* Framework for the Ionic Liquid Assisted Extraction of Gallium (III)

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

In this technology era, there is a boom of inventions in every field. The globe is currently experiencing a serious challenge with the growth of non-biodegradable waste. The management of electronic waste is possible by extraction of precious, rare metals used in electronic waste. Gallium is an important metal in the electronics industry, which is always expanding, drives up manufacturing costs. However, the recovery operation of gallium from electronic waste reduces demand and pricing also. Ionic liquids (ILs) are emerging as a solvent to extract gallium from electronic waste due to their intriguing features. The extraction of gallium from an aqueous acidic solution in this study was modeled using IL-aided liquid-liquid extraction and the expanded Pitzer-Debye-Hückel\* (PDH\*) thermodynamic model from UNIQUAC. The expanded PDH\* model provides a sufficient representation of the long-range electrostatic interactions found in ILs. The model parameters are computed by PCM (Polarizable Continuous Medium) computation, COSMO-RS (Conductor-like Screening Model for Real Solvent), and GA (Genetic Algorithm). For the modeling, 4 co-extraction systems and 4 single gallium metal extraction systems are taken into account. The calculated RMSD (Root Mean Square Deviation) is 0.85-1.5% for co-extraction systems and 0.5-0.8% for single gallium metal extraction systems and 0.5-0.8% for single gallium metal extractio

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# Ru-Pt Loaded 'Black Gold' as Air stable Plasmonic Nanoreactors for Sunlight Driven Acetylene Semi-Hydrogenation

Gunjan Sharma1, Rishi Verma<sup>1</sup>, Shinya Masuda<sup>2</sup>, Tatsuya Tsukuda<sup>2</sup>, Vivek Polshettiwar<sup>1</sup> <sup>1</sup>Tata Institute of Fundamental Research, Mumbai, India. <sup>2</sup>The University of Tokyo, Tokyo, Japan **Gunjan Sharma** 

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**Abstract Category** 

Catalytic studies at atomic, molecular & nano-scales

# Abstract

Catalysts employed in reduction reactions often exhibit instability when exposed to air. In this work, a highly active, selective and particularly air-stable plasmonic reduction catalyst for acetylene semi-hydrogenation was developed by loading Pt-doped Ru nanoparticles on 'dendritic plasmonic colloidosomes (DPC)', also known as black gold. With over 90% selectivity and productivity of 320 mmol g<sup>-1</sup> h<sup>-1</sup> of ethene, the DPC/RuPt catalyst outperformed nearly all previously reported catalysts. The critical role of co-existing metal oxide and metal phase was evidenced by high catalytic activity and long-term stability for at least 100 h, which could only be achieved by providing continuous airflow along with the reactant feed. Plasmon-mediated in-situ reduction and oxidation of the active site were responsible for the unprecedented stability of the catalyst validated by various spectroscopic analyses (XPS, EXAFS, and XANES). Finite-difference time-domain (FDTD) simulations showed a five-fold enhancement in the electric field as compared to pristine DPC due to the near-field coupling between the RuPt nanoparticles and DPC. The KIE measurements in light and dark implied the contribution from the non-thermal effects along with the photothermal activation of the reactants. In-situ FTIR studies provided insight into the molecular reaction mechanism over the oxide surface and highlighted the role of the intermediates in determining selectivity.

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# Catalytic CO<sub>2</sub> Hydrogenation Using Solar Energy via Localized Surface Plasmon Resonance in Hydroxy-Terminated Nickel Nitride Nanosheets

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# **Abstract Category**

**Clean Energy** 

# Abstract

Surface plasmon-enhanced photo-driven  $CO_2$  hydrogenation by hydroxy-terminated nickel nitride nanosheets

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## Harnessing Solar Energy through Defect-Rich Zr-Based Metal–Organic Frameworks

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## **Abstract Category**

**Clean Energy** 

## Abstract

Defect engineering has been strategically employed to modulate the photonic and electrical properties of the UiO-66 framework, as demonstrated in our prior research delving into the influence of these defects. Our experimental findings illustrate that the incorporation of defects in the UiO-66 (UiO-66-D@g-C3N4/Ni) photocatalyst leads to a notable augmentation in the rate of hydrogen generation, reaching 2.6 mmol.g-1.h-1 with an apparent quantum yield (AQY) of 6.41% at 420 nm (Fig. 1). The precise integration of a photosensitizer results in a remarkable 8.8-fold enhancement in hydrogen generation. The empirical data presented in this study establishes a positive correlation between the physical and chemical attributes of the photocatalyst and the distinct rate of H2 generation. To validate our experimental findings, density functional theory (DFT)-based calculations were conducted to explore the interactions between UiO-66-D and g-C3N4 with regard to hydrogen evolution reaction (HER) activity. The presence of defects in UiO-66 was confirmed through various analytical techniques, including FTIR, TGA, EPR, and TEM imaging. Elemental profiling via X-ray photoelectron spectroscopy (XPS) further reveals that a majority of anchored Ni ions predominantly reside superficially, concentrated around near-surface defect regions of the MOF.

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# Synthesis, Characterization and detailed analysis of Titanium dioxide (TiO $_2$ ) nanoparticles by XRD Analysis

Shraddha Admane1, Sandeep Shewale<sup>1</sup>, Nitin Rane<sup>2</sup>

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# **Abstract Category**

Nano Technology

# Abstract

Titanium dioxide particles are produced through a chemical reaction during the manufacture of  $TiO_2$  particles. The  $TiO_2$  nanoparticles are prepared at two different calcination temperature at 50° C and 100° C and the analysis is completed by using X-ray diffraction (XRD) Fourier-transform infrared spectroscopy (FTIR) and Field Emission Scanning Electron Microscope (FESEM). The anatase phase was observed for the values of 20 at peak 25.4°C and 25.52°C respectively. The detailed calculation for particle size, specific surface area, dislocation density, morphology index is calculated in detailed. The comparison of results at two different temperature, it is observed that the nanoparticles prepared at 100° C shows good affinity as compared to nanoparticles prepared at 50° C. By using prepared nanoparticles at two different calcined temperatures i.e. at 100° C and 50° C, the trial for removal of reactive black from wastewater was conducted. It is observed that nanoparticles at 100°C shows 83.75% removal of reactive black dye within 180 minutes while nanoparticles prepared at 50° C shows 62.84%. for removal of reactive black with same time duration.

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# Ultrasound assisted synthesis of n-octyl acetate over H5PW10V2O40 /FAC catalyst

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## **Abstract Category**

Catalytic reaction engineering & scale up

## Abstract

Orange flavour n-octyl acetate was synthesized over H5PW10V2O40 /FAC catalyst in an ultrasound irradiated isothermal batch reactor. Central composite design (CCD) method of response surface methodology was used to study the effect of parameters such as temperature (A), alcohol to acid ratio (B), duty cycle (C) and ultrasound power (D) on the conversion. Various sets of experiments were designed using the design of expert software. A quadratic mathematical model was developed to formulate predictions about the expected conversion under a set of operating conditions. The statistical analysis and analysis of variance were executed to understand the interaction of independent variables and their effect on the conversion. The optimum solution of the maximum conversion of 78.2% in a 180 minute was obtained in presence of US horn at parameters viz temperature (373 K), alcohol to acid ratio (2), duty cycle (80 %) and ultrasound power (100 watt). The intensification by US horn was compared to conventional processes. All inclusive, the intensification using ultrasound helped to establish the optimum conditions.

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Multicomponent synthesis of triazolo quinolines and triazolyl benzamide derivatives using magnetically separable copper oxide nanoparticles

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## **Abstract Category**

New catalytic routes And processes

## Abstract

Triazole moieties and their derivatives are widely used heterocycle compounds as medicinal agents. In this context, synthesizing triazole derivatives using earth abundant metal sources is getting more attention. Here in for the first time we report highly recoverable heterogeneous catalyst for the synthesis of triazoles based quinolines and benzamide derivatives using magnetically separable Fe3O4@piperazine@Cu2O. The material is characterized via various spectroscopy and microscopy techniques. The catalyst offers the formation of C-C and C-N bonds during synthesis along with significant yield. Characteristic studies suggest that, the product formation is due to copper catalyzed reactions of [3+2] cycloaddition followed by SNAr reaction. The piperazine act as surface additives to bind magnetic Fe3O4 and offers facile recovery using external magnet. Further studies on various substrate scope with higher yield enrich our study and proves the material reliability for triazole derivative synthesis.

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## Green Hydrogen Production: A Sustainable Pathway for Clean Energy

Prathamesh Laghane, Muneeb Patni, Pushkar Baraskar

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### **Abstract Category**

Hydrogen generation And storage

#### Abstract

The poster explores the vital role of green hydrogen in achieving a sustainable energy paradigm amid escalating climate concerns. Green hydrogen, generated via renewable-powered water electrolysis, holds significant potential for decarbonizing industrial sectors like transportation, power, and manufacturing. This presentation spotlights innovative strategies and progress in producing green hydrogen through renewable resources. The backdrop highlights current energy challenges and underscores green hydrogen's promise as a high-energy-density, multipurpose fuel for a low-carbon transition. The main focus centers on diverse green hydrogen production pathways, particularly electrolysis methods fueled by solar, wind, and hydro sources. Key enhancements in electrolyzer technology and materials are featured for optimizing both sustainability and economics. Integration aspects, including grid stabilization, energy reservoirs, and hydrogen hubs, are examined alongside successful regional pilot initiatives to underscore scalability and viability. Overcoming challenges and capitalizing on opportunities, such as cost efficiency, policy frameworks, and global cooperation, are discussed. The poster underscores research and development's pivotal role in accelerating green hydrogen's adoption, ultimately steering the energy landscape toward a more sustainable trajectory. In sum, this presentation offers a comprehensive survey of sustainable green hydrogen production using renewable resources. By showcasing technological advances, integration strategies, and global perspectives, it seeks to enrich discussions on leveraging green hydrogen as a fundamental catalyst for ushering in a cleaner, more sustainable energy era.

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# Calcination strategy to design robust automotive catalyst

Deepak Yadav1, Ramita Varshney<sup>2</sup>, Pratichi Singh<sup>3</sup>, Daniel A. Vallero<sup>4</sup>

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# **Abstract Category**

Catalysis in air pollution control

# Abstract

Co-promoted V2O5-WO3/TiO2SCR catalysts using different calcination strategies were prepared by wet-impregnation method, aiming for the SCR of NOx with Carbon monoxide and hydrocarbons in the presence of excess oxygen. Characterization techniques such as low temperature N2 adsorption, X-ray diffraction, X-ray Photoelectron spectroscopy and Scanning electron microscopy with energy dispersive X-Ray were carried out to reveal the influence of Co loadings and calcination strategies on surface properties, physical structures, valence state and acid sites of catalysts, which interpreted the result of NOx reduction in presence of O2. Among differentcatalysts,0.3Co-V2O5/WO3/TiO2 calcined by reactive calcination strategy (4.5% CO in air flowing mixture) exhibited optimal physicochemical properties which has more pore structure, larger specific surface area, higher dispersion and better redox ability. The results of O2 concentration study revealed that 5 vol% of O2 was found suitable for the NO reduction. Reactively calcined 0.3Co-V2O5/WO3/TiO2 could reach 88% NO removal efficiency at a low reaction temperature of 200°C.

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# Access to Pyrimidine Moiety via Acceptorless Dehydrogenative Strategy Catalyzed by $\delta$ - MnO<sub>2</sub> Nanoparticles and its Antimicrobial Activity Studies

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

Cost-effective and step-economic synthesis of pharmaceutically important pyrimidine derivatives was performed using single-phase  $\delta$ -MnO<sub>2</sub> NPs under external ligand-free conditions. The phytochemicals in Areca Nut Husk (ANH) extract were revealed to operate as a reducing agent for the reduction of Mn(VII) to Mn(IV) and then as a supporting agent. The synthesis of  $\delta$ -MnO<sub>2</sub> NPs with an active Mn content of 43.17% w/w was confirmed by P-XRD, FE-SEM, EDX, and ICP-OES analysis. A number of pyrimidine derivatives were synthesized in good to excellent yields under atmospheric circumstances using a one-pot multicomponent synthesis method. Control trials, hot filtration tests, gram scale synthesis, and mechanistic investigations were also discussed.  $\delta$ -MnO<sub>2</sub> NPs and pyrimidine derivatives were also tested for antibacterial efficacy against the gram-negative bacteria *E-coli*.

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## Performance evaluation of an effluent treatment plant using a life cycle assessment approach

Srisangri C, Keyur Moradiya, Sachin Jadav, Kumudini Marathe

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Abstract Category

Life cycle assessment

#### Abstract

The present study aims to assess the environmental impacts of a common effluent treatment plant (CETP) situated at Maharashtra, India using life cycle assessment (LCA). The plant comprises a primary, secondary and tertiary treatment unit along with a sludge handling division. The inventory analysis was performed using the data collected from the plant for a year and averaged and the secondary inputs were taken from GaBi 10.6 database suited for Indian context. The functional unit was assumed to be 1000 m3 treated water. The impact analysis was conducted with the help of CML 2001: Jan 2016 method. It was found that secondary treatment unit offered the highest environmental burden, and the major contributions were towards abiotic depletion potential (ADP) - fossil, global warming potential (GWP) and marine aquatic ecotoxicity potential (MAETP). Electricity was identified as a predominant factor that increased the impacts under each midpoint category. Hence, a scenario analysis was undertaken to estimate the effects of renewable energy sources on ecological hotspots associated with the processes. The impacts generated under such scenario is lower than the original observations, except for the ADP – elemental category. The study emphasizes how LCA helps in optimization of the plant and policy making.

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# Hexagonal Mesoporous Silica Supported Ni/Alumina for the Selective Conversion of Lignocellulosic Xylose into Xylitol

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#### **Abstract Category**

Catalysis in biomass conversion

#### Abstract

Supported metal catalysts have been found to have high catalytic activity due to their dispersion and higher surface areas. In this work, it was shown that a nickel-alumina catalyst supported on hexagonal mesoporous silica (HMS) can be effectively used to transform lignocellulose-derived xylose fraction to the value-added product, xylitol. HMS support was modified by the simultaneous impregnation of nickel (6 wt.%) and alumina (4 wt.%) and it was subsequently oxidized. The catalyst was evaluated for its hydrogenation ability of xylose to xylitol. Identical reactions were carried out with HMS, alumina,  $Al_2O_3$ /HMS and Ni/HMS to ascertain the activity of each moiety in the reaction. Prior to reaction, the catalyst was reduced in a tubular reactor in the presence of hydrogen. Reaction parameters such as metal loading, catalyst loading, speed of agitation, type of precursor, solvent, concentration and temperature were studied and optimized. At 130°C and 20 bar hydrogen, xylose (8.3 mmol/L) with water: isopropanol (1:1 v/v) mixture as solvent, conversion of xylose was found to be 98% with a selectivity of 97% towards xylitol. Kinetic study of the reaction was performed. The transformation of xylose to xylitol using this novel catalyst is a green process since it entails substantially lower metal loading when compared to the conventional Raney nickel catalysts, it does not involve use of noble metals such as Pt, Pd, Rh or Ru, and also does not suffer from the problem of metal leaching, making it superior to those catalysts reported yet.

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# "Green and Efficient Synthesis of Cyclopentanone through Furfural Hydrogenation Using Ni-Cu Bimetallic Catalyst on MOF-5 Support from Biomass-Derived Feedstock"

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

The incorporation of biomass-derived raw materials in the production of fuels, chemicals, and polymers has taken on a pivotal role in advancing the net zero objective. Within the realm of commercial applications, cyclopentanone is synthesized via the selective hydrogenation of furfural, a fundamental chemical component derived from lignocellulosic biomass. In this ongoing investigation, the conversion of furfural into cyclopentanone (CPO) was accomplished utilizing a bimetallic catalyst composed of transition metals nickel (Ni) and copper (Cu), immobilized onto a MOF-5 support matrix. Under conditions of 150°C and 25 bar hydrogen pressure, the 5 wt% Ni-Cu (1:1) @MOF-5 catalyst exhibited full furfural conversion and a 96% yield of cyclopentanone over a 5hour period. The incorporation of nickel and copper onto the MOF-5 structure yielded enhancements in hydro-stability, reduction potential, reinforcement of the CO bond, suppression of furan ring hydrogenation, and mitigation of the formation of a potential byproduct, tetrahydrofurfuryl alcohol (THFA). The introduction of Ni-Cu to the MOF matrix not only heightened reactant adsorption but also introduced subtle Lewis Acid sites, thereby elevating the preference for cyclopentanone formation. Extensive optimization of the procedural parameters was executed, accompanied by a comprehensive exploration of reaction kinetics and mechanisms. A detailed investigation into the virgin and recycled catalysts provided illuminating insights into the reaction pathway and selectivity. This method, serving as a blueprint for producing a valuable chemical entity, stands as an environmentally conscious, sustainable, and biobased approach.

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# Activated carbon derived from tire waste for the removal of Bisphenol from aqueous steams

<u>R Shiva Deepti<sup>1,2</sup></u>, Harsha S R<sup>3</sup>, Phyu Phyu Mon<sup>1</sup>, Phyu Phyu Cho<sup>1</sup>, Subrahmanyam Challapalli<sup>1</sup>

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# **Abstract Category**

Sustainable Engineering

# Abstract

The increased presence of endocrine-disrupting chemicals in water is a major cause of concern for the health of living organisms. Bisphenol A (BPA) is a xenoestrogen that is widely used in the manufacturing of polycarbonate and epoxy resins. BPA has a detrimental effect on human health and the aquatic environment, making it vital to remove from water. This study focuses on utilizing rubber tire waste to remove BPA since both pose a serious threat to the environment. Tire Pyrolyzed Carbon (TPC) was first subjected to activation using varying concentrations of potassium hydroxide (KOH), followed by pyrolysis at a temperature of 700 °C in an inert environment to generate Tire Pyrolyzed Activated Carbon (TPAC). The TPAC was characterized using standard approaches to assess its morphological traits and composition properties. TPAC shows a significant removal efficiency of 75 %, and it sustained adsorption effectiveness throughout a broad pH range. The adsorption of BPA by TPAC has been found to be spontaneous and involve exothermic processes, the kinetics and isotherms are best fitted for pseudo-second order (R2 = 0.99) and Langmuir-type (R2 = 0.98),

respectively. Desorption is efficient with ethanol and adsorbent capacity is notable even after fifth cycle. The findings of this research suggest that TPC has promise as a viable source material to produce activated carbon, which may be used in the removal of BPA from aqueous solution. This presentation will focus on the applications of industry waste product, pyrolyzed tyre carbon for the effective removal of a model pollutant Bisphenol-A.

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# Correlations of Glass Transition Temperature of Ionogel: A Group Contribution Method Approach

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# **Abstract Category**

Sustainable Engineering

#### Abstract

lonogels exhibit potential in driving progress within the domain of electrochemical and energy storage technologies. In this exploration, a technique is devised to determine the glass transition temperature (Tg) of ionogels. This approach entails the combination of silane and titanate with an ionic liquids belonging to the imidazolium class. The study adopts a method referred to as group contribution, where a genetic algorithm is utilized to compute parameters linked to a variety of molecular groups. These derived parameters are subsequently integrated into a non-linear regression process, facilitating the creation of predictive models for Tg. The investigation leverages 26 distinct sets of experimental Tg data, culminating in an average absolute deviation of 1.88% across the entire spectrum of data points.

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# Deciphering the Effect of Fe and Cu in Pd/C Lattice for Oxygen Reduction Reaction

Rashmi Chetry<sup>1</sup>, Rupjyoti Dutta<sup>2,3</sup>, Manash Ranjan Das<sup>2,3</sup>, Pankaj Bharali<sup>1</sup>

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#### **Abstract Category**

**Catalysis For Energy** 

# Abstract

Pd is regarded as a promising candidate for replacing Pt for ORR. The electrochemical performance and utilization efficiency of Pd in ORR will be increased by incorporating transition metals like Fe and Cu. Herein, we present a simplified synthesis method to synthesize uniformly embedded PdFeCu in the carbon support. The NPs are characterized by employing XRD, TGA, SEM-EDX, TEM, XPS, and specific surface area analyses. The ORR performances of the ECs were carried out by using CV, rotating rate-dependent LSV, chronoamperometry (CA), and accelerated durability test (ADT) in 0.1 M KOH solution. The electrochemical results reveal that PdFeCu/C exhibits higher current density, early onset potential, higher electrochemically surface area, and lower shift of E1/2 after 10,000 redox cycles.

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# COD and Color Removal from Binary Mixture of Azo Dyes at Higher Concentrations using Different AOPs: Kinetics and Toxicity Assessment

John Elisa Kumar<sup>1,2</sup>, Mihir Kumar Sahoo<sup>2</sup>

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## **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

## Abstract

The degradation efficiency of a mixture of two azo dyes, Acid Blue 29 and Ponceau Xylidine, at higher concentrations, was investigated using Fenton, Fenton-type, UV-Fenton, and UV-Fenton-type processes. In these processes, hydrogen peroxide (HP) and sodium persulfate (SPS) were used as oxidants, and Fe<sup>2+</sup> was employed as a catalyst. The reactions were conducted in both the presence and absence of UVC light to generate hydroxyl and sulfate radicals. The color and chemical oxygen demand (COD) removal efficiencies of all the systems were studied across a pH range of 3 to 11. Across all systems, the maximum removal efficiency was attained at pH 3. Notably, the highest COD removal efficiency was achieved by the UV-Fenton process, reaching 93.2% after 300 minutes of treatment. Conversely, the Fenton-type process exhibited the lowest COD removal efficiency, at 21.0% after 1500 minutes of treatment. The advanced oxidation processes (AOPs) relying on hydroxyl radicals followed a BMG kinetics model, whereas those involving sulfate radicals adhered to first-order kinetics. The toxicity of the post-treated dye mixture solution was assessed by measuring the inhibition of luminescence (light loss) in the marine bacterium *Vibrio fischeri* (*V. fischeri*) at different treatment stages using various AOPs. Ion chromatography was employed to identify different ions and intermediate products generated during the treatment processes

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# COD removal of Orange RR in homogeneous and heterogeneous oxidation systems – A comparative study

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## **Abstract Category**

**Catalysis For Water** 

## Abstract

A comparative study of homogeneous and heterogeneous catalysts has been examined by using hydrogen peroxide as the common oxidant. Fe<sup>2+</sup> as the homogeneous catalyst and Fe<sub>2</sub>O<sub>3</sub> as the heterogeneous catalyst. Fe<sub>2</sub>O<sub>3</sub> has been prepared by chemical co-precipitation method and the formation of it has been confirmed by performing various analysis such as FTIR, TEM, EDX, VSM, Raman, XRD. The concentration of catalyst and oxidant has been optimised and under the optimum parameters the degree of decolorisation in both the system is similar and raises up to the same extend i.e.,  $\approx$  98 % at 90 min of treatment period. This is due to the rapid cleavage of the azo bond during the first 10 min of the reaction followed by slow cleavage of the azo bond. Under optimal conditions, COD removal was found to be 72.8 and 96.0 % at pH 3.0 in homogeneous and heterogeneous system respectively at 300 min of treatment period. The pH for both the system was varied from 3 to 11 and the desirable pH for maximum COD removal was found to be in its acidic medium i.e., pH 3. For the heterogeneous system, catalyst reusability was performed and it was observed that the catalyst, Fe<sub>2</sub>O<sub>3</sub> can be recycled upto 2 cycles after which the COD<sub>eff</sub> drastically decreases to 7.3 % in the 4th cycle.

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# A sustainable synthesis of palladium nanoparticles supported on waste plastic derived carbon; A step towards the quantification of biothiol compound

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## **Abstract Category**

Catalytic preparation & characterization

## Abstract

Plastic pollution is widely recognized as being one of the most grievous environmental challenges. In order to tackle this problem, it is necessary to consider the reuse of plastic waste, which not only conserves energy but also diminishes the amount of plastic waste. In this respect, we report the synthesis of a new and very promising N-heterocyclic carbene-palladium nanoparticles supported on waste polyethylene terephthalate-based plastic-derived carbon material (PdNPs@PC-NHC) as a nanocatalyst and carried out numerous analytical techniques to the aforementioned material. To check its potential, the material was used to catalyse the oxidation of o-phenylenediamine (OPD) in the presence of hydrogen peroxide (H2O2). The enzymatic characteristics of the synthesized nanocatalyst were methodically examined. The obtained values of Km and Vmax for H2O2 are 4.4 mM and  $3.3 \times 10-8$  Ms-1, while OPD yielded 0.29 mM,  $0.5 \times 10-9$  Ms-1 respectively, demonstrating the significant potential as a nanozyme. Herein, the nanozyme showed exceptional sensitivity of 0.042  $\mu$ mol-1 cm-1 in the detection of the genotoxic sulfhydryl-containing mercaptoacetic acid (MAA) with a detection limit of  $3.17 \ \mu$ M. The PdNPs@PC-NHC mimic holds considerable promise for various biosensing applications due to its advantageous enzymatic characteristics.

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# Ultrasound-Assisted Esterification of Acrylic acid with Methanol using Amberlyst-15.

Vishal Khomane<sup>1</sup>, Jyothi Bandun<sup>2</sup>, Virendra Rathod<sup>1</sup>

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# **Abstract Category**

Catalysis - Prospects & Perspectives

# Abstract

Acrylic esters are versatile monomers and widely used for the production of coatings, adhesives, textiles, and plastics. Acrylic esters are mostly produced by the esterification of acrylic acid with different alcohols. In the present work, the esterification of acrylic acid (AA) with methanol to produce methyl acrylate in an ultrasound-assisted batch reactor has been studied under atmospheric pressure. Amberlyst-15 dry ion exchange resins were used as catalysts. Different parameters, such as the effect of molecular sieve, molar ratios of reactants, temperature, catalyst loading, duty cycle, and power input have been studied in the batch reactor. The comparison between conventional and ultrasound-assisted esterification shows ultrasound is more efficient and gives the highest reaction conversion. Further response surface method was employed to optimize and study the interaction between various parameters.

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# Sustainable Transparent and Bio-based Flame-Retardant Coating for Cotton Fabrics Based on Phosphorus Modified Chitosan BPS Composite.

<u>Akhil Nakhate<sup>1</sup></u>, Pradip Tekade<sup>1</sup>, Ganapati Yadav<sup>2</sup>

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# **Abstract Category**

Sustainable Engineering

# Abstract

Bio-based flame retardants are in high demand due to the increased emphasis on eco-friendly flameretardant finishing of cotton fabrics (CF). For this end, a phosphorous-modified chitosan banana pseudostem (P-CBPS) composite was fabricated on CF via layer-by-layer self-assembly. When exposed to flame, the P-CBPS coated cloth (P-CBPSC) sample preserved its original size and form; moreover, it burned with just a minor amount of smoke and did not catch fire for 3 minutes, but the fabric samples coated with BPS and chitosan [Chitosan coated cloth (CC) and BPS coated cloth (BPSC)] burned entirely within 15 seconds. Uncoated cotton cloth burned completely in 5 seconds, leaving a slight amount of black residue. The flame-retardant (FR) efficacy of a P-CBPS-coated cloth sample (P-CBPSC) was further investigated using precise flame criteria such as the limiting oxygen index test (LOI), vertical flammability test (VFT), and stability at extreme temperatures (e.g., 1500 °C). In comparison to previous work, this work describes the first-ever attempt to construct phosphorous-modified chitosan BPS (P-CBPS) via a simple, low-cost synthetic approach and has the potential to be used as a flame-retardant material for fire protection.

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

#### Yogesh Manivannan

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

As world agencies and governments are marching towards sustainability as a long-term solution, the constant need to re-invent technologies for a safer, greener world is called for. For greener synthesis, Polyethylene Furanoate (PEF) is being explored as a potential replacement for Polyethylene Terephthalate (PET), but there are several technical hindrances because of which PEFs have not yet been taken up into a full- scale commercial product. Furan Dicarboxylic Acid (FDCA) and Ethylene glycol form the monomers for PEF. In this study, the production and separation operation of FDCA was investigated. Life Cycle analysis was used to identify the environmental hotspots and mark critical areas. From the analysis, it was found that acid hydrolysis and 5-HMF synthesis has the most impact across the system. The 'Cradle to Gate' approach was applied to the LCA study. In the list of impact categories, global warming and abiotic depletion continued to be the most impactful among all. This is attributed to the complete dependence on fossil fuels as the only driver for electricity needs. A detailed comparison among different energy sources for the full production sequence is also carried out, showing the ideal way to move forward and further.

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# Modeling and Characterization of Soot Particle Formation and Growth in Methane Pyrolysis Reactor

<u>Akash Shirsath</u>, Manas Mokashi, Patrick Lott, Reihaneh Pashminehazar, Steffen Tischer, Lubow Maier, Jan-Dierk Grunwaldt, Olaf Deutschmann

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**Abstract Category** 

Catalytic reaction engineering & scale up

Abstract

Methane pyrolysis is an appealing and CO<sub>2</sub>-free process for hydrogen production and sequestration of carbon as solid material. In the present work, we have investigated the formation of soot particles in a methane pyrolysis reactor under oxygen-free conditions. The formation process was explored using a one-dimension plug flow reactor coupled with a monodisperse and method of moment model, which includes detailed chemical kinetics of Appel, Bockhorn, and Frenklach (ABF). The soot model accounts for simultaneous chemical reactions, coagulation, surface growth, and sintering. The experimental results uncovered the formation of  $C_2H_2$  and  $C_{16}H_{10}$  species, which are responsible for soot surface growth and nucleation, respectively. In particular, based on experimental and numerical results, C<sub>2</sub>H<sub>2</sub> species dominate soot particle surface growth under oxygen-free conditions. Furthermore, downstream of the hot zone, a rapid increase in soot mass was observed with a decrease in particle number concentration as the particle coagulation process overtakes the particle nucleation process. TEM and Raman spectra of collected soot samples showed that the generated soot consists of rather amorphous agglomerated primary particles with diameters around 150nm, and, DLS analysis showed a PSD ranging from 50-500nm. The soot samples comprise crystalline and amorphous domains, with the graphite-like crystalline domains typically consisting of a few turbostratically stacked graphene layers. Raman spectra and TEM images further verified these results, underscoring the need to consider solid carbon deposition reactions in future research. This detailed study provides pivotal insights into soot formation and growth, setting the stage for subsequent investigations and technological advancements.

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## Lab-on-a-chip: A Novel Analytical Device

#### Bariz Dakhni

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#### **Abstract Category**

Bioprocess engineering aspects, e.g. membrane bioreactors

#### Abstract

The Lab-on-a-Chip (LOC) platform offers a mechanism to study in vitro biochemical reactions and cellular interactions in an environment mimicking normal tissues or organs. By simulating the in vivo microarchitecture, intercellular and cell: substrate connections, and physiological milieu of tissues, the LOC approach provides a near-natural but regulated and measurable environment for biological analysis. LOC platforms are ideal for investigating cellular signaling networks, metabolic dynamics, or intricate biochemical pathways that govern health and disease. LOC takes advantage of customizable design, microfluidic architecture and advantages, and most crucially, the ability to monitor parameters in real-time. These features enable in-depth studies of drug metabolism, protein production, nutrient transport, and complex biochemical networks within an organ or tissue-specific environment. LOC embodies transformational potential as an analytical engine for understanding complicated physiological, pathological, and therapeutic events and mechanisms. Our proposal is to combine real time analytical tools with 3-D cell culture for various drug therapies due to which the pharmacodynamics and pharmacokinetics of a drug can be analyzed with precise accuracy, which will reduce the economic burden on the health care industry and give us the most accurate results that will further help us treat any disease or pandemic in less time. Indeed, an argument can be made for using LOCs as sophisticated analytical tools to bridge the gap between standard in vitro systems and the complexity of in vivo situations.

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# An analytical evaluative study of the oxidation reaction of 1-octanol with $30\% H_2O_2$ : A quantitative approach towards sustainability

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## **Abstract Category**

Catalysis - Prospects & Perspectives

## Abstract

The oxidation of 1-octanol was carried out with 30% H<sub>2</sub>O<sub>2</sub> under heterogeneous, solvent free, semibatch mode conditions using tungstic acid as catalyst. When cetyltrimethyl ammonium bromide, a cationic surfactant was used along with tungstic acid, the conversion improved and the selectivity towards octanoic acid increased. This suggests that the transfer of the peroxo anion across the liquid-liquid interface is the rate limiting step, which indicates mass transfer accompanied with chemical reaction. The oxidation of 1-octanol with 30% H<sub>2</sub>O<sub>2</sub> under heterogeneous conditions, was studied using sodium molybdate as a catalyst and tetra butyl ammonium bromide as a PTC. The effect of pH, studied at 70°C revealed that, 1-octanol is being consumed in ester formation even when the reaction is conducted at neutral pH. No conversion of 1-octanol was observed in the absence of PTC even at  $80^{\circ}$ C. At  $80^{\circ}$ C the selectivity towards esterification increases while at  $40^{\circ}$ C the selectivity towards the aldehyde increases. The organic phase was quantitatively analysed for the 1-octanol, 1-octanol and octanoic acid simultaneously by Gas Liquid Chromatography. The ester formed and the  $H_2O_2$  in the aqueous phase were estimated by titrimetry. The material balance was established. Heterogeneous, oxidation and esterification reactions involving mass transfer accompanined with chemical reaction may lead to runaway reactions due to the heat effects associated with the multiple reactions involved. In order to gain an insight into the manner of 1octanol consumption and product distribution, the present quantitative study has been undertaken, which is a first step towards achieving sustainability in chemical processes.

# **Upload Extended Abstract File**

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# Efficient microwave-assisted synthesis of diphenolic acid from bio-renewable levulinic acid and phenol using mesoporous silica-supported modified heteropoly acid

Rohitkumar Singh, Ganapati Yadav

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#### **Abstract Category**

Catalysis in biomass conversion

#### Abstract

In recent years, the widespread use of bisphenol A (BPA) in polycarbonate plastics and epoxy resins has raised serious concerns due to its potential health hazards, including hormone disruption and an increased cancer risk. Diphenolic acid (DPA) has emerged as a promising candidate due to its structural similarity to BPA, making it a potential replacement in manufacturing processes. This research paper presents a novel approach for DPA synthesis using a solid acid-catalyzed, microwave-assisted method with the Rb<sub>0.5</sub>Cs<sub>2.0</sub>H<sub>0.5</sub>PW<sub>12</sub>O<sub>40</sub>/MCF catalyst. The method offers a solvent-free and efficient process, with a comprehensive investigation of various reaction parameters to optimize yield and selectivity. Under the optimized conditions, an impressive 86.5% conversion of levulinic acid occurs within 4 h, with over 80% selectivity for the desired P, P'-DPA product. The Rb<sub>0.5</sub>Cs<sub>2.0</sub>H<sub>0.5</sub>PW<sub>12</sub>O<sub>40</sub>/MCF catalyst shows outstanding reusability for up to 4 cycles, with minimal reduction in activity and selectivity, supported by various characterization techniques. The kinetic modeling reveals the reaction follows the Langmuir-Hinshelwood-Hougen-Watson (LHHW) mechanism with a second-order reaction, and the activation energy of 10.17 kcal/mol. This study provides a new insight in production of diphenolic acid (DPA) with enhanced efficiency, selectivity and sustainability.

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# Catalytic reductive amination of biomass-derived furfural to furfurylamine using Co supported over hydroxyapatite catalysts

Yogita Yogita<sup>1,2</sup>, P. Mahesh Kumar<sup>1,2</sup>, G. Hariyanandam Gunasekar<sup>1,2</sup>, Nakka Lingaiah<sup>1,2</sup>

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# **Abstract Category**

Catalysis in biomass conversion

# Abstract

In this study, cobalt-supported hydroxyapatite (HAP) catalysts were synthesized by the coprecipitation method to study the reductive amination of biomass-derived furfural to furfurylamine. The synthesized catalysts were characterized through different techniques such as XRD, SEM, XPS, NH<sub>3</sub>-TPD, CO<sub>2</sub>-TPD, FT-IR and HR-TEM to attain their structural properties. As prepared catalysts were tested for catalytic reductive amination of furfural at 110 °C under 1 MPa of H<sub>2</sub> pressure. The catalyst with 7Co/HAP exhibited 100% conversion of furfural with >97% selectivity to furfurylamine in 0.5 h of reaction time. The catalytic activity depended on the Lewis acid-basic properties, metalsupport interaction and presence of enough Co<sup>0</sup> species. The catalysts are easy to separate and reusable with consistent activity.

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# Lanthanum-MOF-Catalyzed Borylation of Alkyl Halides withBis(pinacolato)diboron

Kiran Patil, Shubhankar Bose, Ramesh Bhawar

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#### **Abstract Category**

New catalysis routes

#### Abstract

Organoboranes are a class of vital organic intermediates in a variety of organic transformations.1 In recent years, transition-metal-catalyzed organoborane synthesis has been influentially explored via hydroboration, C-X borylation, diboration, and C-H borylation processes.1-6 However, these methodologies have certain drawbacks, such as necessity of inert atmospheres, contamination of metals in the products and lack of recycling of catalysts and ligands. Therefore, recyclable metal catalyst system has attracted much attention recently. During last decade recyclable MOF supported transition-metal-catalyzed organoborane synthesis is offering great potential to build a diverse array of organoborane derivatives.2 Homoleptic rare earth metal complexes were well explored for hydroboration of carbonyl groups and alkenes.4 However, till date there is no report on rare-earth metal–organic frameworks-catalyzed borylation of alkyl halides. Herein, we report a highly efficient and recyclable easy to synthesise La-metal organic framework catalyzed e f f i c i e nt borylation of alkyl bromides with B2pin2 under mild reaction conditions.7 Key results will be described

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# CeO<sub>2</sub>-modified Oxygen Vacancy-rich Co $_3$ O $_4$ on Graphene Nanoplatelets for Enhanced Oxygen Reduction and Evolution Reaction.

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# **Abstract Category**

Catalysis For Energy

# Abstract

Herein, we have synthesized three graphene nanoplatelet (GNP) supported catalysts viz.  $Co_3O_4/GNP$ , CeO<sub>2</sub>/GNP and Co<sub>3</sub>O<sub>4</sub>/CeO<sub>2</sub>/GNP. A comparative analysis of their electrochemical activities towards oxygen reduction and evolution reactions (ORR, OER) was carried out in 0.1M KOH using a 3electrode system (Pt wire as counter electrode and Ag/AgCl in 3M KCl as reference electrode). The study reveals that the mixed oxide Co<sub>3</sub>O<sub>4</sub>/CeO<sub>2</sub>/GNP generates higher geometric current density (-6.10 mA cm<sup>-2</sup>) for an equal loading of catalyst. The catalyst was also active towards OER which makes it a bi-functional one. This enhanced electrochemical activity of  $Co_3O_4/CeO_2/GNP$  could be attributed to the generation of a  $CeO_2 | Co_3O_4$  heterogeneous interface. Alteration of local coordination of Co ions in the Co<sub>3</sub>O<sub>4</sub> crystal structure is observed in presence of CeO<sub>2</sub>. XPS reveals large quantity of oxygen vacancies in the mixed oxide catalyst Co<sub>3</sub>O<sub>4</sub>/CeO<sub>2</sub>/GNP. XANES of Co K-edge reveals higher average oxidation state of Co atoms in  $Co_3O_4/CeO_2/GNP$  than in  $Co_3O_4/GNP$ . The facile redox couple Ce<sup>3+</sup>/Ce<sup>4+</sup> renders faster movement of electrons via defect oxygen vacancies in crystal structure of the  $Co_3O_4$  unit in  $Co_3O_4/CeO_2/GNP$ . However, EXAFS show no significant change in the bond lengths of first shell Co–O and Co–Co in Co<sub>3</sub>O<sub>4</sub>/CeO<sub>2</sub>/GNP when compared to Co<sub>3</sub>O<sub>4</sub>/GNP. The study provides insightful understanding into the role of CeO<sub>2</sub> in enhancing electrocatalytic activity of Co<sub>3</sub>O<sub>4</sub>.

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# Doped titania nanoparticles for degradation of pharmaceutical drugs.

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#### **Abstract Category**

**Catalysis For Water** 

# Abstract

Nanoparticles are the main source of many nanostructured devices or materials; nanoparticles are regarded as being vital for nanotechnology. Nanomaterials can be created, obtained naturally, or discovered accidentally. One of the few nanomaterials with significant applications in numerous fields of research and innovation is metal oxide nanoparticles (NPs). Due to its physicochemical characteristics and adsorption ability, hydrotalcite is regarded as an effective adsorbent. Hydrotalcite is a porous substance with many hydroxyl groups on its surface, making it a great dispersion for nanoparticles. These nanoparticles have made major contributions, particularly in the biomedical and photocatalysis domains. In this study, I am attempting to study the synthesis of metal oxide nanoparticles ( $TiO_2$ , doped  $TiO_2$ ), characteristics, and applications for photocatalytic degradation of medicines (Paracetamol, Ibuprofen, & Salicylic Acid) contained in wastewater from the pharmaceutical industry. One environmentally friendly, sustainable technology that can offer a better answer is photocatalysis. Due to its excellent chemical stability, high photoreactivity, low cost, and accessibility, TiO<sub>2</sub> is a commonly used photocatalyst. However, because of its large bandgap, it loses effectiveness when exposed to sun radiation. This article includes the manufacture of  $TiO_2$ catalysts as well as various techniques for improving photocatalytic efficiency. Its use as a highly effective photocatalyst has been made possible by the catalyst's unique structural characteristics and several functionalities. The potential of  $TiO_2$ , and doped  $TiO_2$ , as a catalyst in the synthesis of chemicals is also being understood and examined.

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# Dextran Production from Pineapple Waste Extract using *Leuconostoc mesenteroides* NCIM 2198: Integrated Optimization, Structural Characterization and Growth Kinetics

# Ashutosh Tripathy, Mukesh Kumar Patel, Snehasis Chakraborty

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#### **Abstract Category**

Fermentation processes

#### Abstract

This study explores the potential of dextran, a glucose-based homopolysaccharide with biocompatibility and versatile, functional attributes, in various food applications. Dextran acts as a cryoprotectant, thickener, stabilizer, and prebiotic, enhancing nutritional, textural, and probiotic effects. Comprising  $\alpha$ -1-6-linked linear glucose units and  $\alpha$ -1-3-linked branches, with occasional  $\alpha$ -1-2 or  $\alpha$ -1-4 bonds, dextran is extracellularly produced by bacterial species like *Leuconostoc* and Weissella through dextransucrase enzyme mediation. Dextran from Weissella confusa displays favorable dissolution properties and metabolic benefits. Commercial dextran production primarily employs Leuconostoc species through sucrose fermentation. The underexplored potential of pineapple waste, abundant in fermentable sugars, is examined as a substrate for dextran fermentation. This study aims to optimize fermentation conditions and media components using Response Surface Methodology to achieve maximal dextran production by *Leuconostoc* mesenteroides NCIM-2198. Gel permeation chromatography, Fourier transform-infra-red spectroscopy, nuclear magnetic resonance spectroscopy, and scanning electron microscope analyses contribute to characterizing the produced exopolysaccharide. Results indicate that under specific temperature conditions, initial pH, sucrose concentration, and culture volume, L. mesenteroides achieves a maximum dextran yield of 1.47 g·[100 mL]<sup>-1</sup>. Statistical models offer insights into the interaction between variables affecting dextran yield. Logistic and Gompertz equations demonstrate a strong fit with experimental data, reflecting growth kinetics, while FTIR confirms the presence of functional groups. GPC reveals a high molecular weight (Mw 203.1 kDa), and NMR elucidates structural details. This research underscores the potential of pineapple waste as an eco-friendly, cost-effective dextran source and enhances our understanding of the production dynamics, opening pathways for efficient industrial applications.

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# Determination of stability and activity of immobilized lipase for transesterification reaction in fluorous solvent and deducing the reaction mechanism by molecular docking study

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#### **Abstract Category**

Enzyme immobilization & stabilization, particularly in non-conventional media

#### Abstract

The objective of the present study was to immobilize lipase and use it for transesterification reaction in a fluorous solvent. Polymeric substance tylose (Tyl) was chosen as immobilization support. Tylose immobilized lipase from *Candida rugosa* (CRL) was subjected to fluorous solvents treatment and was found most stable in perfluorooctane (PFO). The immobilized Tyl-CRL was characterized for protein loading, solvent stability, surface morphology, restoration of secondary structure, and thermal stability. Immobilized CRL was further applied for the synthesis of phenethyl propionate in a fluorous solvent. All reaction parameters were optimized using the response surface method (RSM). Optimized reaction parameters were substrate ratio 1:3, immobilized lipase quantity 30 mg, and temperature 45°C. Prepared biocatalyst was evaluated for recyclability, and it was found that catalytic activity decreased by 77% up to the fifth recycle run. The optimized synthesis protocol scope was checked to synthesize various flavoring esters. The molecular-level interactions of substrate and lipase were studied using docking.

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# Investigating the Role of Co and Fe in Bimetallic Perovskite Catalysts (LaNiO<sub>3</sub>) for Steam Reforming of Bio-Oil Model Oxygenates: A DFT Study.

<u>Akanksha Goyal</u><sup>1</sup>, Piyush Pratap Singh<sup>1,2</sup>, Tarak Mondal<sup>1</sup>

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#### **Abstract Category**

Computational catalysis

#### Abstract

The world's energy needs require sustainable alternatives to finite and harmful coal and petroleum. Hydrogen offers a clean and efficient solution, outstripping petroleum's calorific value. Yet, current hydrogen production relies on non-renewable methane steam reforming, necessitating more sustainable options. In this context, bio-oil derived from agricultural waste emerges as a strong contender. This study delves into catalytic bio-oil steam reforming to produce hydrogen, focusing on its advantages over other methods. Catalyst selection is a crucial determinant of success in this process, and researchers have explored various avenues, including bimetallic catalysts and perovskite catalysts with unique crystal structures. While experimental studies have affirmed the potential of bimetallic perovskite catalysts, the molecular interactions between complex bio-oil components and these catalysts remain less explored. To address this, Density Functional Theory (DFT) is employed to gain deeper insights into these interactions. The study uses DFT methods to investigate the bio-oil model oxygenates' adsorption on a perovskite catalyst. Substituting transition metals such as Co and Fe within a LaNiO<sub>3</sub> (001) cubic crystal surface examines the bimetallic effect.  $LaNi_{0.8}Co_{0.2}O_3$  displays the optimal binding of molecules among the catalysts. The study also sheds light on carbonaceous specie's role, like CH, in the reaction mechanism, indicating their significant contribution to carbon deposition. In conclusion, the research underscores the stability of adsorption and the potential of bimetallic perovskite catalysts, particularly LaNi<sub>0.8</sub>Co<sub>0.2</sub>O<sub>3</sub>, in enhancing the efficiency of bio-oil steam reforming for hydrogen production. These insights align with experimental observations and contribute to advancing sustainable energy solutions.

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# Alkylation of phenols and thiophenols with various alkenes using solid acid resin catalysts

<u>Prerana Masurkar</u><sup>1</sup>, Pravin Jadhav<sup>2</sup>, Sunil Mokashi<sup>2</sup>, Shirish Naik<sup>2</sup>, Manoj Bhandari<sup>2</sup>, Dinesh Mandhana<sup>2</sup>, Bhalchandra Bhanage<sup>1</sup>

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# **Abstract Category**

Catalysis - Prospects & Perspectives

# Abstract

Catalysts are required for important organic processes to be employed industrially or academically. In this aspect, ion exchange resin catalysts surpass typical inorganic catalysts, particularly regarding product separation from the reaction media, recycling, and recycling. Ion-exchange resins are solid acid heterogeneous catalysts that play a vital role in many advantageous reactions such as

alkylation, esterification, etherification of olefins with alcohols, dehydration of alcohols to olefins or ethers, olefin hydration, and ester hydrolysis. Alkylation is the transfer of an alkyl group from one molecule to another, and it is one of the most significant catalytic processes in the chemical industry since it is widely used in industries such as fuels, cleaning products, and pharmaceuticals. Strongly acidic ion-exchange sulfonic acid resins have been extensively exploited as recyclable acid catalysts for organic syntheses in laboratory and industry since they became commercially available. Among the various solid acid catalysts investigated, ion exchange resins have attracted much attention because of their suitable ion exchange capacity, regeneration, reuse, and simplified product recovery and reduction of undesirable waste streams. We have studied the alkylation of phenol and thiophenol with various alkenes to produce alkyl phenol and alkyl thiophenol using Thermax supplied TULSION T-6813 MP catalyst. Catalyst is inexpensive, efficient, and recyclable. Higher yields of desired products within a short reaction time under solvent-free conditions were obtained. It was found experimentally that the TULSION T-6813 MP gives the best performance for the alkylation of phenol and thiophenol.

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# Ground granulated blast furnace slag-supported biochar composite material for adsorption of 4-Nitrophenol

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# **Abstract Category**

Sustainable Engineering

# Abstract

Water pollution is a significant global challenge resulting from the release of industrial effluents, anthropogenic activities, and natural processes. The use of non-conventional and cost-effective materials has garnered significant interest in the field of wastewater treatment owing to their application in adsorption. The crux of this investigation is to synthesize different composites of GGBS-supported biochar from sawdust and sewage sludge for the removal of model water pollutant 4-nitrophenol. The composite adsorbent was thermally activated at 700 °C in an inert atmosphere. The activated adsorbent was characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and point of zero charge (PZC) analysis. A composite material comprising GGBS, wood sawdust, and sludge exhibits enhanced adsorption efficiency. The kinetics and isotherm analyses were conducted, and it was determined that the second-order model and Langmuir isotherm model exhibited superior fitting. The influence of pH on adsorption reveals that neutral pH conditions exhibit a higher degree of dominance in adsorption compared to acidic and basic pH levels. The thermodynamic analysis indicates that the process of adsorption exhibited spontaneity and was exothermic in nature. The findings of this study show potential for biochar driven by sawdust and sludgesupported GGBS as a feasible source material for low-cost adsorbents that may be utilized to remove 4-nitrophenol from an aqueous solution. This presentation will concentrate on using industrial and household waste-based adsorbents for the removal of 4-nitrophenol.

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#### Kinetics of solid-liquid-liquid oxidation of 4-Methylanisole to p-anisaldehyde

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#### **Abstract Category**

Catalytic reaction engineering & scale up

#### Abstract

Oxidation of aromatic compounds produces chemicals and intermediates useful in pharmaceuticals, perfumes, and agrochemicals. Liquid-phase oxidation is preferred over gas-phase oxidation due to its compact nature. The product of selective liquid-phase oxidation of substituted toluene is usually aldehyde. The aldehyde so formed has a tendency to get oxidized further to acid. Here, we have studied the engineering aspect of the kinetics of the selective oxidation of 4-Methylanisole to p-anisaldehyde along with the effect of various parameters such as agitation, solid loading using MnO<sub>2</sub> as the reagent, reaction time, temperature, substrate concentration, and sulfuric acid concentration on the rate of reaction. The mechanism of interaction between mass transfer and chemical reaction was investigated. We have also discussed two plausible mechanisms for the selective oxidation of 4-Methylanisole. In addition to the above, we have obtained the rate equation for the overall reaction, which will help in industrial-scale reactor design. As a result, the kinetic model for this reaction was developed.

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# Evaluating Environmental Sustainability: A Cradle-to-Grave Assessment of Sodium-Ion Battery Cathode Material

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#### **Abstract Category**

Life cycle assessment

#### Abstract

As the global demand for sustainable energy storage solutions intensifies, sodium-ion batteries (SIBs) have emerged as a promising alternative to conventional lithium-ion batteries. However, to ensure their viability within the context of environmental sustainability, a thorough cradle-to-grave assessment is imperative. [1] This research paper presents a novel and streamlined approach to conducting a comprehensive environmental assessment of SIBs Cathode Active Material (CAM) throughout their lifecycle. The proposed methodology integrates Life Cycle Assessment (LCA) principles with advanced analytical tools, enabling a holistic evaluation of the environmental impacts associated with CAM production, use, and disposal. By carefully considering the extraction and processing of raw materials, manufacturing processes, energy consumption, transportation, and end-of-life management, the environmental footprint of can be accurately quantified. By leveraging existing databases and models, the research minimizes the need for redundant data generation, thus optimizing time and resource utilization. [2] Moreover, sensitivity analyses are employed to identify key parameters influencing the overall environmental performance of CAM, aiding in pinpointing areas for improvement. The findings of this research provide valuable insights into the environmental advantages and potential challenges associated with the adoption of CAM. By presenting a concise yet rigorous assessment framework, stakeholders can make informed decisions regarding energy storage choices, fostering the transition towards a more sustainable energy landscape. This paper contributes to both the academic discourse and industry practices by demonstrating an effective means of evaluating emerging technologies' environmental impacts, ultimately paving the way for the wider integration of sodium-ion batteries in future energy systems.

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### **RL – DDPG Based Temperature Control of Fermentation Bioreactor for Ethanol Production**

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#### **Abstract Category**

Fermentation processes

#### Abstract

This article introduces a methodology for the modelling and control of the temperature in a bioreactor used in the production of ethanol, using reinforcement learning (RL) approaches. The bioreactor plays a crucial role in a wide range of industrial applications, including but not limited to pharmaceutical manufacturing, biofuel generation, and wastewater management. The control of the bioreactor is of utmost importance in order to maximize the efficiency of the production process and maintain the optimum temperature. RL controllers acquire optimum control policies by iterative experimentation within an agent-environment framework, without the need for complex models. The strategies used for training the controller in this study are deep Q-network (DQN) and deep deterministic policy gradient (DDPG). The performance of these agents/controllers is assessed by using the integral squared error (ISE) and integral absolute error (IAE) metrics. The controller based on the Deep DDPG algorithm demonstrates superior performance in terms of ISE and IAE when compared to the DQN.

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# Synthesis and characterizations of P(DADMAC-co-AM) cationic copolymeric surfactant and their application in hair care formulation

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#### **Abstract Category**

Production of fine chemicals & chiral products

#### Abstract

The current investigation involved the synthesis of a cationic polymeric surfactant, namely poly(diallyl dimethyl ammonium chloride-acrylamide) P(DADMAC-co-AM), through free radical aqueous solution copolymerization of two monomers possessing vinyl functionality: diallyl dimethyl ammonium chloride (DADMAC) and acrylamide (AM). The study focused on exploring and optimizing reaction variables, including monomer mole ratio, initiator type and concentration, temperature, and reaction time, to control the copolymerization extent. Optimal conditions were identified as employing DADMAC and AM monomers in a 20:80 molar ratio, with 0.5% 2,2'-azobis(2methylpropionamidine) dihydrochloride as the initiator, at 70°C for 5 hours, yielding the cationic copolymer with a viscosity of 18,436 cp, Mn of 15,936 Da, and a polydispersity index of 1.42. The synthesized P(DADMAC-co-AM) structure was characterized using FTIR and PNMR spectrophotometers. Zeta potential and conductivity analyses were conducted on the monomers and the copolymer to confirm the colloidal stability of P(DADMAC-co-AM)solutions. The surfactant activity of this copolymer cationic surfactant was assessed comparatively against similar copolymer and homopolymer cationic surfactants. Furthermore, the practical application of P(DADMAC-co-AM) as a conditioner in hair care formulations for wet hair was demonstrated by formulating a conditioning shampoo and evaluating its characteristics, including surface activity, physicochemical attributes, and rheological properties, in comparison to a control sample.

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# Synthesis and Characterization of g-C3N4 and boron-doped B-gC3N4 for photoelectrocatalytic water splitting

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# **Abstract Category**

**Catalysis For Energy** 

# Abstract

Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) has gained recognition as a photocatalyst owing to its distinctive electronic structure, narrow bandgap of approximately 2.7 eV, high stability, large surface area, non-toxic nature, and cost-effectiveness. Notably, its bandgap of 2.7 eV is conducive to harnessing a broad spectrum of light, rendering it particularly effective for solar-driven processes. Thermal polymerization for synthesizing both pristine g-C<sub>3</sub>N<sub>4</sub> and boron-doped B-gC<sub>3</sub>N<sub>4</sub>. This approach introduces boron into the g-C<sub>3</sub>N<sub>4</sub>, enhancing light absorption properties, and faster charge transport dynamics. The incorporation of boron serves good photocatalytic potential of the material, enabling it to efficiently harness and channel incident light energy.

The synthesis and subsequent characterization of  $g-C_3N_4$  and  $B-g-C_3N_4$  are conducted through analysis techniques, including X-ray diffraction (XRD), Raman spectroscopy, and Fourier-transform infrared (FT-IR) spectroscopy. The purity of the  $g-C_3N_4$  and  $B-gC_3N_4$  phases, as well as their structural composition, was verified through these techniques. Notably, XRD data reveals distinctive peak

shifts in the case of B-gC<sub>3</sub>N<sub>4</sub>, in comparison to pristine g-C<sub>3</sub>N<sub>4</sub>, corroborating the successful incorporation of boron. The morphological study was also done by scanning electron microscopy. Anchoring the findings, photoelectrochemical (PEC) measurements give insights into the behavior of the materials under illumination. These tests unravel the innate nature of the materials, revealing essential parameters such as photocurrent density and transient responses. Through PEC measurements, the materials' efficiency for solar water splitting is studied to uncover their applicability in this environmental friendly process. Ultimately, the study serves as a straightforward yet scalable synthesis approach for g-C<sub>3</sub>N<sub>4</sub> and its boron-doped variant, B- g-C<sub>3</sub>N<sub>4</sub>.

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# Enhanced COD Reduction in Kitchen Wastewater through Electrooxidation using PbO2-coated graphite electrodes synthesized by the sono-electrochemical deposition method

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**Abstract Category** 

**Catalysis For Water** 

# Abstract

The potential of the electrochemical oxidation (EO) in the mineralisation of high-refractive organic compounds finds more attention in wastewater treatment. This work explores the comparative study of the electrooxidation of kitchen wastewater (KW) using graphite and PbO2 - coated graphite electrodes synthesised by the sono-electrochemical deposition method. The important operating parameters, such as current density, electrolyte concentration, electrode distance and pH, were optimised by examining the COD reduction. A maximum of 96% COD reduction was achieved by PbO2 coated graphite electrode at the optimum current density, electrolyte concentration, electrode distance and pH of 0.75A/dm2, 1.5g/L, 2cm, and 3, respectively. This result demonstrated that the PbO2-coated graphite electrode exhibited an improved COD reduction compared to the graphite electrode by enhancing the generation of reactive oxidizing agents. Also, the PbO2 coating remains stable and durable during the entire electrooxidation cycle. Overall the finding of the study highlights the effectiveness of PbO2 -coated graphite electrodes as promising for the degradation of refractory compounds in wastewater.

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# Synthesis of Transition Metal Oxides Nanomaterials and its Applications in Degradation of Pharmaceuticals

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# **Abstract Category**

**Catalysis For Water** 

# Abstract

Doped semiconductor nanostructures (NSS) have attracted highlighted a promising avenue for an extensive amount of interest as a potential for green, sustainable, and efficient photocatalysis processes. Using a wet chemical technique, magnesium (Mg)-doped zinc oxide (ZnO) nanoparticles (NPs) (MgxZn1-xO (x = 0, 1, 2.5, 5%) have been synthesized and were exhibit improved efficiency compared to pure ZnO. their photocatalytic performance of rapid photodegradation of salicylic acid (SA) and paracetamol (PA) under the illumination of solar light is investigated. The doping of mg2+ and drug degradation. Among previously reported photocatalysts for this process, 5% Mg-ZnO demonstrated outstanding photocatalytic performance. At the optimum condition, without the use of oxidizing agents or additives, 100 mg of salicylic acid and 100 mg of paracetamol in 5% Mg-ZnO demonstrated 100% photodegradation efficiency of 10 ppm of 100 mL of pharmaceuticals after 120 and 180 minutes, respectively. The reusability of these nanoparticles was additionally excellent, with a 97% rate in the fifth cycle.

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A comparative study on sustainability of rice straw lignocellulosic biomass pretreatment for the removal of lignin

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

Mild and effective pretreatments are needed to break down lignocellulosic biomass to obtain lignin for value-added products. This study assessed the effects of hot liquid water, dilute acid, and alkali peroxide pretreatments on the lignocellulosic composition of rice straw. Various process parameters affecting pretreatment were optimized by adopting a Taguchi design. The parameters studied in this work were solid/liquid(S/L) ratio(1:10, 1:15 and 1:20), H2SO4concentration(1%,3%, 5%), Time (30 to 180 min), NaOH Concentration (8 -12%), hydrogen peroxide concentration (8-12%) in terms of lignin removal. Physico-chemical changes of the raw and pretreated rice straw were evaluated by scanning electron microscopy (SEM). Under an optimal condition (15% of S/L ratio and 60 min for hot liquid water pretreatment, 5% of H2SO4, 10% of S/L ration and 30 min for dilute acid treatment, 12% of NaOH,12% of H2O2 and 10 % of S/L ratio for alkali peroxide pretreatment), 66.6%, 16.6% and 63.8% of lignin removal was achieved. The results of this study demonstrate the potential of hot water pretreatment as an effective chemical-free method for the removal oflignin from rice straw.

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# A Sustainable Approach for Soil Amendment using Coal Gasification Waste and Organic Fertilizers: Comparative Studies on the Growth and Development of Okra

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# **Abstract Category**

Sustainable Engineering

# Abstract

Our planet is struggling with many environmental problems which is primarily due to the evergrowing size of the population which on the other side has increased food demand exponentially. The consequence of such a large demand for food is excessive fertilization of soils, often in an uncontrolled manner. The paper presents a comparative overview of the different types of sustainable soil amendment approaches by using coal gasification waste as well as other organic amendments in the form of vermicompost and vermi-effluent. The use of these soil amendment approaches has led to the better growth of okra with banana vermicompost giving the best results in terms of various properties such as plant growth parameters, fruit yield etc. On the other hand, the coal gasified char which till now is considered as a waste has also been successfully implemented for soil amendment owing to its high porous nature thereby increasing the soils capacity to hold more water and also increasing the soils organic carbon content and its effect has been successfully seen in okra plant growth. These types of sustainable soil amendments contribute to a significant reduction in the consumption of commercial inorganic fertilizers, and thus less pollution of the natural environment.

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# EXTRACTION OF FEED STOCK GRADE TIO2 & OTHER OXIDES FROM TITANIFEROUS BAUXITE RESIDUES (RED MUD) OF INDIA

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#### **Abstract Category**

Catalytic reactions in which wastes are converted to useful products

#### Abstract

- The Red Mud (Bauxite Residue) produced by Bayer's Process poses great disposal as well as environmental issues. However some of the Indian Red Muds, especially the Red Muds produced at Renukoot & Muri Refinery of HINDALCO has a great commercial potential as it contains 17 to 19% TiO2 (highest % of TiO<sub>2</sub> found in Red Mud produced anywhere in the world)
- In this process such Titanium rich Red Mud is first subjected to HCl leaching due to which the oxides of Aluminium, Iron, Sodium, Calcium etc. present in the Red Mud get converted in to their respective soluble chlorides & the Titanium di-oxide (TiO2), Vanadium Pentaoxide (V2O5), Silica (SiO2) & REOs (Rare Earth Oxides) being insoluble in HCl get separated as Residue.
- 3. The Residue now contains 55 to 65% TiO2. The Residue is further subjected to 2 more stages of refining to get Feed Stock Grade TiO2 having 88 to 95% TiO2 content.
- 4. The filtrate obtained after Acid Leaching in 1st step contains mainly AlCl3 & FeCl3 is taken to ARP (Acid Regeneration Plant) to get a mixture of Al2O3 & Fe2O3 & the regenerated HCl is used again for leaching in step 1.
- 5. This mixture of Al2O3 & Fe2O3 is then subjected to Alkali Leaching during which Al2O3 gets converted to water soluble Sodium Aluminate (NaAlO2) & Fe2O3 being insoluble settles down. The Sodium Aluminate (NaAlO2) on hydrolysis gives Al(OH)3 which on calcination gives pure Al2O3. Fe2O3 obtained is also pure & used for making Red Oxide Pigment.

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# Impact of Tetrabutylammonium Bromide-Based Deep Eutectic Solvent on the Kinetic Hydrate Inhibition of Methane Hydrate: Experiment and Modeling

<u>Pratham Shah</u><sup>1</sup>, Rahul Sarkhel<sup>2</sup>, Papu Kumar Naik<sup>3,4</sup>, Jitendra Sangwai<sup>2</sup>, Tamal Banerjee<sup>3</sup>, Debashis Kundu<sup>1</sup>

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# **Abstract Category**

Sustainable Engineering

# Abstract

Deep eutectic solvents (DESs) are being considered as potential replacements for ILs, possessing similar attributes. In this investigation, a deep eutectic solvent (DES) is studied as a modern solution for inhibiting methane gas hydrate formation. Here, tetrabutylammonium bromide and ethylene glycol based DES is condsidered, representing a fresh approach to kinetic hydrate inhibition. The dominant interactions driving the formation of DESs play a pivotal role in completely altering the chemical behavior of the system, resulting in delay of hydrate formation. Ultimately, the research

estimates variables including the gas quantity consumed during hydrate formation, the rate at which hydrates form, and the conversion of gas and water into hydrate. Furthermore, the model developed by Klauda and Sandler is employed to forecast the phase equilibrium information for DES based methane hydrate. The projected model aligns well with the empirical data, exhibiting an average absolute deviation (AAD%) of under 7.5%.

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# Hydrogenation and hydrodeoxygenation of biomass-derived oxygenate to liquid products for use as transportation fuels.

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#### **Abstract Category**

**Catalysis For Energy** 

#### Abstract

The decline in fossil fuel reserves and growing concerns about greenhouse gas (GHG) emissions have prompted a quest for alternative, sustainable energy sources. Biomass, an eco-friendly resource, has emerged as a promising material for generating liquid transportation fuels. The primary approach for creating alkanes as transport fuel from biomass involves a series of steps. Initially, carbohydrates are utilized to produce foundational compounds like cellulose and hemicellulose. Carbon-carbon chain elongation processes using acid or base catalysts are employed to establish the carbon structure. Subsequently, hydrodeoxygenation with metal and acid catalysts is used to eliminate oxygen atoms. This study delves into the hydrogenation and hydrodeoxygenation of furfuryl alcohol oligomers to produce viable liquid transportation fuels. The discussion revolves around a single-process, two-step method: acid-catalyzed self-condensation of furfuryl alcohol followed by hydrodeoxygenation to yield liquid products. The research explores the synthesis of a bifunctional catalyst (5% w/w Ni - 20% w/w Al0.66DTP/MCF) possessing highly active acidic and metal sites tailored for the required reaction system. The optimization of reaction conditions for converting furfuryl alcohol is addressed, encompassing temperature, pressure, catalyst selection, and hydrogen feed rate. A variety of heterogeneous catalysts were evaluated for their efficacy in transforming furfuryl alcohol into oligomers, subsequently undergoing hydrogenation to form fuel fractions. All experiments were conducted within an autoclave reactor. To characterize the catalyst, techniques such as XRD, SEM-EDS, BET, FTIR, and XPS were employed to elucidate the interaction among these bimetallic nanoparticles.

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### Insight into Selective Hydrogenation of Eugenol to 4-Propyl Phenol

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

The sustainable production of fine chemicals and fuels from renewable resources is an important process in the current materials and energy crisis scenario. The selective hydrogenation of eugenol into 4-propyl phenol is an attractive transformation to advance the sustainable synthesis of important chemicals. In this study, alumina, titanium nanotubes, SBA-15, and MCM-41 were used to support Ni, Co, Cu, Cr, and bimetallic Ni-Co (with 20% nominal metal loading) and tested for the hydrogenation of eugenol, using isopropyl alcohol as a solvent. The hydrogenation of eugenol was carried out in an autoclave reactor at 225oC using a non-noble catalyst. The effects of the concentration of eugenol, hydrogen pressure, catalyst loading, and temperature on conversion and selectivity were studied. It can be concluded that eugenol was first hydrogenated to 4-propyl guaiacol which then underwent simultaneous demethylation and aromatic ring hydrogenation to form 4-propyl phenol. For characterization of the catalyst, XRD, SEM-EDS, BET, FTIR, TGA-DSC, ammonia TPD, and XPS were used to identify the interaction between these bimetallic nanoparticles and their activity. It was discovered that the catalyst was active, selective, and reusable.

Classification: Green chemistry, Heterogenous catalysis

Key Words: Hydrogenation, Nickel, Cobalt, Copper, Bi-Metallic Catalyst, Alumina, SBA-15, Heterogenous Catalysis, Lignin

Chemical names: Eugenol, 4-propyl phenol

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# Industrial Waste Lignosulphonate a Sustainable Heterogeneous Catalyst for Biginelli Reaction

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# **Abstract Category**

**Biocatalysis** 

# Abstract

A Bio-waste metal-free super acid catalyst (BWC) has been synthesized at higher temperature and used as a catalyst for synthesis of 3,4-dihydropyrimidine-2-(1H)-ones (DHPMs) via one pot three component Biginelli reaction. In the present study, sulfonated carbonaceous material called a green catalyst is synthesized from sodium lignosulfonate which is obtained from the wastage of paper-making industries from the sulfite pulping process. The synthesized green catalyst was characterized by FT-IR, Thermal Gravimetric Analysis (TGA) scanning electron microscopy (SEM), Thermal Electronic microscopy (TEM), and elemental analysis. Catalytic activity was performed as an acid-catalyzed reaction in ethanol. The synthesized compounds were characterized by modern analytical techniques like NMR, MS, FT-IR, CHNS analysis. The satisfactory results were obtained with good yields, shorter reaction time and simplicity in the experimental procedure. The catalysts could be recycled and reused three times without decrease in the catalytic activity significantly.

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# SYNTHESIS OF 6-AMINO-2-NAPHTHOL BY COPPER CATALYZED ULLMANN-TYPE C–N COUPLING REACTION AND PHOTOPHYSICAL STUDIES

Kaustubh Jagushte<sup>1</sup>, Sharmistha Dutta Choudhury<sup>2</sup>, Nabanita Sadhukhan<sup>1</sup>

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# **Abstract Category**

New catalytic routes And processes

# Abstract

6-Amino-2-naphthol (4) is an interesting bi-functional molecule that serves as an intermediate for polariser materials and various pharmaceutics [1]. It is also a photoacid having two protonation sites [2].

We envisioned that synthesis of 4 can be accomplished by copper catalysed Ullmann-type C–N coupling reaction replacing naphthyl bromide with an amine group (-NH2) [3]. In our approach enroute to compound 4, we followed two protocols, i) direct amination, and ii) protection, amination and deprotection of 6-bromo-2-naphthol. We investigated, two different aminating agents, namely aq. NH3 (28-30%), and NaN3 employing various copper catalysts including elemental Cu, Cul, Cu2O, and CuSO4·5H2O. Extensive method optimization revealed that CuSO4·5H2O in presence of Na-ascorbate, NaN3 and NaOH is the superior catalyst. A stable, environmentally friendly, earth abundant and inexpensive catalyst makes the process efficient, sustainable and simple. Successful amination reaction on substituted phenyl, naphthyl, and anthraquinone ring systems proves the generality of this process.

The photophysics of the 4 was investigated in various solvents. Interesting changes were observed in the absorption and emission spectra with change in pH. The presence of NH2 group is found to have significant influence on photoacidity of the naphthol unit [2].

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# Sustainable Transparent and Bio-Based Flame-Retardant Coating for Cotton Fabrics Based on Phosphorus Modified Chitosan BPS Composite

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#### **Abstract Category**

Sustainable Engineering

# Abstract

Bio-based flame retardants are in high demand due to the increased emphasis on eco-friendly flameretardant finishing of cotton fabrics (CF). For this end, a phosphorous-modified chitosan banana pseudo stem (P-CBPS) composite was fabricated on CF via layer-by-layer self-assembly. When exposed to flame, the P-CBPS coated cloth (P-CBPSC) sample preserved its original size and form; moreover, it burned with just a minor amount of smoke and did not catch fire for 3 minutes, but the fabric samples coated with BPS and chitosan [Chitosan coated cloth (CC) and BPS coated cloth (BPSC)] burned entirely within 15 seconds. Uncoated cotton cloth burned completely in 5 seconds, leaving a slight amount of black residue. The flame-retardant (FR) efficacy of a P-CBPS-coated cloth sample (P-CBPSC) was further investigated using precise flame criteria such as the limiting oxygen index test (LOI), vertical flammability test (VFT), and stability at extreme temperatures (e.g. 1500 °C). In comparison to previous work, this work describes the first-ever attempt to construct phosphorous modified chitosan BPS (P-CBPS) via a simple, low-cost synthetic approach, and has the potential to be used as a flame retardant material for fire protection.

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#### Improving Acidic strength of Acidic Aluminosilicate using Gold's Surface Plasmon Resonance

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#### **Abstract Category**

New catalysis routes

#### Abstract

Plastic waste has become a pressing environmental issue due to its enduring presence in both marine and terrestrial ecosystems. Effectively managing plastic waste entails addressing challenges related to disposal, recycling, and pollution prevention. One promising approach is solid acid catalysis, which provides a controlled and potentially less harmful method to break down plastics into smaller, more manageable molecules that can be reintegrated into the environment. Acidic Aluminosilicate (AAS) features Brønsted acidic sites reminiscent of zeolites, coupled with textural properties and high mesoporosity akin to weakly acidic amorphous aluminosilicates. The AAS catalyst boasts a substantial surface area and generous pore volume. This distinctive blend of acidity and accessibility empowers it to catalyze complex reactions more effectively than conventional zeolites. Nevertheless, certain reactions necessitate even greater acidity, prompting efforts to enhance the acidic properties of Brønsted sites in AAS. In this study, we explored AAS coated with gold nanoparticles for the photocatalysis of the Styrene Oxide ring opening reaction. Gold nanoparticles have the ability to augment the electric field in their proximity. We hypothesize that this electric near-field enhancement might elongate the O-H bond at the Brønsted acidic sites, potentially resulting in heightened acidity and improved catalytic performance of the catalyst. The introduction of gold nanoparticles to AAS yielded significant enhancements in conversion percentage and reaction rate within the Au-AAS catalyst. Delving deeper, we aimed to comprehend the precise role played by gold nanoparticles and their Surface Plasmon Resonance (SPR) in amplifying the catalytic activity through various characterization techniques.

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Life cycle assessment (LCA) of marine microalgae cultivation and harvesting process for the Indian context

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#### **Abstract Category**

Life cycle assessment

#### Abstract

Microalgae cultivation is one of the emerging CO2 mitigation technologies and converting it into valuable products. The present study evaluates the environmental impacts of marine microalgae's cultivation and harvesting process with a cradle-to-gate approach from an Indian context. The algal cultivation site of 1000 acres is assumed to be located near the Indian coastal area. The life cycle inventory (LCI) data related to the site was considered based on the literature. The functional unit (FU) for the present study was one kg of dried algae. The evaluation showed that the algal-based technology could mitigate about 1.28 kg CO2 eq./kg algae produced. Among all the impacts, marine aquatic ecotoxicity potential (MAETP) was found to be the most significant one, at 612 kg 1,4-dichlorobenzene (DCB) eq./kg algae. The major contributor to MAETP was the source of electricity. To take into account the uncertainties in the LCI, a scenario analysis was performed with the lower and higher possible process data. The global warming potential (GWP) for 35 g/m2 day productivity was – 1.34 kg CO2 eq./ kg algae, and for 15 g/ m2 day was – 1.11 kg CO2 eq. against – 1.28 kg CO2 eq./kg algae, and for 0.75 g/L, GWP was – 1.39 kg CO2 eq./kg algae. For the consumption change of  $\pm$ 50% in electricity, the change in GWP was  $\pm$  13.85%.

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#### MXene: Promising Material for Heavy Metal Remediation and Wastewater Treatment

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#### **Abstract Category**

Nano Technology

#### Abstract

Despite several technological advances and breakthroughs, wastewater treatment continues to be a major problem on a global scale. If wastewater contains heavy metals, it can seriously harm human health, so getting rid of them is crucial. Due to its adaptable design, simple operation, and reasonable cost, adsorption remains the most used wastewater treatment method for removing heavy metals. One of the largest groups of 2D transition metal carbide/nitride materials is ceramics called MXenes, possessing advanced properties than conventionally used nanoadsorbents like electrical conductivity, high chemical stability, and environmental friendliness. The MXenes were synthesized using a safe route, in which the fluoride salts and strong acids react to form In-Situ etchant. The synthesized MXenes were confirmed by the techniques of Scanning electron microscopy, X-ray diffraction, Fourier Transform Infrared Spectroscopy and Zeta-Potential. The MXenes show promising results for the remediation of the heavy metal ions reported to be highly toxic to the environment. This research shows that the MXenes have a high affinity towards major metal ions like cadmium, chromium, lead and arsenic. The parametric studies for the adsorption like the effect of time, dosage, solution pH and adsorption temperature show that at very little time and dosage, the adsorption of metal ions is comparatively higher than the conventional adsorbents used. The adsorption mechanism was confirmed by adsorption isotherm, thermal modeling and adsorption kinetics. The regeneration and reusability of the MXenes have also been studied.

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# Antimycobacterial, Computational and Spectral Studies of Isoflavonoid and Furanochromone Natural Products

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# **Abstract Category**

Spectroscopic methods For structural characterization

# Abstract

In pursuit of new antitubercular agents, we here report the antimycobacterial (H37Rv) potential of daidzein and khellin natural products (NPs). We procured a total of 16 NPs based on their pharmacophoric similarities with known antimycobacterial compounds. The  $H_{37}Rv$  strain of M. tuberculosis was found to be susceptible to only two out of the 16 NPs procured; specifically, daidzein and khellin each exhibited an MIC of 25 µg/mL. Further, molecular docking study and MD simulation of daidzein indicated that it remained stable inside the cavity of DNA GyrB domain for 100 ns. promising daidzein characterized by Thin layer chromatography (TLC), Melting Point (M.P), Mass spectroscopy, Nuclear magnetic resonance (NMR) spectroscopy, Infra-Red spectroscopy etc.

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# Analysis of Auto garage sample for degradation of PAHs through microbial bioremediation

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#### **Abstract Category**

Clean manufacturing replacing toxic chemicals with environmentally friendly catalysts

#### Abstract

Analysis of Auto Garage Soil sample for degradation of PAHs through microbial bioremediation

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#### Abstract

Polycyclic aromatic hydrocarbons (PAHs) are found ubiquitously in the environment and pose a severe risk to human health. PAHs are highly persistent, mutagenic and carcinogenic properties, hence, it is critical to effectively breakdown PAHs found in the environment. The main sources of PAHs are due to increased anthropogenic and natural activities, such as the incomplete burning of coal and wood, open fires, oil spilling, transportation, mining, and other incidents.

In the present study petroleum contaminated soil samples were collected from six different sites of auto garages located in and around Guntur, Andhra Pradesh, India. Chemical analysis of soil was performed by using Soxhlet extraction to isolate total petroleum hydrocarbons (TPHs). And then it was subjected to column chromatography to separate poly cyclic aromatic hydrocarbons (PAHs). A solvent mixture of DCM and n-hexane was used in the Soxhlet extraction and column chromatography. Approximately thirty pure culture were developed from six soil samples using enrichment culture techniques. To assess the functional groups of contaminants, Fourier-transform infrared spectroscopy (FTIR) was performed. Furthermore, Gas chromatography and Mass spectrometry (GC-MS) was carried out for the confirmation of aromatic hydrocarbons. Results of FTIR revealed various functional groups such as alkanes, alkenes, arenes and alcohols.

Keywords: Soil Analysis, Bioremediation, FTIR, GC-MS

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# Effects of Capping Agents in the Synthesis of Cerium Oxide Nanoparticles by Co – Precipitation Method

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# **Abstract Category**

Nano Technology

# Abstract

The synthesis of CeO2 nano particle was synthesized by co-precipitation method using different polymer capping agent like PVP, PEG, and PVA. The synthesized materials were analyzed by XRD, UV,
TGA and FESEM. Further materials was evaluated by the selective oxidation of cyclohexane using H2O2 as oxidant at room temperatures. Among the materials CeO2 (PVP) nano particle showed high conversion and maximum selectivity. Hence, the influence the capping agent in synthesis of CeO2 nano particle correlated to conversion of cyclohexane and selectivity of the product towards cyclohexanone.

## Upload Extended Abstract File

### Effect of pin-to-plate atmospheric cold plasma on the activity and conformation of papain

Ms. Jayashree Potkule<sup>1</sup>, Dr. Uday Annapure<sup>1,2</sup>

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#### **Abstract Category**

**Biocatalysis** 

#### Abstract

The effect of pin-to-plate atmospheric cold plasma (ACP) treatment at different voltage inputs ranging from 170V to 230V with exposure time of 5 min to 20 min on the enzyme activity and conformation of papain were investigated. The residual activity of ACP treated papain samples were found to be decreased from 100 to 72 % with increasing voltage inputs; while the effect of treatment time was marginally observed. According to the conformational analysis of Fourier transform infrared spectroscopy, fluorescence spectroscopy and circular dichroism spectroscopy; side chains of amino acids, amide transitions,  $\alpha$ -helical elements and  $\beta$ -structure domain of papain were influenced by pin-to-plate ACP treatment. The intrinsic and extrinsic fluorescence intensity of papain was also observed to be affected by ACP treatment. The results suggest that the exposure of reactive plasma species to the papain sample during pin-to-plate ACP treatment leads to modifications in the weak interactions between the peptide linkages, secondary and tertiary structure of papain. These modifications can results in the denaturation of protein, and subsequent loss of enzyme activity. This findings indicated that the activity of papain could be inactivated after pin-to-plate ACP treatment due to the variation in their secondary and tertiary structures.

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## A Comparative study between NH2 MIL 88B and ZIF-67 nanozymes: H2O2 detection and unlocking the intrinsic peroxidase activity.

#### Santosh Sethi

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## **Abstract Category**

Nano Technology

#### Abstract

Nanozymes are a class of MOFs that possess the ability to mimic the catalytic activity of natural enzymes. MOFs are high-efficiency and economical enzyme mimics due to their outstanding surface area and abundant active sites. A comparative study includes synthesis and intrinsic peroxidase activity of two different nanozymes; Fe-based NH2 MIL 88B and Co-based ZIF-67 is reported for the detection of H2O2 an important biomarker for biomedical diagnostics. The rod-shaped NH2 MIL 88B crystals were produced through mixing of FeCl3·6H2O and NH2-BDC in 100 mL of NN-Dimethylformamide (DMF) by solvothermal method. Synthesis of ZIF-67 using Co (NO3)2·6H2O and 2-methylimidazole in 40 ml methanol by biomineralization method. The successful synthesis of both MOFs was characterized by SEM, DLS, UV-VIS, FTIR, and XRD. We used a UV spectrophotometer to assess changes in absorbance at 650 nm, allowing precise quantification of the nanozymes. Optimized the concentrations and explored the effect of pH on the peroxidase activity of both the MOF ranges from 2.5 to 8.5 pH and also investigated the effect of temperature and different solvents on the catalytic activity of the ZIF-67 and NH2 MIL 88B crystals. Both MOFs exhibited outstanding repeatability as evidenced by the resulting Coefficient of variation in the batches being less than 10%. The LOD achieved was 26 nM and 29 nM H2O2 for NH2 MIL 88B and ZIF-67.

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## Industrial Grade Resin as Reusable Catalyst for Amidoalkylation of y-Hydroxy Lactams

#### Jyotiranjan Mishra

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#### **Abstract Category**

Industrial catalysis

#### Abstract

Despite the significant progress on catalytic/stoichiometric methodologies for amidoalkylation reactions between  $\gamma$ -hydroxy lactams and a nucleophile, the associated substrate-specific reactivity, catalyst reusability, difficulty in separation of the desired product and catalyst from the reaction mixture are remained with some unresolved issues, which needs to be addressed.1-3 Herein, we disclose a selective, versatile, accessible, cost-effective and highly efficient cation-exchange industrial grade INDION 130 resin as a reusable catalyst for the synthesis of 3-substituted isoindolinones involving various  $\gamma$ -hydroxy lactams and a variety of C, N, O, and S nucleophiles under mild reaction conditions. Mechanistic studies evaluated from in-situ monitoring of the reaction progress, control studies, and Hammett studies suggested the generation of a different kind of kinetically and thermodynamically controlled intermediates/eliminated products, which further converted to their corresponding products depending upon the nucleophile, reaction parameter and nitrogen substitution (benzyl vs. aryl) of the substrate (succinamidals vs. phthalimidals). The easy synthesis, efficient reactivity and selectivity, broad substrate scope (68 examples) with verities of C, N, O, and S nucleophiles, and efficient recycling make the catalyst and the protocol economical and sustainable.

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## Utilization of waste for catalyst synthesis and its application in biodiesel production

### **Dhairyashil Santre**

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#### **Abstract Category**

Catalytic reactions in which wastes are converted to useful products

#### Abstract

In the present work, a heterogeneous calcium oxide catalyst is synthesized from the waste marble. Transesterification of waste cooking oil with synthesized calcium oxide as a catalyst was carried out to produce fatty acid methyl esters (FAME). The effect of various operating parameters such as molar ratio (9:1 to 18:1, Methanol to oil), catalyst loading (3-5% w/w of oil), reaction temperature (50-70 °C) and power (60-90 W) on biodiesel synthesis using methanol by the conventional and advanced method has been studied. The highest yield of biodiesel was obtained at a molar ratio of 9:1, catalyst loading 4 wt%, reaction temperature 65°C, and power of ultrasound 70W. Thus, it can be interpreted that waste marble-derived calcium oxide is an effective catalyst for the transesterification of waste cooking oil to produce biodiesel.

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## Hydrogenation of biomass-derived oxygenates to important fuel additives

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#### **Abstract Category**

Catalysis in biomass conversion

#### Abstract

The use of furfuryl alcohol as a starting material, already produced commercially from hemicellulosederived pentoses, is commercially important. Oligomerization of furfuryl alcohol to form dimers and trimers was carried out using  $H_2SO_4$  under ambient pressure and temperature. The resulting mixture of oligomers was analyzed and further hydrogenated under 2.5 MPa pressure and 130°C using Ni-Cu supported on Reduced Graphene Oxide as catalyst under constant stirring for six hours. The final products obtained were a mixture of some important fuel additives like Methyl Levulinate, Dimethoxyhexane, and Butyric Anhydride. Various parameters were optimized to achieve good conversion and selectivity.

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## Manganese supported on Sr induced AIO4 and AIO6 catalyst for complete oxidation of pollutants: Effect of preparation methods

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## **Abstract Category**

Catalysis in air pollution control

#### Abstract

The complete oxidation of propene was done by using a series of MnAl and Sr doped MnAl catalysts prepared by deposition precipitation after the coprecipitation method. The concentration of Mn2O3 and SrAl2O4 active phases increases with the relative content of reactive oxygen species. These species enhance the reducibility of catalysts, which further increases the activity of C3H6 oxidation at relatively low temperatures. Characterization techniques like XRD, FTIR, BET, XPS, H2-TPR, HR-TEM, and 27Al NMR were used to determine the physicochemical characteristics of the catalysts. The complete propene oxidation activity was observed on MnSr0.3Al at 237 oC. The effect of preparation methods indicates that the coprecipitation-deposition precipitation approach strengthens the interaction between Sr and Mn. It also improved the dispersion of Sr and Mn on the surface of Al2O3 compared to the successive impregnation and deposition precipitation method.

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Abstract ID : 151

## Extraction of phenolics from Spilanthes Acmella: Kinetic studies using Peleg's model

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## **Abstract Category**

Sustainable Engineering

## Abstract

## Extraction of phenolics from Spilanthes Acmella plant: Kinetic studies using Peleg's model

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## ABSTRACT

This study focuses on the stirred batch extraction of Total Phenolic Content (TPC) from the Spilanthes Acmella L. plant and its optimization with kinetics. The study investigates the effect of various parameters such as extraction solvents (n-butanol–water), solid-to-solvent ratio (1:10–1:50), speed of agitation (100–500 rpm), pH (5–8), and extraction temperature (30–60°C) on the extraction of total phenolic content from Spilanthes Acmella powder. The optimized parameters for the stirred batch extraction of total phenolic content from Spilanthes Acmella L. dried plant powder are solid to solvent ratio of 1:30, speed of agitation 300 rpm, pH 5, extraction temperature of 50°C with a maximum phenolic content of  $18.91 \times 10^{-3}$  g GA/g. The cost and energy requirement of the batch process was less than that of the Soxhlet technique. The study also investigates the kinetics of the extraction by using Peleg's model. The extraction rate constant, initial extraction rate, and equilibrium concentration for all experimental conditions have been predicted. The mathematical model applied showed a good agreement with the experimental results, depicting the course of an experiment in an accurate manner.

*Keywords: Spilanthes Acmella L.*, batch extraction, total phenolic compounds, kinetics, Peleg's model.

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### Abstract ID : 152

## Sulfated Spinel for Catalytic Acetylation of Glycerol

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## **Abstract Category**

Catalytic reactions in which wastes are converted to useful products

## Abstract

The issue of global warming has gained widespread attention, particularly with regards to CO2 emissions resulting from the burning of fossil fuels. One potential solution is the use of biodiesel, which is a domestically produced, clean-burning, and renewable alternative. However, the rapid expansion of the biodiesel industry has led to an oversupply of glycerol, causing decreased prices and environmental problems with the disposal of contaminated glycerol. As a result, there is a pressing need to extract value from glycerol by subjecting it to various processes to obtain valuable products. Glycerol's replaceable alcoholic groups allow it to undergo several chemical reactions, such as reforming, steam reforming, hydrogenolysis, esterification, ammoxilation, oxidation, and dehydration, to produce valuable products. In this research endeavor, a diverse set of catalysts have been prepared, including CuFe2O4, CuFe2O4/Al2O3, and CuFe2O4/CeO2 in sulfated and nonsulfated form. The main focus is to investigate the efficacy of each catalyst for glycerol acetylation. To achieve this objective, a comprehensive array of experimental reactions will be conducted, manipulating critical reaction parameters like temperature, time, glycerol/acetic acid molar ratio, and catalyst loading. The ultimate goal is to optimize glycerol conversion while ensuring excellent selectivity towards the acetins. The findings from this study hold significant promise for advancing the field of catalysis and establishing sustainable methodologies for the production of valuable chemicals and renewable resources.

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# CeO2-Nanorods Catalyzed Additive- Free Borylation of Alkyl Chlorides Bromides and Aryl Halides with Bis (pinacolato) diboron

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#### **Abstract Category**

New catalytic routes And processes

#### Abstract

CeO<sub>2</sub>-Nanorods Catalyzed Additive- Free Borylation of Alkyl Chlorides Bromides and Aryl Halides with Bis (pinacolato) diboron

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## Abstract:

Organoboranes are a class of vital organic intermediates in a variety of organic transformations.<sup>1</sup> In recent years, transition-metal-catalyzed organoborane synthesis has been influentially explored *via* hydroboration, C-X borylation, diboration, and C-H borylation processes.<sup>1-</sup>

<sup>6</sup> However, these methodologies have certain drawbacks, such as necessity of inert atmospheres, contamination of metals in the products and lack of recycling of catalysts and ligands. Therefore,

recyclable metal catalysts with a high surface to volume ratio have attracted much attention due to their potential use as catalysts. During last decade transition metal catalyzed organoborane synthesis is offering great potential to build a diverse array of organoborane derivatives.<sup>2</sup> Homoleptic rare earth metal complexes were well explored for hydroboration of carbonyl groups and alkenes.<sup>4</sup> However, till date there is no report on rare earth metal catalyzed borylation of alkyl halides. Herein, we report a highly efficient and recyclable easy to synthesise CeO<sub>2</sub>-nanorods catalyzed efficient borylation of alkyl chlorides, bromides and aryl halides with B<sub>2</sub>pin<sub>2</sub> under mild reaction conditions.<sup>7</sup> Key results will be described.

Keywords: Borylation, Alkyl halide, Boronate, Cerium, Boryl.

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## Approach for the commercialization of the production of Biodiesel

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#### **Abstract Category**

**Bio refinery** 

#### Abstract

The rate of energy consumption is higher than the rate of population growth. Fossil fuels, coal, natural gas, liquified petroleum gas etc are the finite sources of useful form of energy and these are de-pleating at the faster rate. Biodiesel (bioenergy) is considered as one of the options to these fossil fuels because it can be manufactured from renewable resources. The hurdle with the production of biodiesel is that the cost associated with the edible oils is generally high if these are used as a raw material. As edible oils are highly expensive then there is a need to use waste cooking oil (WCO) or non-edible oils as a raw material for carrying out the production of biodiesel because these are comparatively less expensive. Therefore, there is a need for alternative less expensive raw material which is available in tremendous form from which biodiesel can be manufactured without affecting the agricultural economy. Palm FFA is the rich source of free fatty acids (FFA) from which biodiesel can be manufactured via esterification followed by trans-esterification. The technical hurdle with carrying out the esterification reaction is the selection of suitable catalyst. Biodiesel can be manufactured with minimum cost, and it should be available at an affordable market price in developing and underdeveloped countries.

Keywords: esterification, trans-esterification, homogeneous catalyst, heterogeneous catalyst, reaction rate, edible oils, non-edible oils, Palm FFA, sulphuric acid, corrosion.

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# Hydrogenation Involving Two Different Proton- and Hydride-Transferring Reagents through Metal–Ligand Cooperation: Mechanism and Scope

Rahul Patil, Sanjay Pratihar

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#### **Abstract Category**

Homogeneous catalysis

#### Abstract

The goal of controlling active metal center properties through a defined ligand system is pursued to modulate reactivity for specific substrate activation.1 Understanding pre-catalyst activation, binding mode, and key catalytic cycle steps is crucial for achieving superior catalyst activity. While hydrogenation of nonpolar alkenes and alkynes relies on H–H bond cleavage through oxidative addition, recent advances have shown transition metal catalysts capable of hydrogenating both nonpolar and polar substrates via metal–ligand cooperation (MLC).2 For polar substrates like alcohols and amines, the reverse reaction between metal hydride and protonated ligand during H2 elimination is pivotal in dehydrogenation. In this study, we introduce a stable bifunctional Ru(II) catalyst for selective unsaturated carbonyl/aldehyde hydrogenation, employing hydride and proton transfers from distinct sources (silane and methanol).3 This is achieved through interconvertible coordination modes (imino N  $\rightarrow$  Ru and amido N–Ru) of the catalyst. The system is further applied to synthesize saturated ketones and  $\alpha$ -methyl saturated ketones from  $\alpha,\beta$ -unsaturated ketones using a solvent and base-dependent switchable process. The catalyst demonstrates strong performance across 69 examples, enabling diverse transformations such as monomethylation, hydrogenation, double methylation of ketones, and N-methylation of amines.

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## MEMBRANE SEPARATION-BASED RECOVERY AND REUSE OF TEXTILE WASTEWATER

Ankita A. Yadav<sup>1</sup>, Pritesh S. Patil<sup>1</sup>, Nitin V. Thombre<sup>2</sup>, Yagna Prasad K.<sup>3</sup>, Anand V. Patwardhan<sup>1</sup>

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Abstract Category Sustainable Engineering

## Abstract

The textile industry is one of the oldest sectors and consumes different dyes and harmful chemicals for the process. It involves various processes and requires a substantial amount of water to carry out these processes, therefore, it is causing a large amount of water pollution. In the present study, we have successfully treated the textile effluent using membrane separation. The effluent was collected from a local effluent treatment plant (ETP) and treated on commercial polymeric, commercial ceramic, and novel synthesized composite ceramic membranes. Detailed analyses of each membrane were carried out. The effluent received from ETP and treated effluent was characterized in terms of pH, TDS, COD, BOD, Conductivity, Turbidity, and Osmolality. A reduction in all the measured parameters of water was achieved. COD was reduced by around 40% after the treatment of effluent. Overall, our novel synthesized composite ceramic membrane shows better results and is comparable to the commercially available membranes.

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#### Valorization of industrial and domestic waste into useful products

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

This research investigates the valorization of organic waste, including custard apple waste, ice apple waste, and food waste, as alternative energy sources and sustainable waste management practices. The study aims to replace lignite coal with biomass pellets derived from these waste materials. Proximate analysis reveals the composition and characteristics of the waste samples, with average final moisture contents of approximately 6.630%, 10.756%, and 4.367% for custard apple waste, ice apple waste, and food waste, respectively. The total solid content is approximately 93.370%, 89.244%, and 95.663%, and the ash content is approximately 12.280%, 4.623%, and 14.790% for the corresponding waste samples. Moreover, ice apple waste exhibits the highest calorific value among the samples, making it a promising energy source. The optimization of pelletization processes focuses on parameters such as pellet durability, moisture content, and binder selection, with ice apple waste pellets demonstrating high durability. Comparative analysis shows that ice apple waste possesses the highest energy content per unit weight, making it a potential alternative to lignite coal for biomass pellet production, promoting sustainable waste management practices, and reducing environmental impact. The impact of binders, such as waste cooking oil and waste lubricating oil, on the pellet strength of organic waste is investigated, revealing the potential to improve pellet quality and durability. Overall, this research contributes to the understanding of waste valorization and underscores the significance of incorporating organic waste into the circular economy to promote sustainable resource utilization and waste management practices.

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## Synthesis and Characterization of Gelatin and Silica/Titania/Zirconia Based Mesoporous Nanohybrid Material

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#### **Abstract Category**

Micro- And meso-porous catalysts

#### Abstract

Organic-inorganic hybrids are materials prepared by combining organic and inorganic building blocks . Gelatin as one of the main component of hybrid materials is an attractive option. It is biodegradable; biocompatible; non-toxic; bio-adhesive and contains many active groups such as -NH2, –COOH, in the biopolymer backbone makes these hybrid materials important in various technological applications. The synthesis of a series of gelatin-based nano-hybrid mesoporous materials was carried out using gelatin as the bio-polymeric backbone, silica, titania or zirconia; SDS as surfactant for o/w emulsion, TEOS as silulation or cross-linker material to obtain different hybrid materials for different applications. Hydrochloric acid (HCl) was used as catalyst, n-hexane as the solvent and sodium dodecyl-sulphate (SDS) as a surfactant for oil-water emulsification. The sol-gel technique was used to prepare the gelatin-based mesoporous nano-hybrid materials as a promising and efficient method. Thus, four kinds of different gelatin-based hybrid materials: gelatin-silica, modified gelatin-silica, gelatin-titania and gelatin-zirconia based hybrid materials were synthesized. The effect of post-calcination on the properties of the as-synthesized hybrid materials was also studied and confirmed from various characterization techniques such as: elemental analysis, scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-Ray diffraction studies (XRD), thermo-gravimetric analysis (TGA), energy dispersive X-ray (EDX) and Fourier transform infrared (FTIR) spectroscopy and BET surface area analysis. These materials nano-hybrid mesoporous materials have high surface area and good candidates for many frontline applications.

**Keywords:** Biopolymer, Gelatin, Sol-gel, Nano-hybrid, Mesoporous, FTIR, TGA, XRD, TEM, EDX, SEM, BET

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Abstract ID : 161

## A sustainable catalytic route for the synthesis of five-membered dioxolane as a fuel additive using modified boehmite catalyst

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## **Abstract Category**

Catalysis in biomass conversion

## Abstract

The choice of active site and support medium decides the activity of a catalyst. Modifications on either of these will have a significant impact on the reactivity and selectivity. On the other hand, every 100 Kg of biodiesel production generates 10 Kg of crude glycerol as a major by-product. Flooding of such additional glycerol in the already saturated market, downgrade its market value. To address this, significant efforts have been devoted to bridge the gap between sustainable production of biodiesel and valorisation of glycerol for its potential applications. Among the diverse chemistry, acetalization of glycerol with carbonyl compounds has gained significant interest to construct fivemembered dioxolane (solketal) and six-membered dioxanes (cyclic acetals/ketals). Here we have synthesised WO3 loaded boehmite and applied them for acetalization of biomass derived bulk chemical, glycerol. The well-characterized acid catalyst, exhibit a selective acetalization of glycerol with good conversions to five-membered dioxolane product. The cyclability of catalyst upto six times with retention of catalytic activity ensures the heterogeneity of the material.

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# Unmixed Combustion: A novel solution to addressing conventional combustion related energy and environmental issue simultaneously

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#### **Abstract Category**

Sustainable Engineering

#### Abstract

The enthalpy associated with conventional combustion has over the years been utilized in several important process applications. This process however suffers from a drawback of flue gas generation and reduced thermal efficiency. Although several researchers have attempted to address the above issues in a segregated manner, very little has been done to change the fundamental nature of the combustion process itself. Unmixed Combustion (UMC) referred to as the "alternative to fire" offers an exciting alternative to address the above dual problem. It is brought about by alternately exposing zero air and fuel to an Oxygen Storage and Release Material (OSRM) that undergoes cyclic oxidation and reduction reactions. The net energy released in these reactions can be potentially used for process applications. This work presents results from studies that demonstrate the potential of UMC for 3 important process applications, i.e., process heating, syngas production and CO to CO2 conversion.

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## A Paradigm Shift: Examining the Viability of Transition from Batch to Flow Processing in Drug Discovery and Manufacture of Pharmaceuticals

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## **Abstract Category**

Sustainable Engineering

#### Abstract

Flow (continuous) processes have been well-established in numerous manufacturing sectors as they afford superior flexibility, quality control, safety and environmental sustainability. Reduced costs coupled with higher operational efficiency provide more rationale to prefer flow processes over batch reactions. The pharmaceutical industry however, has predominantly relied on batch processes and the evolution to adopt flow chemistry is slowly gaining traction. Requirements for increased throughput and highly specific properties of certain pharmaceutical products are some driving forces for this transition. Recent innovations in highly automated flow processes have rendered batch processes to be increasingly inefficient. In this review, emphasis is placed on how benefits of flow processes outweigh those of batch processes and a detailed overview on recent advances in the transition from batch to flow reactions in the fields of drug delivery and pharmaceutical manufacturing are discussed. Specific recent and relevant instances of the merits of flow processes, their reaction mechanisms and industrial setup is also presented.

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### Nanoparticle Integration in Cosmeceuticals: Advantages, Limitations and Prospective Trajectories

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#### **Abstract Category**

Nano Technology

#### Abstract

Nanotechnology is one of the fastest growing technologies in the field of food, pharmaceuticals, nutraceuticals and cosmeceuticals. It has highly captivated the global market for its high value usage and almost immediate results. The usage of this nano-technology has its advantages and limitations that have many consequences for the future prospects. Efficacious achievement of safe and precise administration of therapeutic agents and cosmetic compounds through nanoparticles. Utilization of carrier mechanisms, drug delivery, in nanotechnology provides added benefit of enlarged dermal permeation, deposition phenomenon, and prolonged positive results. Gold nano particles has extensively been used in barrier restoring sheet masks and silver nano particles in ultraviolet visible spectroscopy protection cream. Titanium dioxide and Zinc oxide are excellent nano emulsion components in products formulated concerning UV protection. There are advantages of nano sized particles to penetrate better and have high performing anti-aging cream formulations on an extensive user-based scale, however production of reactive oxygen species (ROS) is a potential risk due to the very small size of particles. Oxidative stress, and damage to RNA and DNA is a possibility. The evolution and market integration of nanotechnologies have emerged as a pivotal complement to conventional industries, driven by escalating consumer exigency for enhanced and innovative commodities.

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## Oxidative Dehydrogenation of Cyclohexane over phosphorus modified catalyst: in-situ DRIFTS Studies and effect of preparation method

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## **Abstract Category**

Spectroscopic methods For structural characterization

#### Abstract

oxidative dehydrogenation of cyclohexane investigated over phosphorus-modified bimetallic copper-manganese oxide catalyst. The catalysts were synthesized using incipient wetness impregnation. Catalysts were characterized through XRD, BET, Raman spectroscopy, and H2-TPR. It was observed that copper-manganese oxide and phosphorus remained dispersed at lower loading levels, with a reduction in phosphorus oxide crystallite size as loading increased. The catalyst exhibited a mesoporous nature, although impregnation of copper manganese oxide led to decreased surface area due to pore blockage. Raman spectral analysis indicated the formation of a CuMnOx solid solution and isolated phosphorus oxide phase formation. The reactivity of the catalyst was examined through in-situ DRIFTS, revealing various intermediate species on the catalyst surface. Notably, the presence of phosphorus hindered the formation of CO2, suggesting a role in controlling oxidation pathways. The in-situ DRIFTS spectra unveiled several surface-bound species, including Cyclohexanolate, Enolate, Phenolate, Carboxylate, and Bidentate carbonate.

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## Analytical method Development and Validation of RP-HPLC Stability Indicating potential impurities Quantification Method for Rivaroxaban in Active Pharmaceuticals Ingredient

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## **Abstract Category**

Spectroscopic methods For structural characterization

#### Abstract

Rivaroxaban is Anti-hypersensitive drug. In this study Stability indicating RP-HPLC method for quantification of potential impurities in Rivaroxaban was developed and validated as per ICH guidelines. For this analytical method, the HPLC column used was Inertsil ODS 3V (250 mm X 4.6 mm X 5  $\mu$ m) column temperature was kept at 35°C. The mobile phase used was 0.01M potassium dihydrogen phosphate buffer and a Mixture of Buffer: ACN mixture with gradient elution. The flow rate was 0.9 ml/min. The wavelength used was 240 nm Injection volume was set to 10  $\mu$ l. Run time kept at 60 minutes. The developed analytical method there is no interference with the degradation product. The analytical method found specific, and linear over the range of 300 ppm to 2250 ppm, The method was precocious, robust, and stability indicating.

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## Sulfated Spinel for Catalytic Acetylation of Glycerol

## **Abstract Category**

Catalytic reactions in which wastes are converted to useful products

## **Abstract Title**

Sulfated Spinel for Catalytic Acetylation of Glycerol

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## Abstract

The issue of global warming has gained widespread attention, particularly with regards to CO2 emissions resulting from the burning of fossil fuels. One potential solution is the use of biodiesel, which is a domestically produced, clean-burning, and renewable alternative. However, the rapid expansion of the biodiesel industry has led to an oversupply of glycerol, causing decreased prices and environmental problems with the disposal of contaminated glycerol. As a result, there is a pressing need to extract value from glycerol by subjecting it to various processes to obtain valuable products. Glycerol's replaceable alcoholic groups allow it to undergo several chemical reactions, such as reforming, steam reforming, hydrogenolysis, esterification, ammoxilation, oxidation, and dehydration, to produce valuable products. In this research endeavor, a diverse set of catalysts have been prepared, including CuFe2O4, CuFe2O4/Al2O3, and CuFe2O4/CeO2 in sulfated and nonsulfated form. The main focus is to investigate the efficacy of each catalyst for glycerol acetylation. To achieve this objective, a comprehensive array of experimental reactions will be conducted, manipulating critical reaction parameters like temperature, time, glycerol/acetic acid molar ratio, and catalyst loading. The ultimate goal is to optimize glycerol conversion while ensuring excellent selectivity towards the acetins. The findings from this study hold significant promise for advancing the field of catalysis and establishing sustainable methodologies for the production of valuable chemicals and renewable resources.

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## Synthesis of Iron Doped Nickel Vanadate for Electro catalyst for Oxygen Evolution Reaction

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**Abstract Category** 

**Catalysis For Energy** 

Abstract

Synthesis of Nano catalysts has gained more recognition in these past couple of years due to its numerous applications in various fields including electrocatalysis. Electrocatalysis of water known as water splitting reaction is mostly used method for obtaining hydrogen in its gaseous form but, the amount of potential energy required is not yet affordable for large scale production of hydrogen due significant over potential i.e., difference between theoretical and actual value of voltages. Hence, in order to get efficient results of hydrogen evolution an attempt will be made in research work using electrocatalyst which will be incorporated for water splitting reaction. This might give better hydrogen gas evolution while using less amount of energy (potential) required for splitting of water molecule.Here,enhancing the rate of Oxygen Evolution Reaction (OER) is done by introducing iron doping in synthesis of nickel vanadate electrocatalyst prepared using Successive Ionic Layer Adsorption and Reaction (SILAR) method. In order to transfer current 10mAcm-2 as well as 100mAcm-2, this has confirmed ultra low over potentials of 180mV and 305mV in our work. In our current work, doping of iron in Nickel Vanadate electro catalyst increases the electrochemical active surface area, also intrinsic activity of active sites, interacting electronically with the Fe as well as Ni catalytic centers. Iron doped Nickel Vanadate electro catalyst also produces a large surface wettability as well as low gas bubble adhesion for accelerated large scale transport. This doping also gives more gas bubble dispersion at high current densities, vanadate variation also increases the OER activity.

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# Microwave-assisted synthesis of a flavor ester: Citronellyl propionate from $\beta$ citronellol by enzymatic catalysis in non-aqueous media

## **Abstract Category**

Enzyme immobilization & stabilization, particularly in non-conventional media

## **Abstract Title**

Microwave-assisted synthesis of a flavor ester: Citronellyl propionate from  $\beta$  citronellol by enzymatic catalysis in non-aqueous media

## Abstract

Citronellyl propionate (a terpene ester) is widely used as a flavor and fragrance material. In this work, citronellyl propionate was successfully synthesized under microwave irradiation via transesterification of  $\beta$ -citronellol (as nucleophile) with methyl propionate, ethyl propionate and vinyl propionate (as acyl donors) using immobilized CALB (Candida antarctica B lipase), TLL (Thermomyces lanuginosus) lipase and CRL (Candida rogusa lipase). Various reaction parameters were optimized, compared and screened for an optimum conversion and yield. Organic solvents such as heptane, toluene and 1,4 dioxane were compared to get the best catalytic activity. CALB-Immobead 150A lipase showed the highest activity among those studied. The optimized reaction system consisted of the following conditions: CALB Immobead 150, heptane as solvent, 400 rpm agitation speed for the lab reactor, an equimolar ratio of citronellol and vinyl propionate and 70 °C reaction temperature. The initial reaction rate was intensified by 21% by microwave irradiation than conventional heating due to the significant increment of collision frequency factor. The process parameters were optimized using a mixed approach of one factor at a time, multiple regression and black box-based machine learning models. The simultaneous effect of temperature and pH on lipase activity was also studied. The optimum reaction system was studied to overcome mass transfer and intra-particle diffusion limitations to determine intrinsic kinetics. It was found that the reaction is enzyme kinetics limited. A ping pong bi-bi non sequential model was fitted based on a double reciprocal plot.

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## **ACKNOWLEDGEMENTS**









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