APPLIED CATALYSIS: ENERGY ENVIRONMEN AND SUSTAINABILITY

Applied Catalysis: Energy, Environment and Sustainability

Proceedings of the 1st online International Conference on Emerging Trends in Catalysis for Sustainable Chemical Processes (ETCSCP-2021)

26th- 28th August 2021)

Edited By

R R Siva Kiran
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Kulbhushan Samal

RAMAIAH
Institute of Technology

Jointly Organized by
IIChE, Bangalore Regional Centre
Catalysis Society of India, Bangalore Chapter
Department of Chemical Engineering, M.S. Ramaiah Institute Of Technology, Bangalore
Poornaprajna Institute of Scientific Research, Bangalore
Department of Chemical Engineering, Dayananda Sagar College of Engineering, Bangalore

Applied Catalysis

Energy, Environment and Sustainability

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About Conference

1st Online International Conference on "Emerging Trends in Catalysis for Sustainable Chemical Processes (ETCSCP - 2021)", from 26th to 28th August 2021 was jointly organized by IIChE - Bangalore Regional Centre, Catalysis Society of India - Bangalore Chapter, Department of Chemical Engineering, M S Ramaiah Institute of Technology, Bangalore, Poornaprajna Institute of Scientific Research (PPISR) and Department of Chemical Engineering, Dayananda Sagar College of Engineering. Eight plenary speakers from across the globe addressed the audience and shared their research experience on application of catalysis encompassing energy, environment and sustainability.

The National Organizing Committee comprising of Prof. G.D. Yadav, ICT Mumbai, Dr. R. V. Jasra, Senior Vice President at Reliance Industries Limited, Dr. R. Rajeswar, Director, Sabic Research & Technology Centre, Dr. Kishan Gurram, Sravathi Advance Process Technologies Pvt. Ltd, Dr. Laxmi Narasimhan, Shell Technology and Dr. N. V Choudhary, HPCL contributed in disseminating the emerging trends in the field of catalysis. The chief patrons and patrons immensely contributed towards the event.

The local organizing committee comprising of Dr. Archna, Chairman, BRC, IIChE, Dr. R. Ravishankar, Vice Chairman, BRC, IIChE, Sri K. A. Badarinaryana, Secretary, BRC, IIChE, and Dr. Ganapati Shanbhag, PPISR, Dr. Y.J. Rao, BRC, IIChE, Dr. K.S. Rajanandam, BRC, IIChE, Prof. G.A. Shareef, BRC, IIChE, Dr. R. Vetrivel, PPISR, Dr. S. Sivakumar, M/s Sravathi, Advance Process Technologies Pvt. Ltd, Sri. P.T. Raghuram, BRC, IIChE, Sri. G Kishore Kumar, BRC, IIChE, Dr. V Venkateswam, BRC, IIChE, Dr. G.M. Madhu, BRC, IIChE, Dr. Brijesh, BRC, IIChE, Dr. V. Sravanthi, MSRIT, Dr. Rama Sivakiran Reddy, MSRIT, Dr. J. Koteswara Rao, BRC, IIChE, Dr. G.K. Mahadevaraju, BRC, IIChE, Ms. Priya S, DSCE, Mr. Karthik K V, BRC, IIChE, Ms. Deepa. A, DSCE and Sri. Sagar. J.S, MSRIT bought together several elite researchers working in the area of catalysis from industry and academia together.

In the three days' conference, 350 participants joined on the virtual platform and more than 40 scientific papers were presented by the young researchers from India and abroad. Overall, the international conference created a euphoria in the research community across the globe.

Message from President, Catalysis Society of India, Bangalore Chapter

We are happy to organize for the first time an Online **International Conference on "Emerging Trends in Catalysis for Sustainable Chemical Processes (ETCSCP-2021)"** in association with the Indian Institute of Chemical Engineers - Bangalore Regional Centre **(IIChE, BRC).** It is my great pleasure to welcome all the delegates who are attending this conference on behalf of The Catalysis Society of India as well as Bangalore Chapter and also IIChE, BRC**.** We have invited renowned international plenary speakers and also some outstanding speakers from industry. Applied catalysis and technologies play a very important role in the well-being of humanity for producing sustainable energy, driving towards a cleaner environment, manufacturing of low cost materials, etc. Technologies development through discoveries in catalysis make a huge impact the world economy and on mankind. The basic inventions in the field of catalysis need to be bridged with process design and development, with a synergy between scientists, engineers, academia and industry. In this backdrop, the symposium plans to bring together the researchers in academia and industry to cover the broad spectrum of topics in catalysis.

The frontier topics chosen for International conference are methane activation to value generation, hydrogen production through Biomass, renewable energy, biomass conversion to value added chemicals, novel mesoporous catalyst for fine specialty chemicals, etc. We have also invited two experts in the area of petrochemicals as well as various polymer catalyst developments. They will share their experience from concept to commercialization.

This symposium aims for disseminating knowledge on the recent advances in the field of catalysis encompassing energy, environment and chemicals. We have invited several young research scholars to present oral as well as poster presentations based on their research findings.

The organizing committee members have made a lot of efforts for bringing together several academic/industry catalysis researchers for this forthcoming ETCSCP-2021 and also for disseminating knowledge on the recent discoveries in the field of catalysis encompassing energy, environment and sustainable chemical processes.

I hope that all the members spare their valuable time by way of discussions and interactions with fellow researchers and on Industry – Academia collaboration so that all efforts that have been put forth in the Symposium will enormously benefit the catalysis researchers both in academia and industry.

Dr Anand B Halgeri
President – Catalysis Society of India-Bengaluru Chapter
Director, Poornaprajna Institute of Scientific Research.

Message from Chief Executive, M S Ramaiah Institute of Technology, Bangalore

I am delighted to know that the Department of Chemical Engineering, M S Ramaiah Institute of Technology, Bangalore in association with professional bodies IIChE, BRC and catalysis society of India is going to bring out the proceeding of the 1st International Conference on “Emerging Trends in Catalysis for Sustainable Chemical Processes” (ETCSCP-2021) organized during the 26th – 28th August 2021. I commend the Department of Chemical Engineering, MSRIT for taking initiative to create a platform despite a challenging situation of Covid -19 to bring ideas that are concrete and will invoke changes in the catalyst applications for sustained development of society.

The Department of Chemical Engineering, M S Ramaiah Institute of Technology in association with professional bodies IIChE and Catalysis Society of India, Bangalore Chapter has put great deal of effort into the arrangement of the conference and the organizers are privileged to have distinguished resource persons in the field of catalysis from industry and academia. The paper presentations and plenary lectures will enrich the participants on the latest developments and challenges in this field.

I congratulate the Organizers of ETCSCP-2021 for conducting the conference with its application towards sustainable development theme. I wish that participants have fruitful outcomes from the three day deliberations.

Shri B S Ramaprasad
Chief Executive
M S Ramaiah Institute of Technology Bangalore

Message from Principal, M S Ramaiah Institute of Technology, Bangalore

I am delighted to note that Department of Chemical Engineering, M S Ramaiah Institute of Technology, Bangalore is organizing first Online **International Conference on "Emerging Trends in Catalysis for Sustainable Chemical Processes (ETCSCP-2021)"** in association with Indian Institute of Chemical Engineers – Bangalore Center, Catalysis Society of India Bangalore Chapter, Poornaprajna Institute of Scientific Research (***PPISR***), and Dayananda Sagar College of Engineering, Bangalore from 26th – 28th August 2021.

Catalyst is the key element in many of the current industrial chemical and biological processes for efficient economical production of valuable compounds. Both academicians and industries work relentlessly to meet this need by developing new catalyst materials. In this regards it is essential to create an ecosystem where researchers from academia and industry come together on the same platform with a common goal to strengthen the catalyst research for application in the field of energy and environment, thereby, contributing to the development of the nation as well as humanity.

I wish the conference to succeed in providing a vibrant platform for the participants to brainstorm on the various thrust areas of the conference.

Dr. N V R Naidu
Principal
M S Ramaiah Institute of Technology Bangalore

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Message from Principal, Dayananda Sagar College of Engineering, Bangalore

I am happy to note that Bangalore Regional Centre, IIChE in association with Catalysis Society of India, Bangalore Chapter, and Department of Chemical Engineering M S Ramaiah Institute of Technology, Poornaprajna Institute of Scientific research and Department of Chemical Engineering Dayananda Sagar College of Engineering has organized 1st Online International Conference on **Emerging Trends in Catalysis for Sustainable Chemical Processes 2021 (ETCSCP–2021)** between 26th – 28th August 2021. I am sure that this International Conference ETCSCP–2021 will be beneficial for participants, students and faculty. I complement the organizing committee of this international conference and wish the conference a grand success.

Dr. C P S Prakash
Principal
Dayanada Sagar College of Engineering Bangalore

Message from Chairperson, IIChE Bangalore Regional Centre

On behalf of the organizing committee, I am elated to extend a warm welcome to all for the first Online **International Conference on “Emerging Trends in Catalysis for Sustainable Chemical Processes (ETCSCP-2021)”** organized by the Indian Institute of Chemical Engineers – Bangalore Center in association with Catalysis Society of India Bangalore Chapter, Poornaprajna Institute of Scientific Research (***PPISR***), Department of Chemical Engineering, M S Ramaiah Institute of Technology, Bangalore and Dayananda Sagar College of Engineering, Bangalore from 26th – 28th August 2021.

Indian Institute of Chemical Engineers – Bangalore Center has always provided insights to the chemical engineering fraternity in the upcoming interdisciplinary areas. Research activities across plethora of chemical fields has been the priority for IIChE, BRC and as one step towards that this conference has been planned to bring the experts from premier institutes and industry across the globe to share their expertise in the area of Applied Catalysis and related technologies.

This conference emphasis on disseminating knowledge on the recent advances in the field of catalysis encompassing energy, environment and chemicals. Several young research scholars have been given opportunity to present oral as well as poster presentations based on their research findings.

On behalf of IIChE, BRC and MS Ramaiah Institute of Technology, Bangalore, I appreciate the organizing committee for showing a keen interest in making all the necessary arrangements for the Conference. The Academia and industry collaboration, well knitted by the organizers will enormously benefit the catalysis researchers.

Dr. Archna
Chairperson, IIChE -Bangalore Regional Center,
Professor and Head,
Department of Chemical Engineering MSRIT Bangalore

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PLENARY SESSIONS

Plenary Session 1

Bipin V. Vora,
Consultant,
Adjunct Professor, IIT-Chicago
Retired UOP/Honeywell Fellow, Elected to NAE-USA, NAI-USA, INAE-India

Dr. Bipin Vora, Recipient of 2013 Platts Global Lifetime Achievement award and 2011 Chemtech-India Technology Leadership Award was inducted into National Academy of Engineering (NAE) in 2018. He is elected as a Foreign Fellow of Indian National Academy of Engineering December 2020 and elected to National Academy of Inventors, USA in 2021. After 48 years at UOP, Bipin joined IIT as an adjunct professor in Chemical and Biological Engineering Department. Products produced today employing technologies developed under leadership of Bipin Vora are valued at more than 30 billion US dollars per year.

He received B. Sc. (Hons) in Chemistry from University of Mumbai in 1963, followed by B.S and M.S. degrees in Chemical Engineering from the University of New Mexico, Albuquerque, NM, and joined UOP in 1967. Bipin has been credited to leading development and commercialization of several new process technologies, among them UOP Oleflex™ process for propane and isobutane dehydrogenation; higher conversion Pacol™, DeFine™ and UOP/Cepsa Detal™ alkylation processes for the production of linear alkylbenzenes, a raw material for synthetic detergents; and UOP/Hydro MTO™ process for conversion of methanol to olefins.

He holds 95 US Patents and over 200 international patents. He has over 150 publications in various technical and trade journals, including contributions to Kirk-Othmer Encyclopedia of Chemical Engineering, Encyclopedia of Chemical and Process Design, Handbook of Detergents, Handbook of Heterogeneous Catalysis, Handbook of Industrial Catalytic Processes, Applied Catalysis, Handbook of Petroleum Refining, Advances in Carbon Management Technologies and Studies in Surface Science and Catalysis.

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Success Factors in Catalyst Development to Commercialization

Abstract:

Catalysis plays a critical role in virtually every industry so does the process design innovation. This presentation takes one through weaving the chemistry, catalysis, and various aspects of process and reaction engineering, from laboratory to pilot plant, to a commercial design and to a successful start-up.

From invention of a catalyst to a commercial success is a long journey. What makes such process a success is to have an entrepreneurial team leader taking the project from concept, weaving art of various disciplines. One should note essential success factors for this journey.

Success Factors

Work on Right Project,
Meet Safety, environmental and social needs
visionary Management
Entrepreneurial Team Leader
Set Boundaries, Goals, targets for each task at the beginning
Right experiments & Coordination with engineering and other disciplines.
understating experimental results
Be skeptical of Data
Four Eyes are better than Two
Out of Box thinking members of Various Disciplines
Putting pieces together, Art of weaving catalysis, Chemistry and engineering.
Supportive and Forgiving Management

These success factors for catalyst development to commercial success are highlighted with an example of development and commercialization of catalytic dehydrogenation of propane to Propylene and other personal experiences of the author.

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Plenary Session 2

Virendra Kumar Gupta
Reliance Research & Development Centre, Reliance Industries Limited, Navi Mumbai 400 701 India

Dr Virendra K Gupta, R&D Head - Polymer & Senior Vice President, Reliance Industries Limited is an accomplished Scientist & Technologist who has successfully translated his fundamental work in Catalyst & Material Science in to Commercial Technology implemented first in India.

Dr Gupta is an inventor / coinventor of 200 patents and commercialized 30 Technologies in Petrochemicals and Polymer Sectors. He has 80 Research Publications in Peer Reviewed Journals and 90 Invited and Contributed Presentations in International and National Conferences. He is a recipient of VASVIK Award, Acharya PC Ray Awards for Development of Indigenous Technology and 20 Other Technology and Product Development Awards from Govt. of India and Industrial Organizations.

Dr Gupta obtained Ph.D. from Banaras Hindu University and worked also at Indian Petrochemicals Corporation Limited and Gharda Chemicals Limited after Teaching and Research Assignment at University of Alabama at Birmingham, USA. He has 40 years Professional Experience covering Teaching, Petrochemicals Research, & Technology Development and Management.

Indigenously Developed High- Performance Catalyst Technology for Polyolefin Materials: Invention to Commercialization

Abstract:

Discovery of transition metal-based catalyst for olefin polymerization in 1950's by Karl Ziegler and Giulio Natta have made enormous scientific, technological and societal impact through industrial production of polyolefin materials. The scientific contribution of Ziegler & Natta is recognized by awarding the Noble Prize in 1963.

Continuous innovations in catalyst and polymerization technology has resulted in current global production of olefin based polymer touching to ~190 million ton / annum. It is close to 60 % of total synthetic polymer produced worldwide annually. The applications of polyolefin materials cover most of high growth sectors like packaging, transportation, agriculture, automobile, defense etc.

The present talk presents the development of advanced catalyst technology for homo and copolymers of ethylene as well as propylene [1-10]. The production of polyolefin materials is accomplished through homo and copolymerization processes catalyzed by organometallic compounds controlling different polyolefin product characteristics such as molecular weight, thermal, rheological etc.

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Plenary Session 3

Sander van Bavel

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Dr. Sander van Bavel is currently leading the long-range research program of Methane to Products at Shell. Since early 2018, he was also been appointed as Principal Science Expert in Catalysis. Previous roles were mainly in heterogeneous catalysis with a strong focus on basic research, specifically in Fischer-Tropsch Synthesis (GTL technology) and olefin epoxidation. Sander was one of the inventors of an improved catalyst currently deployed in the Shell's Pearl GTL plant and co-inventor of a newly implemented technology at the same plant. He has joined Shell's Innovation, Research & Development department in 2006 after obtaining his Ph.D. in Chemistry from the Eindhoven University of Technology, the Netherlands. Sander is co-author of tens of scientific papers and patents.

Methane Utilization – an industrial perspective

Abstract:

In the coming decades the share of renewable energy in the energy mix will expand substantially worldwide. This development is supported by the strong cost reductions of solar and wind energy. As a consequence, it can be expected that renewable electricity will become more abundantly available at competitive prices – and strongly contribute to the power sector, hydrogen economy (e-H_2) and as a direct source of energy. This energy transition will thus substantially impact the value and use of methane as its current main outlet is in power generation and in hydrogen production (grey hydrogen). In this paper we will discuss some areas of research to position methane and natural gas as an advantaged feedstock for chemicals, and as source for low carbon-intense hydrogen.

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Plenary Session 4

Prof. Kamal Kishore Pant
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Prof. Kamal Kishore Pant, is currently Petrotech Chair Professor and Head of the Department of Chemical Engineering at IIT Delhi, Adjunct Faculty at University of Saskatchewan, Honorary Faculty at the University of Queensland, Australia and Joint Faculty in Centre for Rural Development at IIT Delhi. Prof. Pant's research contribution involves a wide range of innovative studies covering both theoretical and experimental aspects of heterogeneous green catalysis for coal to chemicals, biomass and fossil hydrocarbon conversion to hydrogen and fuels, CO2 capture and conversion, waste to wealth and value-added chemicals. Prof. Pant is a part of research consortium which is developing a technology for conversion of high ash Coal to Methanol in collaboration with Thermax. Prof. Pant has over 30 years of academic and research experience during which he has published 175+ Journal articles having 9500 citations (google H index 50), Three Books and granted several national and international patents. Prof. Pant has successfully completed over 50 high impact projects and consultancies valued more than 1.5 billion Indian Rupees from India's and worlds top most premier companies and organization such GAIL, HPCL, DRDO, TATA Chemicals, NOVOD, MHRD, CSIR, IARI, Ministry of Defense, SERB, Ministry of Fertilizers, DST Government of India and Petrotech Society of India. Owing to his outstanding contribution the academia and research Prof. Pant is frequently invited as an expert member in several national and international scientific committees such as SERB, DST, CPCB, Ministry of Electronics, Ministry of New and Renewable Energy, etc.

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Tuning the Cu^0 and Cu^+ ratio on Mg/Mn/Ce promoted Cu-based catalysts for conversion of CO_2 rich syngas to methanol and dimethyl ether

Abstract:

Thermocatalytic conversion of CO/CO_2 to green fuels viz. methanol and dimethyl ether (DME) has been considered as one of the topmost research priorities all over the world to mitigate the levels of these hazardous oxides in the atmosphere. Moreover, methanol/DME may not only help in minimizing the environmental impacts but also reducing the dependency on non-renewable resources and meeting the energies supply demand simultaneously. Currently, the Indian coal reserves have a significant potential for producing methanol and DME via gasification process in which the coal is gasified to CO_2 rich syngas which is subsequently converted to methanol/DME. The catalytically active material for this reaction include metals, metal oxides and intermetallic compounds. Since CO_2 emissions from direct coal combustion pose a significant problem in coal utilization, coal gasification has attracted extensive attention. The present study provides a comprehensive view of the significant advances of binary and ternary catalysts for methanol/DME synthesis through CO_2 rich syngas hydrogenation. Additionally, significant challenges in developing robust catalytic systems with excellent catalytic performance and long-term stability are discussed thoroughly. Moreover, efforts are made to develop various Cu/Cu^+ based catalysts with novel synthesis approaches using Mg, Mn, (for CO_2 rich syngas) and Ce, Zr (for pure CO_2) as co-promoters. These catalysts were characterized in terms of structural, morphological, textural and chemical features by sophisticated multi-technique approach. Characterization results revealed that the use of promoters enable the modification in crystallinity, modulation of surface structures, and stability of active centers of catalysts. The activity results demonstrated promising behavior of the catalysts for the CO/CO_2 conversion as well as valorization of the CO_2 since it outperforms the conventional catalysts. In addition to this the importance of in-situ characterization and theoretical studies on understanding mechanistic insights and in designing improved catalysts are presented.

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Plenary Session 5

Dr. Ajay K. Dalai,
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Dr. Ajay K. Dalai research focus is the novel catalyst development for gas to liquid technologies, biodiesel production, hydrogen/syngas production, hydroprocessing, value-added products from biomass, and pollution control. He has supervised over 150 M.Sc., Ph.D., and Post-doctoral Fellows and has received over 35 million dollars for his research over the past 25 years. Dr. Dalai has published over 550 research papers mostly in heterogeneous catalysis and catalytic processes in international journals and conference proceedings. He has submitted several patent applications. His ground-breaking research has led to over 31500 citations of his work and H-index of 82. He serves in Editorial Board of several prestigious journals. Professor Dalai has received fellowship from different societies such as Royal Society of Canada, Royal Society of Chemistry in UK, International Association of Advanced Materials, American Institute of Chemical Engineering, Canadian Academy of Engineering, Chemical Institute of Canada, Engineering Institute of Canada, and Indian Institute of Chemical Engineers. Professor Dalai is also a Fulbright Fellow from USA, DAAD Fellow from Germany and JSPS Fellow from Japan. Professor Dalai has received several national and international awards. Recently, he has received Indian Institute of Chemical Engineers DRC Life Time Achievement Award, Canadian Society of Chemical Engineering R.S. Jane Memorial Award for outstanding contributions to Chemical Engineering Profession, Royal Society of Canada's Miraslow Romanoswki Medal for Outstanding Contribution to Environmental Science, and University of Saskatchewan's George Ivany Internationalization Award.

ISBN: 9789391131449

Bioprocessing Technologies for Clean Sustainable Energy Production

Abstract:

Biofuels are gaining attention as renewable energy sources to address the rising energy demands, fluctuating crude oil prices and greenhouse emissions from fossil fuels. Biofuels can be produced from a wide variety of renewable feedstocks and biogenic wastes through thermochemical, biological and hybrid conversion technologies. This presentation will highlight the candidacy of a variety of bioprocessing technologies for a wide range of waste feedstocks such as lignocellulosic biomass (e.g. agricultural crop residues and woody biomass), energy crops, sewage sludge, municipal solid waste, food waste, waste cooking oil, waste tires as well as petroleum residues (e.g. heavy/light gas oils, bitumen, asphaltene and petroleum coke) to produce clean sustainable energy production. Although these waste residues are available in considerable amounts worldwide, their potential for resource recovery is least realized. This presentation will highlight some notable research studies conducted in the Catalysis and Chemical Reaction Engineering Laboratories (CCREL) over the past 25+ years at the University of Saskatchewan on biomass-to-gas (BTG) and biomass-to-liquid (BTL) conversion technologies to produce synthetic transportation fuels and carbon-rich solid products. The potential and performance of integrated clean technologies, especially hydrothermal gasification, liquefaction, pyrolysis and Fischer-Tropsch synthesis will be discussed along with the upgrading of biocrude oils through catalytic hydrotreating. Synchrotron-based advanced structural chemistry studies on the synthesis, characterization and application of novel catalysts and nano-catalysts used in BTG and BTL technologies will be comprehended. The current progress, challenges and knowledge gaps in the R&D of BTG and BTL technologies for the production of synthetic hydrocarbon fuels from waste resources as well as their opportunities to Canadian bio-economy will be comprehensively reviewed.

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Plenary Session 6

Dr. 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. E-mail: skannan@csmcri.res.in

Dr. Kannan Srinivasan specializes in the area of Heterogeneous Catalysis & Materials Chemistry. He obtained M.Sc from IIT Madras, Chennai, India in 1990, Ph.D. from IIT Madras, Chennai, India in 1995, followed by Post-Doctoral Fellowship at National Chemical Laboratory, Pune, India in 1996. His current affiliation is with CSIR-Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI; www.csmcri.res.in) as Director. He is also Professor, Academy of Scientific & Innovative Research (AcSIR), India. He has authored more than 80 research publications with over 2600 citations and h-index of 32. He has authored a book on catalysis entitled “Catalysts and Surfaces: Characterization Techniques”. He has several book chapters and is the primary inventor of eight original patents which includes five granted US Patents. He was a member of the delegation representing the country in the field of catalysis and has handled several research projects.

He is the recipient of CSIR Young Scientist Award and INSA Medal for Young Scientist – 1998. He was awarded Alexander von Humboldt Fellow - 2001-02, Prof. H. Knozinger, LMU, Germany and JSPS-INSA Research Fellow - 2003-04, Prof. T. Hattori and Prof. A. Satsuma, University of Nagoya, Japan. He was Raman Research Fellow – 2009, Prof. Tom Mallouk, The Pennsylvania State University, USA and Dharamsi Morarji Chemical Company Visiting Fellowship by Institute of Chemical Technology, Mumbai for the year 2013-14. He also was Secretary, Catalysis Society of India 2011-2013 and Executive Committee Member, Catalysis Society of India 2009-2015. He was Affiliate member, Royal Society of Chemistry from 2012-16 and American Chemical Society Member, 2015-18, 2020. He is part of the editorial board of various journals. He was a fellow of Royal Society of Chemistry, 2016 and Gujarat Science Academy, 2016 & Vice President, GSA, 2020. He is the recipient of CRSI Bronze Medal – 2018.

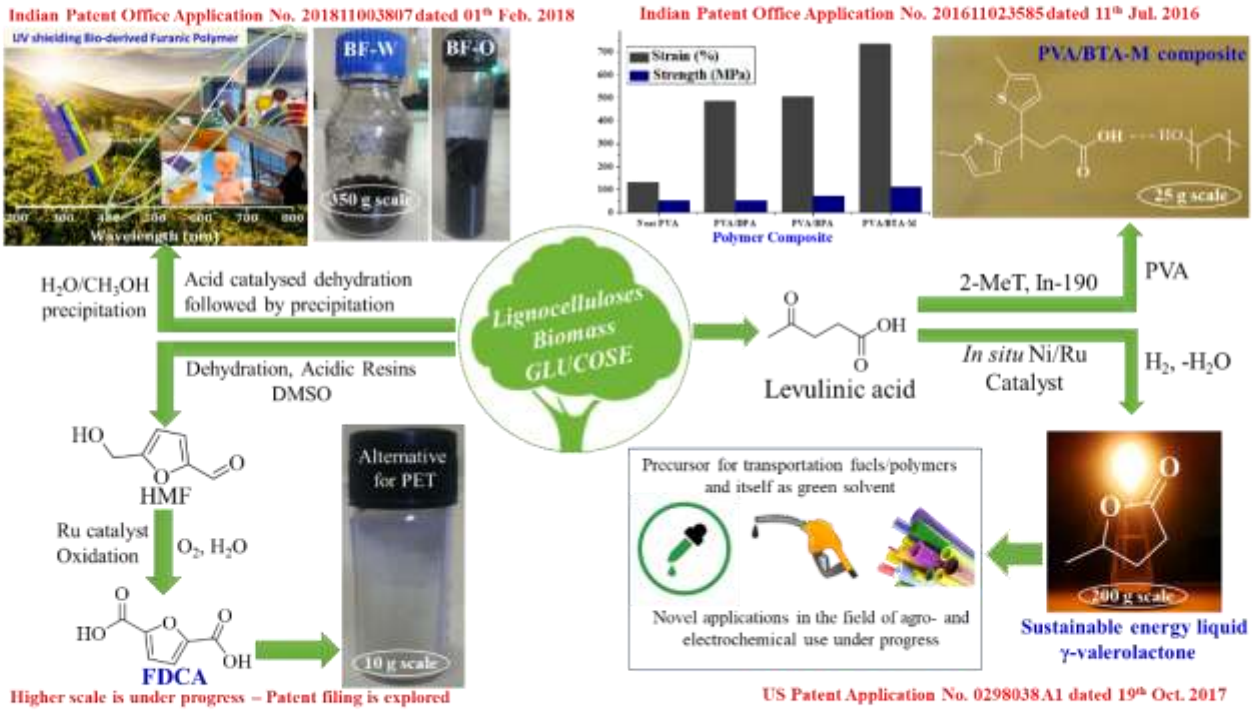
ISBN: 9789391131449

Biomass to Chemicals and Polymers – Opportunities & Challenges

Abstract:

Currently world’s energy and chemicals requirement are largely met through fossil resources like petroleum, coal and natural gas. The demand for the energy and quality of life is continuously growing that makes the world to look for alternate solutions. Sustainability, probably the “*word of this century*”, will be the prime mover in stimulating scientists and technologists while looking at such alternate options in making fuels, chemicals and polymers that are indispensable in our daily lives. Biomass is the only renewable source that has useful carbon atoms that could fervently be explored with significant potential for the production of chemicals that includes polymers. This is *de facto* an attractive option considering the balance between the availability and consumption patterns. The approach also has an intrinsic advantage of reducing indispensability on fossil fuels to an extent besides reducing CO_2 emission thereby positively contributing to climate change. Researchers across the world have made considerable advancements on biomass value addition for producing chemicals. India with its strong roots on agriculture, diverse availability of enormous forest/agro resources and vast coast line for marine macro/micro algae, 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 few of the ongoing work in the domain of biomass to chemicals and polymers carried out at this institute with an emphasis on γ-valerolactone, levulinic acid derived plasticizers, 2,5-furandicarboxylic acid (FDCA) and furanic polymers that have impending opportunity (at the same time with challenges) in establishing new chain of industries.

Keywords: Biomass valorization; Furan compounds; Levulinic acid derivatives



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Plenary Session 7

Dr. K. Seshan obtained his PhD in 1980 in Materials Science from Indian Institute of Technology, Bombay, India, followed by career as Research Scientist, R&D, Indian Petrochemicals Corporation, India from 1980 – 88. He joined as Faculty Member, University of Twente, The Netherlands in 1988. Currently he is working as Professor in the area of Renewable Fuels & Chemicals. He has 354 Publications in International peer reviewed Journals, 21 Reviews/Book chapters and 11 Patents.

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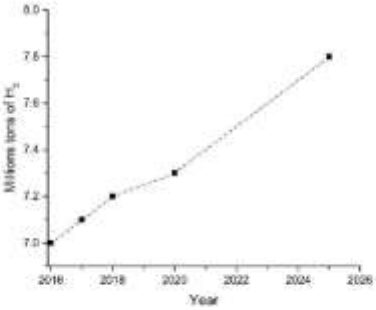
Hydrogen from biomass wastes via Aqueous Phase Reforming

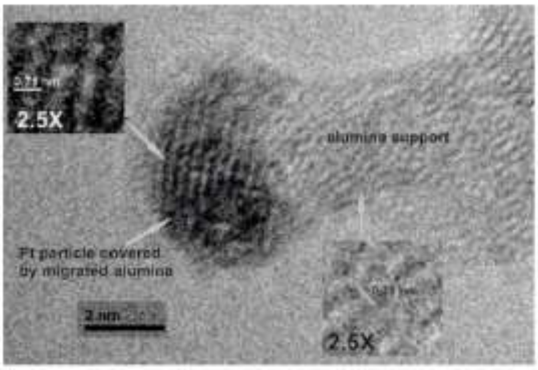
Abstract:

Demand for hydrogen is ever increasing and environmental legislations require that a major part of this is “green hydrogen”. Waste water streams from, e.g., food industries or bio refineries have aqueous effluents that contain dissolved organics, usually in the range of 5-20 wt%. Aqueous Phase Reforming (APR, Gasification in hot compressed water), allows for the generation of hydrogen from these, e.g., sugars, $C_6H_{12}O_6 + 2H_2O \dashrightarrow 4CO + 2CO_2 + 8H_2$.

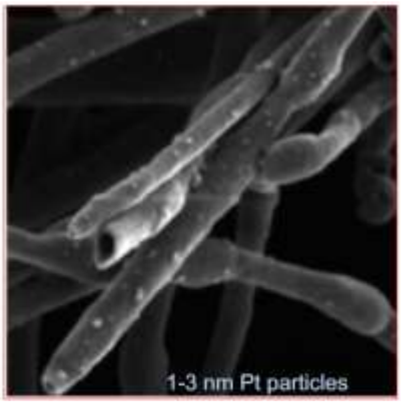


During APR, steam reforming of dissolved oxygenates occur at milder temperatures in pressurized liquid water (225-270 °C, 30-60 Bars). As these conditions also favour the Water Gas Shift reaction ($CO + H_2O \dashrightarrow CO_2 + H_2$) hydrogen yields are maximized during APR.

In general, Hydrogen selectivity due to the competing formation of alkanes (e.g., $CO + 3H_2 \dashrightarrow CH_4 + H_2O$) is one problem. Catalyst (typically metals on oxide support) stability under these harsh conditions is another issue for commercialization of the process. They relate to sintering of metal particles, leaching of the metal, support (and subsequent migration to cover metal particles as seen on the figure right) and/or coke formation due to oligomerisation of the intermediates formed during reaction, e.g., olefins, aldehydes, etc. Extensive research work carried out at our



laboratories have allowed us to develop stable metal particles and supports and that are suitable for APR catalysis.



In this presentation let us look at the reasons for the problems that affect the performance of the catalyst during APR of oxygenates found in bio waste streams. A thorough understanding of the processes happening on the catalyst surface allows ways to overcome these limitations. Genesis of a catalyst that maximizes hydrogen yields and at the same time shows resistance to deactivation will be presented. The aim of this lecture is to present to young researchers, a methodology that can be applied to be successful in catalysis research and thus be relevant to industrial application.

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Plenary Session 8

Dr. Pramod Kumbhar
President and CTO,
Praj Industries Ltd.

Dr. Pramod Kumbhar, is working with Praj Industries, as President and Chief Technology Officer for last 9 years at Praj Matrix – R&D centre leading 90+ scientists and engineers. After working for 20+ years in petrochemical (hydrocarbon) industry made a shift to biotechnology led renewable fuels and chemicals industry. Focused on driving innovations in biotechnology to make biofuels and bio chemicals. Ph.D. in Chemical Engineering from Institute of Chemical Technology (formerly UDCT), Mumbai. UAA-ICT Distinguished alumnus award (Research) for 2020 from UDCT Alumni Association and Institute of Chemical Technology, Mumbai. VASVIK Award for 2020 in chemical Science and Technology, Received the Green Chemistry award from IGCW 2019 for the furfural process. Post-doctoral stints at CNRS laboratories in Montpelier and Institute of Catalysis, Lyon in France. Fellow of Maharashtra academy of sciences. Received the ICI process development award from Indian Institute of Chemical Engineers. Worked at General Electric R&D Centre in Bangalore and SI Group (formerly Schenectady chemicals, USA) in various positions including last assignment as R&D director for Asia Pacific. 30+ International patents. Received Bronze and silver medals from GE for patent filings. More than 30 publications in peer reviewed scientific journals.

Role of Reaction engineering and Catalysis in sustainable bio-processes

Abstract:

The talk will mainly focus on emerging technologies and processes where catalysis and reaction engineering (CRE) can significantly contribute to solving the energy and single use plastic pollution problem. Enhanced process efficiency via intensification and multifunctionalization of biomass conversion will be the major topics covered. The role of CRE in overcoming some of the challenges in the energy and materials arena will be illustrated with examples. Emphasis will be placed on how biocatalyst development and reactor/fermenter design can be used for production of renewable chemicals and fuels from biomass.

ORAL PRESENTATION

P-001

Enhanced one-pot selective conversion of cellulose to ethylene glycol over mesoporous NaZSM-5 supported metal catalysts

Sreejith Sreekantan,[a] Arun Arunima Kirali,[ab] Banu Marimuthu*[ab]
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[b] Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh.

Abstract:

The demand for liquid transport fuels and chemicals is growing continuously and they are produced from fossil resources, which are limited and non-renewable. Their production from renewable feedstocks such as inedible biomass is attractive, as this approach can lead to carbon-neutral technologies. The study on the catalytic conversion of cellulose was initiated in 1980s and achieving a renewable carbon based economy by the resourceful utilization of this complex polysaccharide is still challenging. In 1917, the production of ethylene glycol (EG) was semi commercialized and the global market volume for EG is escalating since then. The polyesters, particularly PET used widely for clothes and for packaging, the demand for glycols specifically EG is furthest up. Furthermore, EG is also a used as coolant, antifreeze agent, heat transfer agent and desiccant. Currently, ethylene glycol is manufactured from ethylene attained by petroleum cracking. Zeolite supports are the popular for its stability, pore structure and ranging acidity. The reports on zeolite supported catalyst for cellulose conversion are limited. G. Liang et al reported 91.2 % selectivity of hexitols over Ni-ZSM5. However, the challenges to be overcome in the present study includes retaining the stability of the catalyst and obtaining high conversion of cellulose and high yield of EG at milder reaction conditions. In the present work, the mesopores interconnected with microporous NaZSM-5 was synthesised by sol-gel method. The reactions on cellulose using the different bimetallic and trimetallic combination of nickel, aluminium and tungsten metals supported on NaZSM-5 have been carried out. The different weight percentages (wt%) of Al-Ni-W were loaded on NaZSM-5 support by wet impregnation method. The prepared catalysts were characterized by using PXRD, FE-SEM, HR-TEM, BET and XPS confirmed the presence of mesopores, textural properties, metal loading and active oxidation states. The catalytic activity of xAl-yNi-zW/NaZSM-5 (where x, y, z are the wt % of Al, Ni, W metals respectively) supported catalysts was studied for one-pot conversion of cellulose into ethylene glycol under at 220 °C temperature and pressure of 70 H_2 bar (at reaction temperature), in water (as a solvent). The 5%Al-8%Ni-25%W/NaZSM-5 catalyst exhibited the highest cellulose conversion of 100% with ethylene glycol yield as high as 89% (C mol%) at moderate reaction conditions has been reported for the first time. The Al^{3+} in the catalyst hydrolysis the cellulose, W^{5+} species acted as an acid centre which facilitated the retro-aldol condensation reaction and eventually led to an increased EG yield in the presence of Ni. The catalyst was stable after four consecutive run for 6h, 220°C, at 70 bar H_2 reaction pressure. The high yield at moderate reaction conditions promises the process to be energy efficient and economically feasible.

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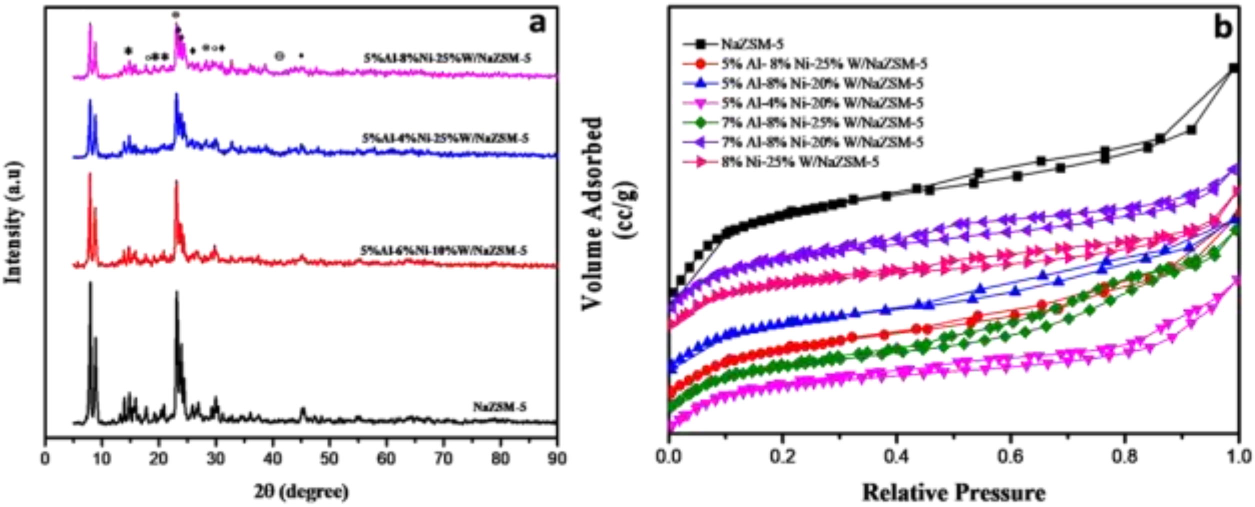

Fig. 1 (a) The XRD patten of NaZSM-5 support and metals supported over NaZSM-5. The peak labelling is as follows: ◆ for WO_3, ○ for $NiWO_4$, * for $Al_2(WO_3)_4$, ⊕ for Ni, ⊗ for Al_5W (b) The BET adsorption isotherm of support and metals supported over NaZSM-5 support.

Entry #	Conversion (%)	Reaction Parameters				Yield[b] (%)				
		Catalyst : Cellulose ratio	T (°C)	P (bar)	Time (h)	EG	PG	Glu	Sor	Total glycol (EG+PG)
1	100	0.3:1	220	70	6	36.9	22.4	19.7	-	59.3
2	100	0.75:1	220	70	6	70.8	10.0	12.8	2.3	80.8
3	100	1:1	220	70	6	74.1	8.4	12.8	2.9	82.5
4	85.1	1:1	220	70	1.5	59.8	9.2	20.1	2.4	69.0
5	**100**	**1:1**	**220**	**70**	**12**	**89.0**	**0.8**	**6.5**	**0.4**	**89.8**
6	100	1:1	220	50	6	63.2	7.3	14.1	4.4	70.5
7	100	1:1	220	60	6	65.9	12.2	14.4	2.7	78.1
8	45.6	1:1	200	70	2	52.9	7.8	26.0	7.4	60.7
9	66.7	1:1	200	70	6	59.6	10.3	19.4	2.7	69.9
10	97.3	1:1	200	70	12	70.0	10.0	12.3	4.0	80.0

Table 1. Catalytic activity data of 5%Al-8%Ni-25%W/NaZSM-5 catalyst in the conversion of cellulose to ethylene glycol.[a] ; [a]Reaction conditions : Cellulose: 0.20 g; Catalyst: 0.06–0.2 g; water: 20 ml; pressure: 50-70 bar H_2 (at reaction temperature); temperature: 200 -220 °C; time: 1.5 -12 h; stirring speed: 1000 rpm; [b]EG= Ethylene glycol, PG= 1,2-Propanediol, Sor= Sorbitol , Glu = Glucose.

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P-002

Catalyst-Engineered and Multi-Dimensional Covalent Organic Frameworks as Sustainable Photo-Catalysts for Aerobic Cross-Coupling Reactions

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Abstract:

Recent advancement in developing unprecedented methodology for the construction of new classes of carbon–carbon bonds will overwhelmingly dictate overall synthetic efficacy of organic synthesis, wherein visible-light driven cross-dehydrogenative coupling (CDC) rank top priority with enhanced catalytic ability.[1] However, from the standpoint of sustainability and economic viability, such systems should be recyclable, and operate under environmentally green condition in highly synergistic and atom-efficient manner.[2a] To this end, covalent organic frameworks (COFs) have attracted much attention because of their large porosity, high stability, and prospects to effective band-gap modulation for photocatalysis. Especially, applications that aim sustainable catalysis have surfaced as hottest areas of research, wherein incisive amalgamation of active homogeneous catalyst over COF backbone benefit pore-environment modulation for atom-economic and recyclable CDC reactions.[2b]

Aiming at visible light mediated direct α-arylation of glycine derivative for rapid access to indolylglycines without the aid of bases, a chemo-robust two-dimensional (2D) imine COF is designedly built from [2,2']bipyridyl (Bpy) unit functionalized pores. Integration of Bpy unit benefits anchoring of active homogeneous complex Ru(Bpy)$_2^{2+}$ over the framework backbone to devise Ru-2DCOF that acts as unprecedented visible light photocatalyst towards coupling of secondary amines with indoles in excellent yield at room temperature, under aerobic condition.[3a]

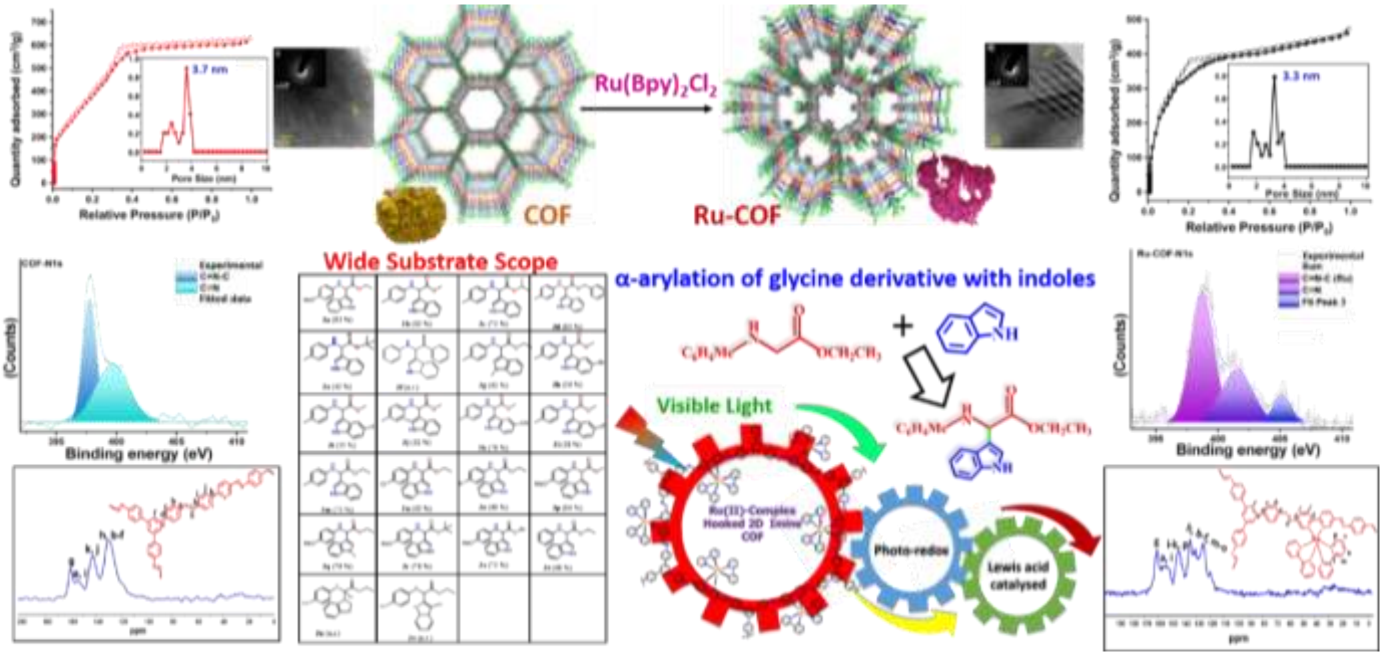

Figure 1: Structural engineering in pre-functionalized covalent organic framework via anchoring active Ru(II)-complex for visible-light triggered and aerobic cross-coupling of α-amino esters with indoles.

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Ru-2DCOF shows admirable reusability and superior activity to that of homogeneous catalyst Ru(Bpy)$_3$Cl$_2$, while substrate variation studies delineate wide ranges of functional group tolerance. To the best of Ru-2DCOF, atom-economic C−H functionalization is realized in a way that iminium ion intermediate is in situ generated. The photocatalytic route is detailed from astute modulation of optical band-gap in light of density-functional theory studies and experimental results, which validates single-electron-transfer pathway.

Then again, size-selectivity in CDC reaction for synthesizing important building blocks is almost non-existent that urges the involvement of 3D COFs, where reaction site accessibility within pre-designed pores impose barriers to diffuse larger-sized substrates. In this regard, a three-dimensional, amine-based COF is fabricated surmising on the combination of tetrahedral (T_d) amine vertex and N-functionalized linear strut. The 3D COF features diamondoid network with high architectural robustness. Involvement of [2,2']bipyridinyl units provides an opportunity to graft homogeneous catalyst Ru(Bpy)$_2$Cl$_2$ devising first-ever 3D Ru-COF that acts as visible-light mediated photocatalyst for oxidative cyanation reaction of tertiary amines in excellent yields at room temperature in green solvent H_2O, using molecular oxygen as selective oxidant.[3b] Admirably, atom economic photocyanation reaction is realized through in situ generated iminium ion intermediate, and diminishes additional steps of conventional Strecker reactions. The activity of this catalyst engineered COF compares favorably well to homogeneous counterpart, while separation difficulty of photocatalyst are excluded. Importantly, outstanding conversion and selectivity are maintained for a range of tertiary amines, while larger sized substrates exhibit insignificant conversion, demonstrating poe-fitting-induced size selectivity.

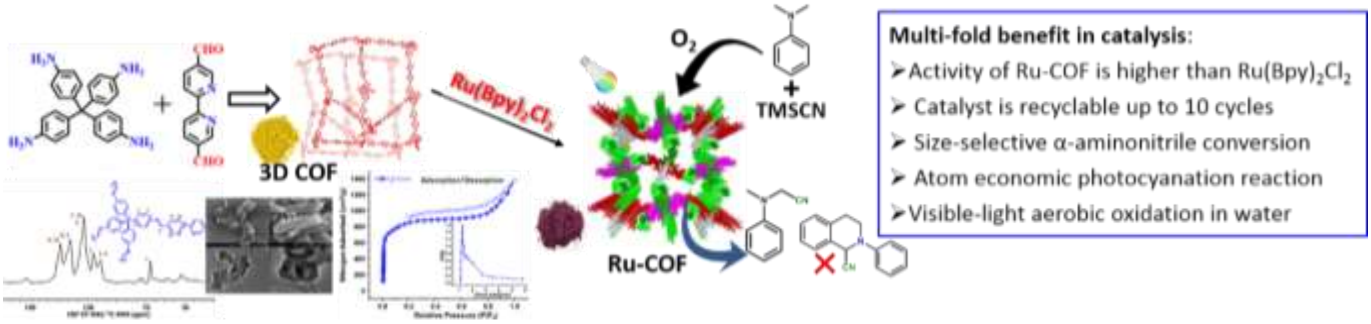

Figure 2: Post-metalated covalent organic framework for size-selective photo-cyanation through sustainable route.

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P-003

Green Synthesis of Ag-ZnO nanocomposites using “Amaranthus Viridis” plant extract for catalytic, electro-catalytic and photo-catalytic applications.

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Abstract:

In contemporary research, nanocatalysts plays an important role in extracting varied properties and resulting in more effective, efficient and diversified applications. The present work focuses on green nanocatalysts of Ag/ZnO nanocomposite using the plant extract of “**AMARANTHUS VIRIDIS**”. The synthesized nanocomposites were characterized using XRD, FTIR, SEM analysis. The obtained nanocomposite assembly was used for **catalytic, electro-catalytic and photo-catalytic applications.** 4-Nitrophenol Reduction and methylene blue dye degradation were taken as model reactions for catalytic /electro-catalytic and photocatalytic studies.

The opted plant extract has a good amount of phytochemical constituent of flavonoids and phenols which will act as the reducing agent in the process of converting the precursor solution to the equivalent Metal/Metal Oxides. Fig.3a& Fig.3bareXRD and FTIR characterization results confirms the formation of the Ag/ZnO Nanocomposite, and other characterization techniques like UV – Visible spectrophotometer, SEM analysis was also done for the obtained nanoparticles. It was seen that the Ag/ZnO Nanocomposite show a higher efficiency in the reduction process of the 4-Nitrophenol to 4-Aminophenol when compared to the individual performance of the Ag and ZnO Nanoparticles as a catalyst. The Outcome of this work helps to understand the mechanism of the green synthesis but also helps to achieve the low-cost catalyst for further applications.

Keywords: Nanocatalysts, Ag, ZnO, Green route, 4-NP.

Experimental Methodology:

- A 20g of fresh green leaves of Amaranthus Viridis was taken and washed with tap water once and distilled water twice to remove dust and soil content over the leaves. Then add those leaves with 150ml of Distilled water is taken in a 500ml beaker and keep this mixture for heating for 20mins at 70^{0}C. After that filter the leaf extract using Whatman filter paper no.1 and store the leaf extract in a cool atmosphere for further use.

- Take 100ml of leaf extract in a round bottom flask and add the required amount of $AgNO_3$&$Zn(CH_3COO)_2.2H_2O$ and add 2ml of Fresh Lemon juice extract for the precursor solution and close the flask with aluminum foil and keep it under the sunlight for 4hrs. Later collect the solution and do centrifugation process and keep those samples in the hot air oven for overnight to remove moisture content in samples and later keep those samples in the muffle furnace for calcination process at 450^{0}C for 5hrs. Later collect the samples and make them into a fine powder using mortar & pestle and store the samples in sample holders for further use.

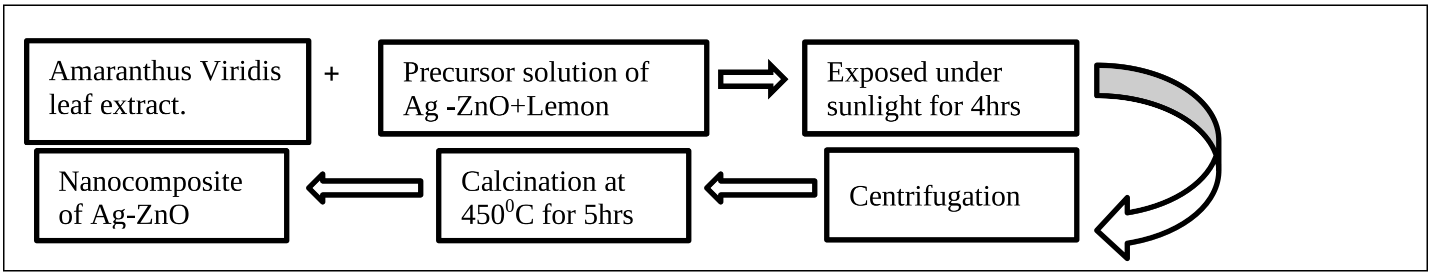

Figure1: Block Diagram representation of Ag-ZnO Nanocomposite.

❖ The 4-Nitrophenol studies were performed for synthesized nanocomposites of Ag-ZnO, collect required amount of 4-NP solution in a beaker then add a few amounts of $NaBH_4$ solution for the same keep them under stirring for few minutes. Later add a small amount of Ag-ZnO nanocomposites to the solution under stirring then we will notice the rapid Colour change of the 4-NP solution i.e. from Dark yellow to the colorless solution that which indicates the reduction of 4-NP to the 4-AP.

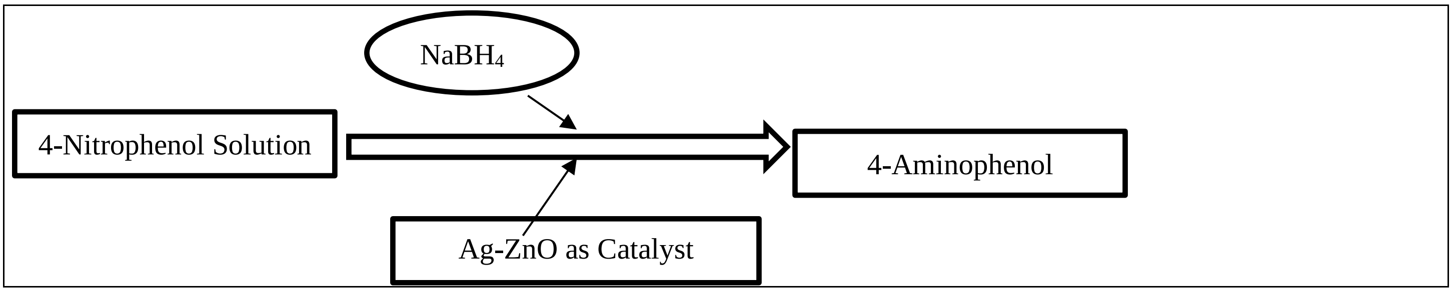

Figure2: Block Diagram representation of 4-Nitrophenol Reduction.

Results:

❖ The preliminary characterization techniques like XRD and FTIR confirm the formation of Ag/ZnO Nanocomposites. Fig.3a indicates the XRD peaks of Ag-ZnO Nanocomposites with the theta angles of Ag with 38.18^0, 44.25^0, 64.72^0, $77.40^{0,}$ and ZnO with 31.84^0, 34.52^0, 36.38^0, 47.64^0, 56.7^0, 63.06^0, 68.1^0 respectively. Fig.3b represents the FTIR Result of Ag-ZnO with the wavenumbers of 2113, 1091, 593nm of Alkyne, CN stretch, C-S stretch respectively.

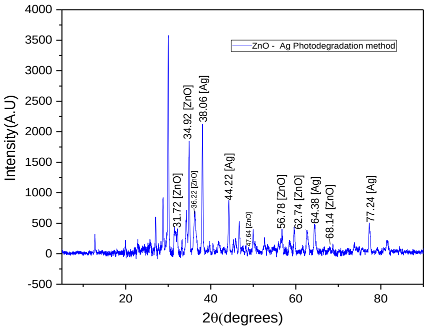

Figure.3a: XRD Result Ag-ZnO Nanocomposite

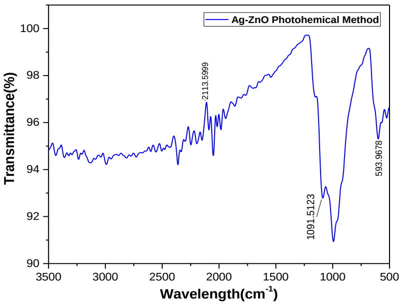

Figure 3b: FTIR Result Ag-ZnO Nanocomposite.

Conclusion:

❖ The further characterization techniques like UV – Visible spectrophotometer, SEM analysis were need to be done for the obtained nanoparticles. It was seen that the Ag/ZnO Nanoparticles show a higher efficiency in the reduction process of the 4-Nitrophenol to 4-Aminophenol when compared to the individual performance of the Ag and ZnO Nanoparticles as a catalyst. The Outcome of this work helps to understand the mechanism of the green synthesis but also helps to achieve the low-cost catalyst for further applications in the future.

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P-004

Solvent-Free Synthesis of Bimetallic Nickel-based Hydrotalcite Type Materials and Their Application on Hydro-treatment of Anisole

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Abstract:

Hydrotalcites a potential catalysts and catalyst supports, conventionally synthesized by the co-precipitation of M^{2+} and M^{3+} metal cations at a low temperature and a constant pH.[1] However, the large scale production of these materials at the industrial level by this method has disadvantages, such as the need for large amounts of water, the treatment of metal salt effluents, and the significant differences in the hydrolysis rates of different metal salts, lead to undesirable inhomogeneity in the product.[2-4] The preparation of HTs through a solid-state reaction is an alternative route to solution-phase synthesis; it proceeds through mechano-chemical methods, an environmentally friendly, simple, quick process, and does not require large solvents. This method also avoids the loss of chemical components (i.e., it is an atom-efficient route).[5,6] The nickel-based catalysts are known as a potential for hydro-treating processes in various petrochemicals and biomass hydrogenation.

Thus, the object of the present work focused on preparation of a series of bimetallic nickel-based HT materials (NiAl-HT, NiRh-HT, NiRu-HT, and NiIr-HT, respectively.) by a solvent-free, environmentally friendly, and atom-efficient method. The physico-chemical properties of the developed materials were investigated using various spectroscopic and analytical techniques.

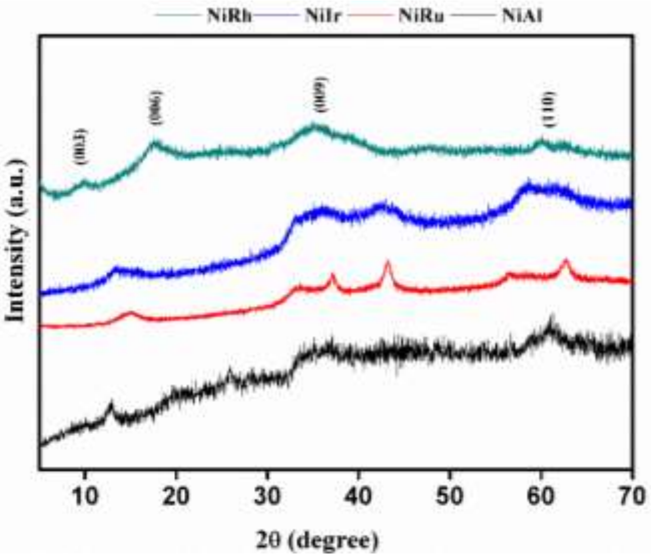

Figure 1 Powder XRD patterns of solvent-free synthesized nickel-based HT materials:

The powder XRD patterns of all the solvent-free synthesized bimetallic nickel-based HT materials (Fig. 1) show that the diffraction patterns correspond to the layered structure of HT. The XRD patterns of all samples show diffraction peaks at approximately 12.9°, 25.7°, 33.2°, 36.9°, 44.3°, 58.7°, and 60.3°, corresponding to the (003), (006), (009), (015), (018), (110), and (113) planes of the HT structure, respectively. This suggests that the samples prepared by the solvent-free approach had a well-developed layered structure with good crystallinity.[7] After calcination (400℃), the nickel-based HT materials were evaluated regarding their activity in the hydro-treatment of anisole, which serves as a lignin model

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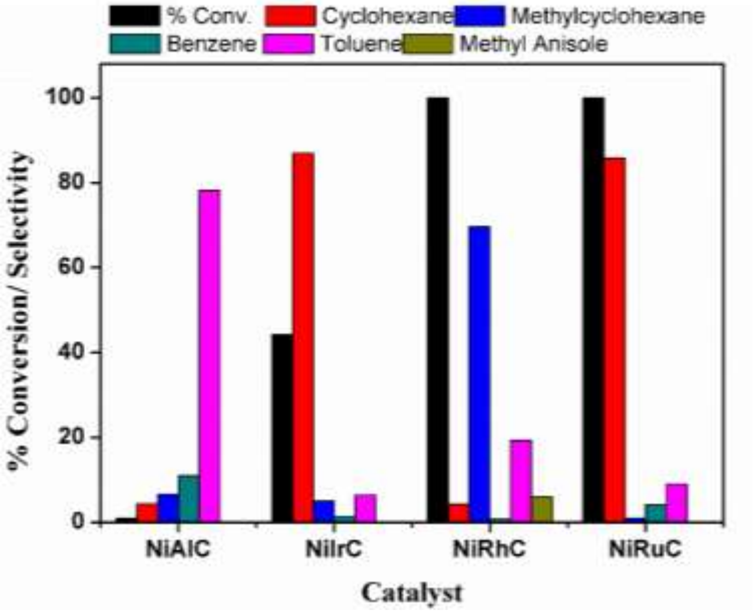
compound (Fig.2). After optimization in mesitylene, reactions were performed at 170 °C under 2.5 MPa H_2 pressure, using 0.05 g of catalyst for 6 h in a 50 mL Teflon-lined autoclave (high-pressure stirred reactor system SR1323, KLB India). Gas chromatography (GC) analysis revealed the primary products to be cyclohexane, methylcyclohexane, benzene, toluene, and methyl anisole.



Reaction conditions: catalyst, 0.05 g; substrate, 5.0 mmol, anisole; solvent, 5 mL, mesitylene; T = 170 °C; H2, 2.5 MPa; t = 6 h.

Figure. 2 Hydro-treatment of behaviors of the bimetallic nickel-based catalysts prepared by a solvent-free method regarding the hydro-treatment of anisole.

Among the various catalysts studied, the bimetallic nickel catalysts containing noble metals exhibited the highest activity and selectivity in the hydro-treating of anisole (Fig. 2). This proves that there was a positive synergistic interaction between nickel and noble metal catalysts, which increased the conversion of the hydrotreatment of anisole. Hydrogen spillover occurred more easily on the surfaces of noble metal-Ni catalysts. Among the various noble metal incorporated HT, the bimetallic NiRu and NiRh catalysts achieved the complete conversion of anisole, with cyclohexane and methylcyclohexane being the major products, respectively.

A simple method on preparation of nickel-based HT was prepared and explored for hydrotreatment of anisole. The preliminary result showed best activity occurred on Ni-Ru based catalyst.

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P-005

One Pot Synthesis of Oxazolidinone Isomers: Three Component Reaction of Amine, Epoxide and CO_2 by Efficient Mixed Metal Oxide Catalyst

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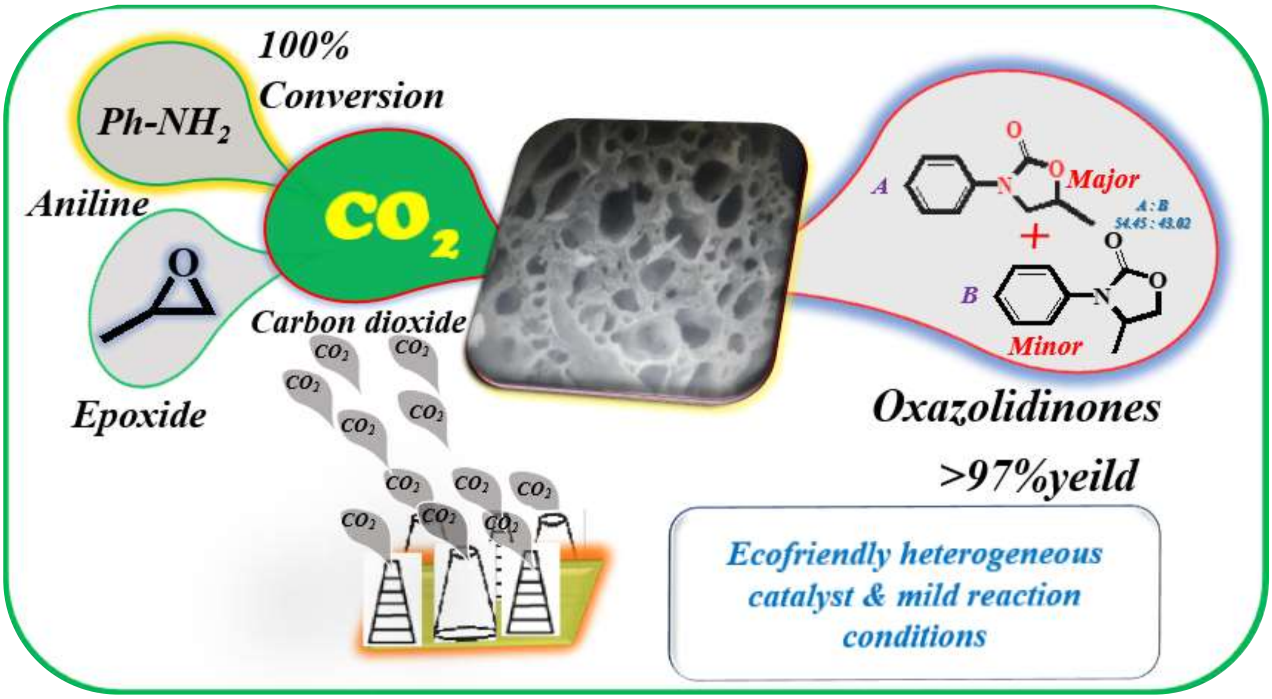
Abstract:

Greener synthesis pathway of value added chemicals from CO_2 utilization is very trending research topic, in viewpoint of sustainable and green chemistry concepts owing to its vast industrial applications. Given this industrial interest, development of low-cost, less-toxic, highly active and stable catalysts enabling the optimum reuse of CO_2 for the preparation of chemicals is vital. In the present work, the mixed metal oxide catalyst was synthesized by using a facile combustion method and used for oxazolidinone synthesis through three component reaction between terminal epoxides, CO_2 and aryl amines. The catalyst was characterized by various techniques such as XRD, SEM, TPR/TPD, FT-IR and BET surface area analysis. To our delight, metal oxide catalysts presented appreciable activity with 100% conversion without base and solvent. Moreover, various reaction parameters such as effect of time, temperature, pressure, catalyst loading and molar ratios was discussed extensively and the reaction products confirmed by GC-MS data. Based on the experimental evidences and reaction results, the tentative catalytic mechanisum of oxazolidinone synthesis from CO_2, aniline, and propylene oxide was proposed. A variety of anilines and epoxide substrates were studied using the protocol with prominent conversion and excellent yield of desired oxazolidinones product. Intrestingly, the catalyst displayed impressive performance in recyclability study without significant loss of its initial activity.

Graphical abstract



P-006

Development of Novel Catalysts for n-Hexane Isomerization

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Hindustan Petroleum Green R&D Center, Banaglore

Abstract:

Hydrocarbon isomerization reactions are of significant relevance to the petroleum refining industry and are utilized in the production of Gasoline and Lubricants. Light Naphtha Isomerization process is used to enhance the octane of low RON naphtha to high RON Isomerate. Typically, noble metal based chlorided alumina catalysts are used for this process. They are highly acidic and therefore active at low temperatures such as 140°C. However, these catalysts suffer from disadvantages such as high sensitivity to poisons S/N/H_2O and low-down times due to operation issues.

Recently, noble metal-based zeolite catalysts have been developed and commercialized globally. This catalyst possesses advantages such as relatively better resistance to poisons and consistent operation performance. However, these catalysts operate at relatively higher temperatures around 250°C leading to a RON penalty of 2 units due to severe operating conditions. Therefore, there is an immediate need for catalysts which are highly active at low temperatures and have better stability against poisons.

In this work novel bifunctional noble metal-based catalysts were developed using heteropoly acids supported on mesoporous materials such as SBA-15, MCM-41, MCM-22, MCM-48, Mordenite and Reduced Graphene Oxide. Catalysts were characterized using X-ray diffraction, scanning electron microscopy (SEM), temperature programmed desorption (TPD), thermo gravimetric analysis (TGA) and nitrogen adsorption (BET).

This work put insights on the morphological transitions which enhanced the metal impregnation. Figure 1 and 2 shows the morphological transition of Heteropoly acids (HPA) and reduced Graphene Oxide Assisted HPA respectively.

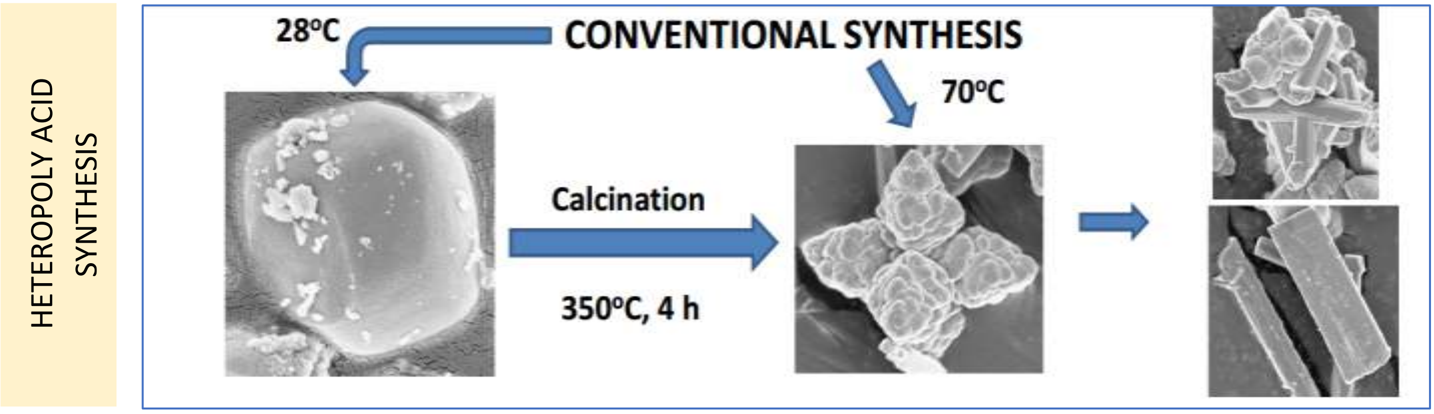

Figure 1. Morphological transition of Heteropoly Acids

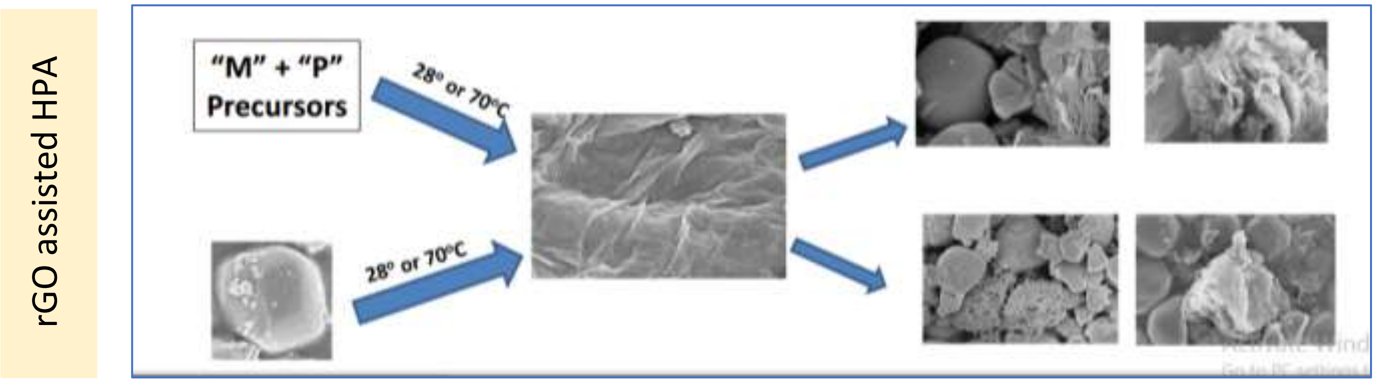

Figure 2. Morphological transition of Heteropoly Acids (HPA) assisted by reduced Graphene Oxide (rGO)

Reaction conditions were optimized with respect to temperature, pressure and WHSV. The mesoporous structure of support as well as the composition was observed to play in vital role in controlling the reaction temperature and selectivity towards the formation of high RON isomers. It was observed in this study that novel materials like rGO and HPA were synthesized and their kinetics, morphological transitions were studied by varying synthesis parameters. The crystallization behavior of HPA was improved over refluxing conditions. Secondly, composite catalysts with HPA and rGO were synthesized and the % metal loading and the type of metal loading was optimized for n-hexane isomerization. Also, a high RON isomerate was produced with better conversion with rGO-assisted HPA catalyst. In this study, alternative to Pt/MOR catalyst i.e., rGO assisted-Ni-HPA catalyst was developed. Lastly, the optimum temperature for n-hexane isomerization with the catalyst in our study is 250^0C and optimum pressure is 30 bar.

P-007

Mg-Fe-Mo ternary oxide-based material as potential catalyst for oxidation of biomass model component isoeugenol

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Abstract:

Layered double hydroxides or hydrotalcite (HT) materials are well known as potential catalyst precursors and supports for several organic transformations [1]. HT materials have been widely used as ion exchangers, catalysts and catalyst precursors, pharmaceuticals, UV stabilizers, adsorbents etc. Hydrotalcite materials are layered materials consisting of positively charged two dimensional sheets with water and exchangeable charge-balancing anions present in the interlayer region. The general formula of the hydrotalcite materials is $[M^{2+}_{1-x}M^{3+}_{x}(OH)_2]^{x+}(A_{x/n}^{n})\cdot mH_2O$, where M^{2+} and M^{3+} respectively represent divalent and trivalent cations, A is the interlayer anion with charge n, and x is the fraction of trivalent cations[2]. Hydrotalcite like materials are used as catalysts or catalytic supports in reduction, oxidation, alkylation, condensation, hydroxylation, transesterification, isomerisation, epoxidation, hydro-isomerisation and reforming [3]. Numerous such materials have been developed by varying framework divalent and trivalent metal ions, and interlayer anions.The intercalation of silicate,phosphate,molybdate etc., may broaden the scope of the materials. Molybdenum compounds have been widely used in various catalytic applications such as hydrodesulfurisation, epoxidation, propene hydration etc., [4]. The objective of the present work is to introduce molybdate species into the Mg-Fe-HT materials and the resultant Mg-Fe-Mo ternary oxide-based materials to explore for the oxidation of biomass model compound, viz., isoeugenol.

Molybdate was introduced into the Mg-Fe-HT by *in-situ*hydrothermal method during the synthesis using metal nitrate salts in presence of ammonium hydroxide and ammonium heptamolybdate at pH = 9. A series of molybdenum intercalated magnesium iron hydrotalcite catalysts(HMFeMo) having different molybdenum ratio were successfully prepared and characterized by FT-IR spectra, X-ray diffraction (XRD), UV-VIS studies.

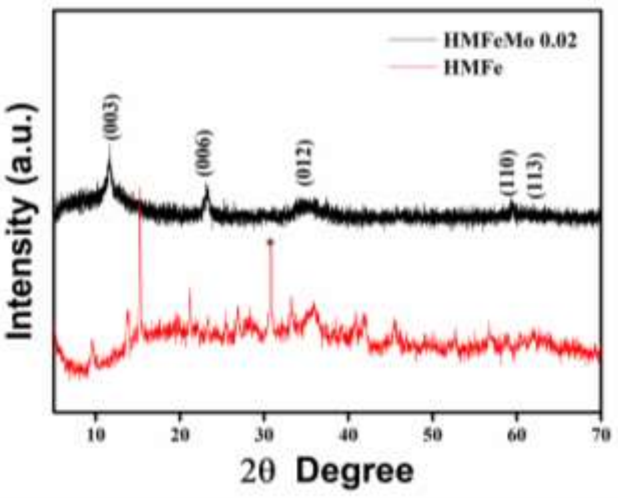

Figure 1. Powder XRD pattern of (a) Mg-Fe-HT and (b) Mg-Fe-Mo-0.02 HT.

The presence of interlayer water and carbonate ions were evident from FT-IR vibration band appeared between 4000-3000 cm^{-1}(γ_{O-H})and at 1380 cm^{-1}(CO_3^{2-}) respectively. Presence of molybdate ions is confirmed from the observed vibrational peak near 840 cm^{-1}. The powder XRD pattern of the synthesized materials also confirm the intercalation of molybdate anions (Figure 1).The broad peaks at 2θ of 11.5°, 23.1°, 34.7°, 59.5°, and 61.2° in the XRD patterns of the as-synthesized HMFeMo samples corresponded to the (003), (006), (012), (110), and (113) planes, respectively, of layered hydrotalcite materials. The uniform distribution of molybdate species with the presence of molybedenum in its higher oxidation state (+5 and + 6) was evident from DRUV-Visible and XPS studies (not shown here). The Mg-Fe-Mo ternary materials have surface area around 175 m^{2}g^{-1}.

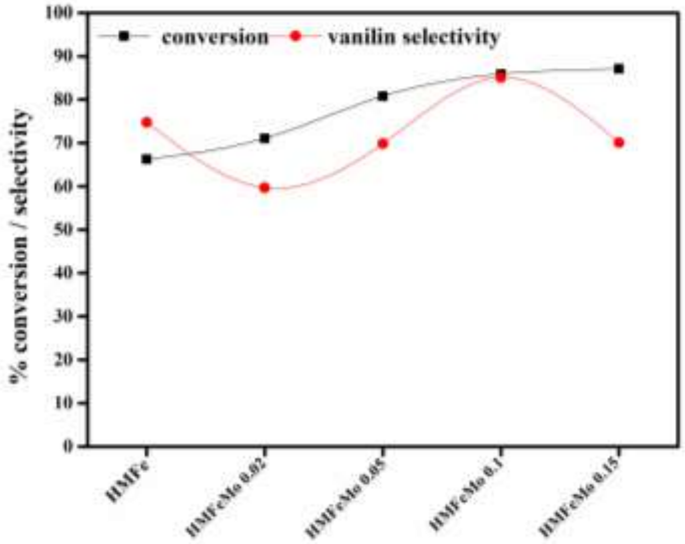

Figure 2. The role of molybdate ion concentration on oxidation of vanillin.

The resultant materials both in the as-prepared and calcined forms were studied for the conversion of biomass model compounds into valuable chemical. One such study is the conversion of isoeugenol to vanillin using tertiary butyl hydroperoxide as the oxidizing agent.The reaction conditions were systematically optimized at different temperature, duration, catalyst amount etc. Under the optimum reaction conditions, the concentration of molybdate ion concentration in reactivity was explored (Figure 2). The isoeugenol conversion and selectivity toward vanillin of HMFeMo0.1 were 86% and 83%, respectively at ambient reaction conditions. The activity remain intact for several hours.

To summarise, this is the first report on molybdate intercalated magnesium iron hydrotalcite for the production of vanillin from isoeugenol[4].

Acknowledgement: Author thank to CSIR and DST-SERB-CRG (Project No: CRG/2019/004624) for financial support.

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P-010

Graphene Oxide (GO) as a flexible adsorbent for Crystal Violet Dye degradation: Batch and Continuous column studies

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Abstract:

The effluents from textile industries contain toxic dyes which are not only consume dissolved oxygen and leading to destroy the aquatic life but also contaminate the environment. Adsorption is one of the most effective and economical method for treatment of waste water containing dyes. Graphene Oxide (GO) is highly effective adsorbent of Crystal violet and has been studied well for removal from aqueous solutions. Graphene Oxide has functionalized with oxygen containing groups and attracted resurgent interests because of its superior properties such as large surface area, mechanical stability. Herein, we report GO as a flexible adsorbent synthesized via Modified Hummer’s method for crystal violet dye degradation studies. The synthesized GO is characterized by XRD, UV-VIS Spectroscopy, SEM, and TEM. The Batch and Continuous Column studies were carried out to understand the effect of various parameters such as contact time, pH and adsorbent dosage. The outcomes of this article will help to understand the molecular mechanism of dye degradation.

Keywords: Crystal Violet dye, Graphene Oxide, Adsorption, Batch and Continuous Column studies, Modified Hummers Method.

Experimental methodology:

Graphene Oxide (GO) was synthesized using Modified Hummer’s method as shown in fig.1. This modified Hummer’s method of synthesis involves both oxidation and exfoliation of graphite sheets due to thermal treatment of solution. An Amount of Graphite(2g), sodium nitrate(1g) and 90mL of sulphuric acid (98%) were mixed in a 1000 ml volumetric flask and kept under in ice bath(lower than 5°C)with continuous stirring the mixture was stirred for 1hr and then add 12 g of potassium permanganate to the suspension very slowly. The rate of addition was carefully controlled to keep the reaction temperature lower than 15°C.After that remove ice bath, the heat of the suspension temperature brought up to 35°C and it had kept for 30 minutes. At the end of the 30 min 184 ml of water added slowly(drop wise) to that suspension, causing violet effervescence and an increase in temperature up to 98°C.After 10 min, the temperature changes to 30°C which gives that brown colored solution. After that 40 ml of H_2O_2 was added slowly and color changes to bright yellow, and add 184 ml of water to the solution and kept for 1hr. it is then kept without stirring for 3 to 4 hrs. When the particles settled at the bottom and remaining solution is poured to filter. The resulting mixture can washed several times with 10%HCl and then with deionized water until it forms like a gel substance (pH-neutral).After filtration, the gel like substance can dry at 80°C more than 8 hours then GO produced.

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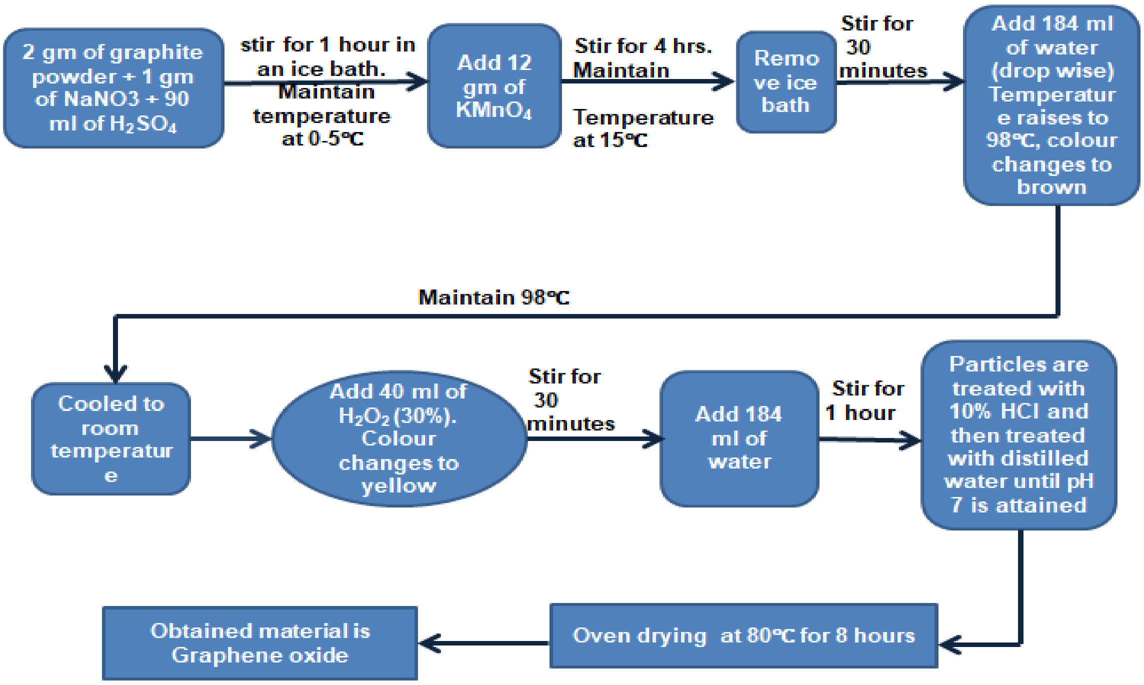


Figure 1-Schematic diagram for the synthesis of GO

Experimental setup:

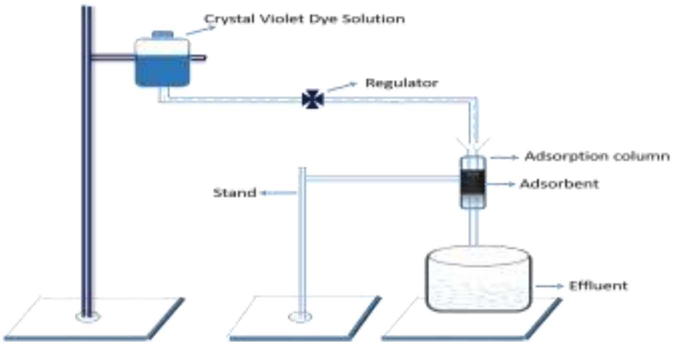


Figure 2- Column studies

Continuous column studies were conducted using a glass tube placed at a certain height. A schematic of the experimental setup used for the column study was shown in fig. 2**.** A regulator was used to maintain the desired flow rate. Due to gravity the crystal violet dye solution was passed through the adsorption column in order to remove the impurities from the adsorbent. The treated effluent is collected from the bottom of the column at different time intervals and the concentration of the dye was determined using UV-visible spectrophotometer.

Results: The batch and continuous column studies were conducted systematically and the preliminary characterization technique of XRD pattern obtained for as graphite, partially graphene oxide and synthesized graphene oxide (GO) shown in fig 3. XRD shows the peak for graphite in 2θ=32.81º, peak for partially graphite oxide 2θ=11.6º, 32.81ºand peak for GO in 2θ=10.52°, 42.38°, which is mainly due to the oxidation of graphite.

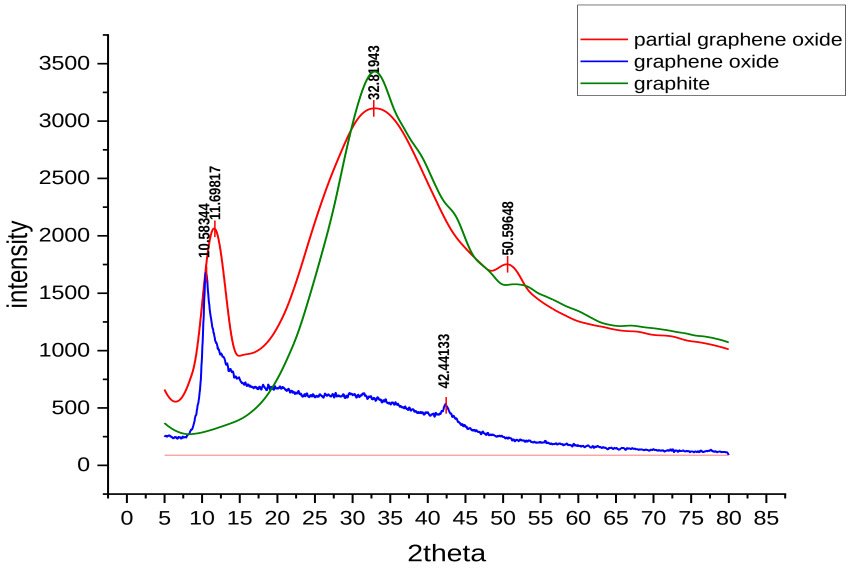
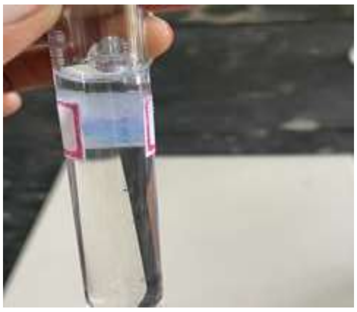


Figure 3-XRD result of Graphene Oxide

Degradation process:

Before degradation



After degradation

Conclusion:

The further characterization techniques like SEM and TEM analysis were needed to be done for the obtained synthesized GO Nano particles. The Batch and Continuous Column studies were carried out to understand the effect of various parameters such as contact time, pH and adsorbent dosage. The outcomes of this article will help to understand the molecular mechanism of dye degradation.

P-012

Formation of homojunction between g-C_3N_4 and P doped g-C_3N_4 for photocatalytic hydrogen production from water decomposition

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Abstract:

The type II heterojunction with g-C_3N_4 based photocatalysts plays a major role in hydrogen production owing to its tuned chemical potential between the two semiconductors. Thus results creation of strong internal electric field to enhance the charge carrier across the interface. Herein, we have developed isotype heterojunction between g-C_3N_4 and P-g-C_3N_4 by forming the surface P-C bond was confirmed by XPS results. The maximum hydrogen production of 1590 $\mu molh^{-1}g^{-1}$ is obtained for the optimized heterojunction catalysts which is 5.3 and 2.6 times higher than pristine g-C_3N_4 (300 $\mu molh^{-1}g^{-1}$) and P-g-C_3N_4 (600 $\mu molh^{-1}g^{-1}$). The achieved hydrogen production was mainly attributed to formed surface P-C bonds which simultaneously increase the spatial charge separation and prolonged carrier life-time. This was confirmed from PL, TRPL and photocurrent measurements. Besides the tuned electronic band structure and modified work functions of P-g-C_3N_4 which are also responsible for the improved photocatalytic activity.

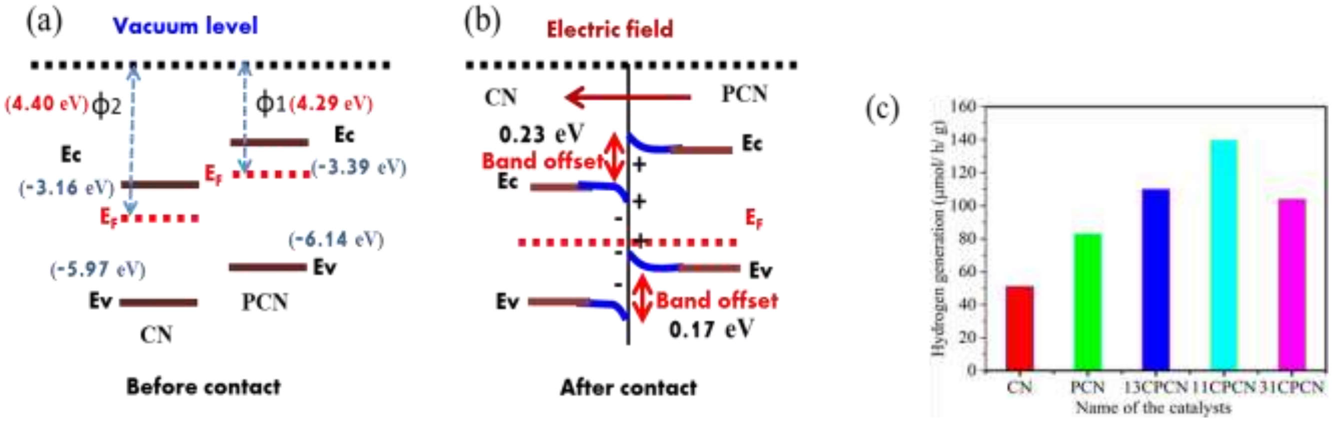

Figure 1. (a) Work function (b) band offset potential of CN and PCN (c) Photocatalytic activity of CN, PCN and CPCN catalysts

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P-016

"Synthesis and characterization of TiO_2 anatase nanoparticles for preparation of ethyl cellulose mixed matrix membranes (MMMs)"

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Abstract:

Polymer blending strategy is used to develop integrated membranes with new prospective benefits by adding the advantages of two compatible polymers. Although the method seems to be straightforward from the mixing point of view it is having limitations related to miscibility and interactions between the blending polymers. From the literature studies it is understood that, researchers are focusing on development of alternate and cost-effective polymeric membrane materials for use in industrial separations. New strategy of developing new membrane materials is enhancing polymer morphology by adding inorganic fillers such as TiO_2, graphene oxide, SiO_2 etc. The combination of polymer and inorganic phases is having advantages of both the phases and also results in highly potential membranes, mixed matrix membranes (MMMs) for use in separations with high efficiency.

In the present study, it is aimed to synthesis TiO_2 anatase nanoparticles and as prepared nano particles are used as filler material to blend with ethyl cellulose to cast ethyl cellulose/ TiO_2 mixed matrix membranes. TiO_2 anatase nanoparticles are synthesized and membrane is casted using 2 wt% TiO_2 of Ethyl cellulose dispersed in ethyl cellulose. The XRD results confirms that the formation of TiO_2 anatase nanoparticles which are matched with JCPDS database. XRD of 2 wt% filler incorporated in ethyl cellulose/ TiO_2 membrane clearly shows that the presence of both cellulose and TiO_2 nano particles confirming the polymer composite MMM system for various applications.

Keywords: Polymer Blend, Mixed Matrix Membranes, TiO_2 anatase nanoparticles, Ethyl Cellulose

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P-017

Rh-Porphyrin Complex Grafted Materials as potential Catalysts for hydrogenation of biomass model compound

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Abstract:

Porphyrins and metallo-porphyrins are fascinating macro-molecules, which are involved in a number of synthetic transformations and have great interest in industry and academic researchers. Porphyrin and its derivatives are well-known example of naturally occurring macrocylic compounds and play a significant role in biological life cycles. These compounds have strong affinity towards the metal ions and these are known as potential tool on biological, bio-chemical, photochemical applications [1-3]. On the other-hand transition metal (Co, Fe, Ni, Ru, Rh, Pt, Pd, Ir, etc.) based organo-metallic complexes, in particular group VIII-based complexes are shown great impact on various chemical, pharmaceutical processes due to their immense redox potential [3]. It will be interesting to introduce group VIII metals such as Ir3+, Rh3+ etc., into the cavities of porphyrin and porphyrin derivatives and encapsulate on functionalized surface materials and subsequently explore its catalytic behavior in various organic transformations. The preset work focuses on preparation and surface grafting of a rhodium (Rh) containing *meso*-tetraphenylporphyrin and explore its catalytic behavior in industrially important organic transformations i.e. hydrogenation reaction.

meso-Tetraphenylporphyrin (TPP) was prepared as per the standard procedure described in literature [1-4]. Metalloporphyrin (M-TPP, M = Rh) were prepared by refluxing equi-molar mixtures of respective macromolecules with corresponding metal salt in presence of a solvent. The resultant M-TPP was heterogenized by encapsulating M-TPP on amino functionalized SBA-15 molecular sieves (M-TPP-SBA-AM) [1, 2, 4-7]. Both homogeneous and heterogeneous macro-molecular catalysts were thoroughly characterized by various analytical and spectroscopic techniques such as FT-IR, UV-Vis, TGA, powder XRD, 1H NMR, Mass, CHNS studies. The catalytic activity of material was screened for hydrogenation of biomass derived levulinic acid.

The formation of TPP and metallo-porphyrin (M-TPP) were evident from 1H-NMR, Mass spectrum, UV-Vis and CHN studies. The surface grafting of M-TPP/M-TCPP were evident through powder XRD, N2-sorption, FT-IR, UV-Vis and NMR spectral studies. M-TPP/M-TCPP and the corresponding heterogeneous catalysts are shown as promising catalyst for hydrogenation of biomass derived levulinic acid to industrially important γ-valerolactone and 1,4-pentanediol with complete conversion at moderate reaction conditions. The product was confirmed by GC and FT-IR spectroscopic methods. All homogeneous catalysts were studied for several cycles. γ-valerolactone and 1, 4-pentanediol were obtained as the major products. The homogeneous catalysts showed conversion levels of 90–100 % even after several cycles. For the heterogeneous catalysts the conversion was decreased considerably after

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the third cycle. This loss in activity might be due to the chemisorption of reactant molecules on the surface of mesoporous materials, which block the active sites.

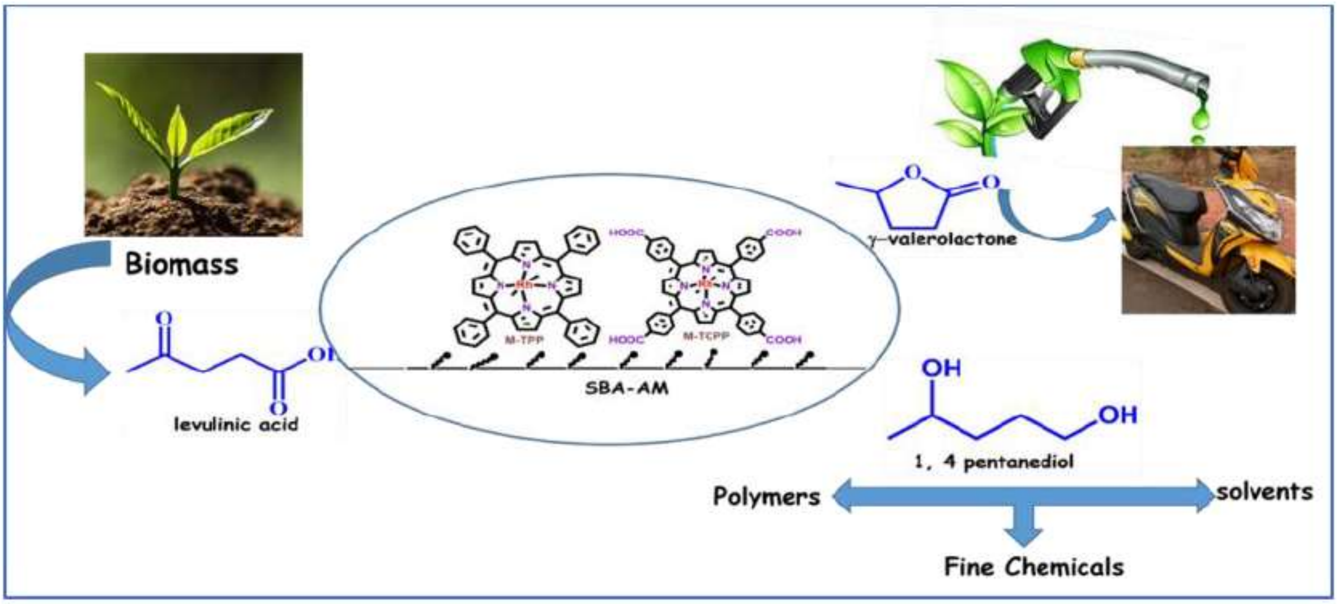

Figure 1: Conversion of levulinic acid using Rh based porphyrin catalysts

To summarize, rhodium containing porphyrins were prepared and encapsulated on the surface of functionalized mesoporous silica materials. The homogeneous porphyrins complexes and the corresponding heterogeneous catalysts were demonstrated as potential catalysts for industrially important biomass hydrogenation reactions as shown in figure 1.

Acknowledgements

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P-018

Hydrogenation and Valorization of Levulinic acid to γ-Valerolactone Using Cu/CeO_2-Al_2O_3 Catalyst

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Abstract:

The synthesis of fine chemicals like γ-valerolactone from the biomass derived levulinic acid through hydrogenation and valorization involved pathway is a promising approach towards the sustainable synthesis of value added products. This work demonstrates the development of Cu based CeO_2-Al_2O_3 heterogeneous catalysts for the effective hydrogenation and valorization of levulinic acid into γ-valeroalctone. The catalysts were prepared using impregnation protocol in a greener way avoiding the use of large amount of solvents. The successful synthesis and structural transformations was further characterized using spectroscopic and analytical tools. The catalytic activity resulted in 99% conversion of levulinic acid and 100% selectivity towards γ-valerolactone at 250 °C under vapor phase conditions. Further, various parameters were tested namely the feed rate, flow rate of H_2 gas to name a few. Additionally, upon the time on stream analysis it was revealed that the catalyst showed appreciable activity up to 5 h beyond which the conversion dropped to 10% after 7 h. This work provides an insight on the sustainable route for synthesis lactones, which can be adapted for scale-up applications.

Keywords: Levulinic acid valorization, γ-valerolactone, Hydrogenation.

P-019

Selective synthesis of furfuryl acetate from biomass derivative furfuryl alcohol over solid acid catalysts: Active site exploration using Density Functional Theory

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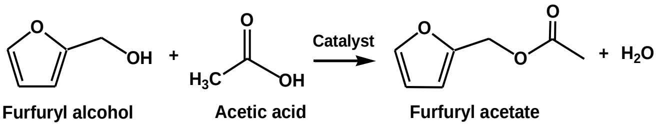
Introduction:

The impact of energy crisis on the renewable resources like solar, wind, water, and biomass has redefined the focus of scientists for the betterment of the mankind. Furfuryl alcohol (FA), a renewable biobased feed stock can be used to target the production of furfuryl acetate (FAc) (Scheme 1) that has application in the fragrance, flavour industry and as a potential biofuel and/or additive[1]. The present investigation embarks to find the conventional solid catalysts to identify the nature of active sites responsible to improve catalytic efficiency by study over porosity and acidity of the varied active sites. Screening of different solid acid catalysts (Zeolite-Y, H-Beta, ferrierite, SAPO-11, sulfated zirconia, Al-SBA-15 and amberlyst-15) showed that sulphated zirconia is the most efficient catalyst due to its mild acidity inhibiting the polymerization of FA. Post-calcination washing of the leachable sulfate species of sulphated zirconia and the optimization of the reaction conditions were studied to arrive at the best FAc yield reported so far.



Scheme 1 Esterification of Furfuryl alcohol to produce Furfuryl acetate

Materials and Methods

Sulfated zirconia, SAPO-11 and Al-SBA-15 catalyst were synthesized using the reported procedure from literature [2-4]. Additionally, the physisorbed sulfate ions in sulfated zirconia (S Zr) were removed by post calcination washing. Various physicochemical properties of the catalysts were investigated using techniques such as PXRD, NH_3-TPD, N_2 sorption studies, FTIR, ICP-OES and SEM. The samples of the reaction mixture were quantitatively analysed by gas chromatography (GC) and product identification was performed using Gas chromatography–mass spectrometry (GCMS).

Results and Discussion

Esterification of FA to FAc was carried at 70°C in liquid phase batch regime. Amberlyst-15, being a pure Brönsted acidic catalyst, showed poor results in terms of TON (Figure 1). As FA is prone to polymerization at the stronger acidic sites of catalyst, recyclability of catalyst always becomes a major issue to be addressed as the thermal stability of the catalysts is always expected to be above 300°C [5]. The strength of Brönsted acidity in most of the zeolites tested was strong because of which there was a pronounced effect of formation of humins. SAPO-11 inheriting displayed TON of 75 and has disadvantages of having presence of weaker phosphate type of acid sites and the steric constraints. S Zr with a lower surface area compared to most of the catalysts screened, had the combination of high acid

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site density, mild acidity synergistically helping to get high conversion and low polymerization of the FA. Therefore, S Zr with the highest TON of 126 was opted for further studies. S Zr catalyst showed 95% FAc yield at 24h at optimized reaction conditions (Figure 2) which is the best compared to the only reported catalyst[1] Fe-DTP@ZIF8 with FAc yield of 76%. DFT calculations were performed for the adsorption studies for the esterification of Fa to FAc mechanism over catalyst surfaces of S Zr, SAPO-11 and Al-SBA-15. The DFT calculations correspond with the conclusion derived from experimentation.

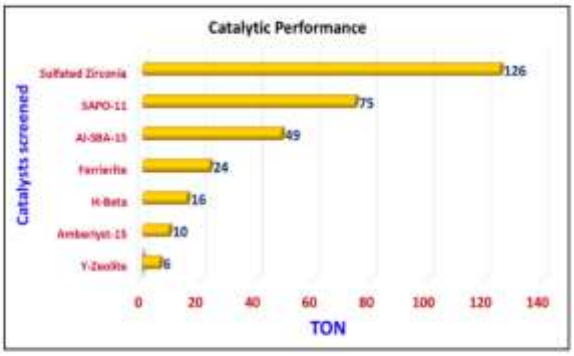

Figure 1. Catalyst screening. catalyst conc- 1.5wt%, T-70°C, time- 4 h, mole ratio- 1:10

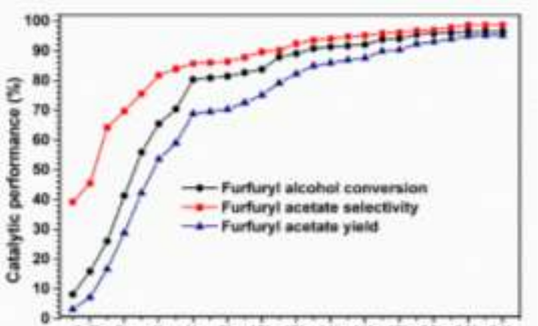

Figure 2. Reaction conditions: T-100°C, catalyst conc-0.37wt%, mole ratio- 1:10

Conclusion

Various solid acid catalysts with different physicochemical properties were studied to understand the nature of active sites required to efficiently convert FA to FAc. It was concluded that, moderate number and strength of acidity, high thermal stability and mesoporosity were found to be the optimum qualities required for the catalyst to obtain high yield towards FAc. These properties are inherently present in sulfated zirconia as it demonstrated excellent catalytic activity of 96% FA conversion and 98% FAc selectivity. DFT calculation was performed for adsorption studies for the mechanism over catalyst surface which supported the experimental results. DFT calculations also explained the difference in the type of active sites in different catalysts in terms of adsorption energies for the substrate molecule. Sulfated zirconia is a potential candidate as it has shown the best catalytic performance at the most desirable reaction conditions which promotes the green chemistry principles.

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P-020

Effect of acid modulators on catalytic activity of MIL-101 (Cr) in Prins condensation of β-pinene with paraformaldehyde

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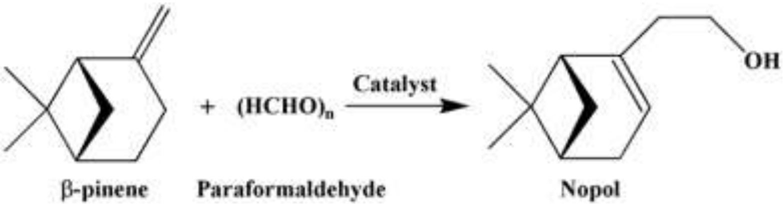
Abstract:

The development of efficient and sustainable strategies that evades the utilization of petroleum reserves is highly challenging yet inevitable today. In this context, biomass is a sustainable source of carbon that can be used to minimize the catastrophic effects of fossil resources on the environment [1]. Variety of chemicals, fuels and fuel additives can be obtained from the lignocellulosic biomass [2]. Among them, pine tree derived α and β-pinene have driven the significant research interest for being important bicyclic hydrocarbons from the commercial standpoint [3]. In this regard, the conversion of pine tree derived β-pinene to highly recognized nopol is particularly attractive owing to the widespread applications of nopol (scheme1).

Scheme 1: Reaction scheme for nopol synthesis by Prins condensation:



Herein, we describe an approach that enables the selective synthesis of nopol with extraordinarily high activity of MIL-101(Cr) catalyst. In particular, the MIL-101(Cr) materials having different textural properties have been synthesized using the three mineralizing agents by hydrothermal method. Four catalysts were characterized by various techniques and tested in the nopol synthesis from β-pinene and PFA condensation. Among the MIL-101(Cr) catalysts screened, the MIL-101(AA) (5 wt.% catalyst concentration) demonstrated the superior catalytic activity for the selective nopol synthesis (figure 01). This remarkable catalytic activity of MIL-101(Cr) is ascribed to its high specific surface area (SSA), accessible active sites in the mesopore architecture and unsaturated Cr^{3+} Lewis acid sites.

We have established a correlation between the superior catalytic performance and textural properties of the materials, which can be tuned by using different mineralizing agents. To realize the unprecedented catalytic activity, the influence of reaction parameters, solvent properties and mineralizing agents have been investigated systematically. To the extent of our knowledge, the catalytic activity of MIL-101(AA) (AA-Acetic acid) is superior to most of the reported materials for this transformation to date. The characterizations of catalytic materials reveal a good correlation between the textural properties and catalytic activity of MIL-101(Cr) catalysts. The MIL-101(AA) catalyst showed consistent results in the recycling experiments (Up to 5 recycles) (figure 02).

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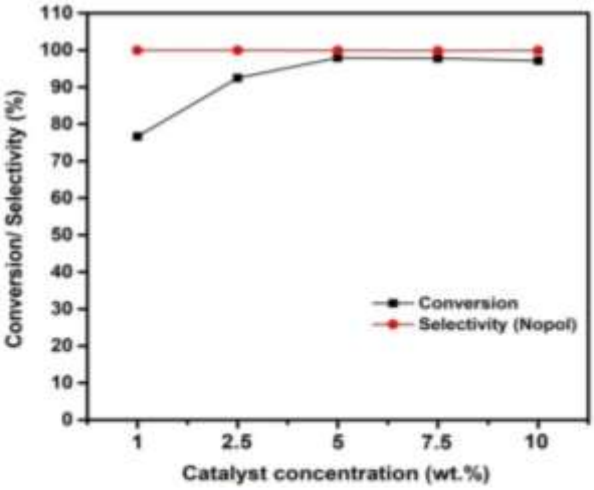

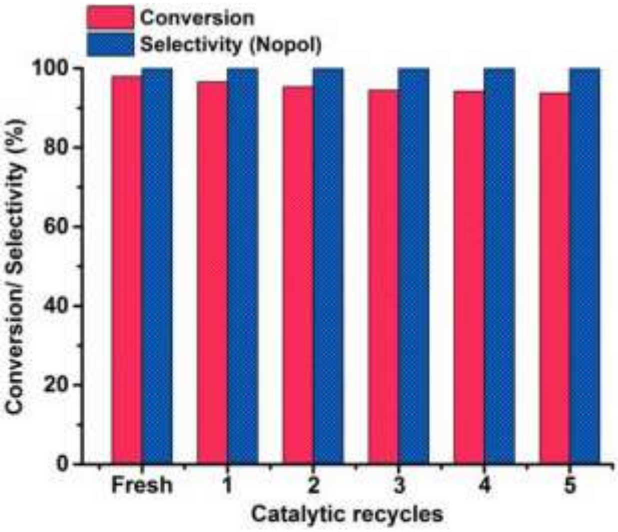

Figure 1: Effect of catalyst concentration

Figure 2: Recyclability studies

Default reaction conditions: Catalyst- MIL-101(AA), catalyst concentration- 5 wt.%, mole ratio- 1:2 (β-pinene: paraformaldehyde), solvent- benzonitrile (5 mL), reaction temperature- 90 °C, reaction time- 6 h, conversions were calculated with respect to limiting reagent (β–pinene).

The results of catalyst recycle and hot filtration experiments have emphasized that the catalyst is resistant towards leaching of active sites and retained its original catalytic activity beyond four recycles. MIL-101(AA) is found to be highly efficient, inexpensive and selective heterogeneous catalyst for the nopol synthesis by β-pinene condensation with paraformaldehyde. This approach opens up new avenues for the efficient conversion of biomass-derived molecules to vale added chemicals.

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P-022

Modified-Silica as an Efficient Catalytic Material for Probing Effective CO_2 Conversion into Cyclic Carbonates

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Abstract:

Carbon dioxide (CO_2) has been projected as an ultimate carbon building block for organic synthesis as CO_2 is considered as an abundant renewable carbon feedstock, non-toxic nature, and contributing to a more sustainable use of resources. Several protocols have been reported for catalytic CO_2 fixation with epoxides to yield cyclic carbonates. However, achieving efficient activity and selectivity over economical catalysts remains challenging. In this context, we present synthesis of metal oxide engineered dendritic nano-fibrous silica as a promising catalyst for the fixation of CO_2 in to epoxide to produce cyclic carbonates. The physicochemical properties of this bi-functional catalyst were investigated with the assistance of several characterization techniques after which the catalyst was tested for its efficient activity towards the synthesis of cyclic carbonates by conversion of CO_2 with epoxide. Additionally, the effect of reaction parameters such as temperature, pressure, amount of catalyst and metal loading, were also studied. The catalyst demonstrated appreciable yield towards the desired product under mild reaction conditions. The presence of acidic-basic sites in the developed catalyst possibly contributed to the ring opening of epoxide and activation of CO_2 under mild reaction condition as proposed in the plausible mechanism. Further, the catalyst displayed substantial recyclability performance for several recycles without considerable loss in its catalytic activity.

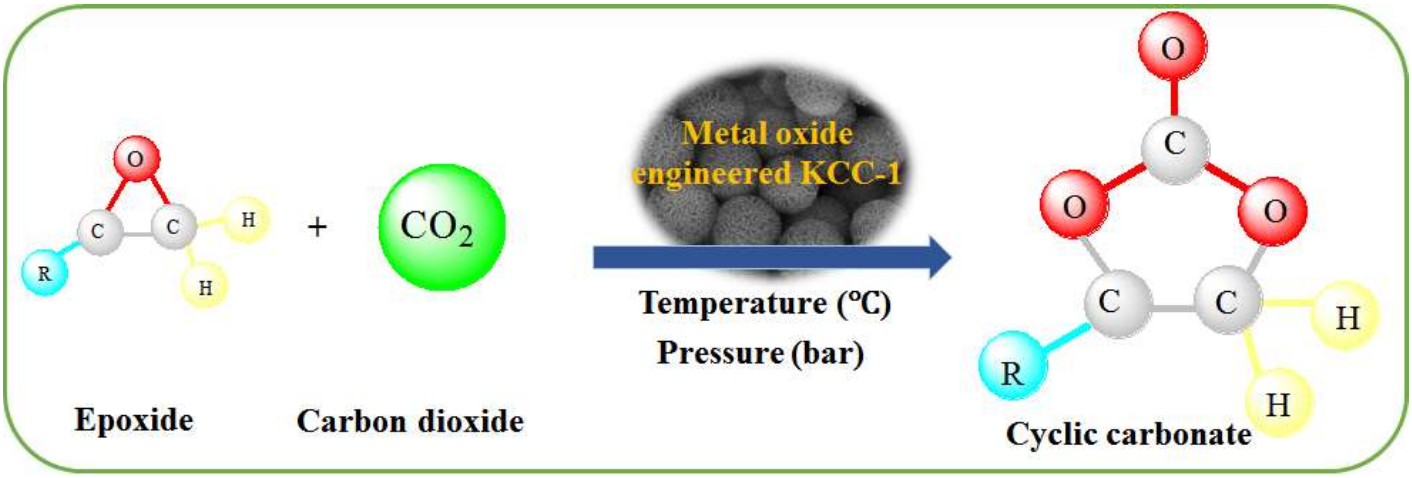

Figure 1. Catalytic fixation of CO_2 with epoxide in to cyclic carbonates.

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P-023

Production of γ-Butyrolactone from Selective Vapour Phase Dehydrocylization of Biomass-Derived 1,4-Butanediol over Cu/ZnAl$_2$O$_4$-CeO$_2$ Catalyst

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Abstract:

A spinel-based ZnAl$_2$O$_4$-CeO$_2$ support was prepared by co-precipitation method and then Cu was impregnated by standard wet-impregnation method to obtain Cu/ZnAl$_2$O$_4$-CeO$_2$ catalyst with different Cu loading. The catalysts were characterized by XRD, H$_2$-TPR, FTIR, CO$_2$-TPD NH$_3$-TPD, FE-SEM and H$_2$ pulse chemisorption studies and then were tested for the production of γ-butyrolactone by dehydrogenation of 1,4-butanediol. Further, various reaction parameters were optimized and their effect on the catalytic activity were studied to obtain maximum yield towards the desired product at ambient reaction conditions. The results revealed that the metallic Cu species and CeO$_2$ as a promoter were highly dispersed on ZnAl$_2$O$_4$ support with appreciable surface area. Additionally, CeO$_2$ as a promoter prevented agglomeration and increased the basic character of catalyst to selectively obtain γ-butyrolactone product. The 10 wt% Cu/ZnAl$_2$O$_4$-CeO$_2$ exhibited excellent yield (96%) towards γ-butyrolactone product and it has shown consistent activity and selectivity during 24 h time on stream study. Further, the 10 wt% Cu/ZnAl$_2$O$_4$-CeO$_2$ catalyst displayed substantial recyclability performance up to seven recycles without much loss in its catalytic performance making the catalyst feasible at industrial scale.

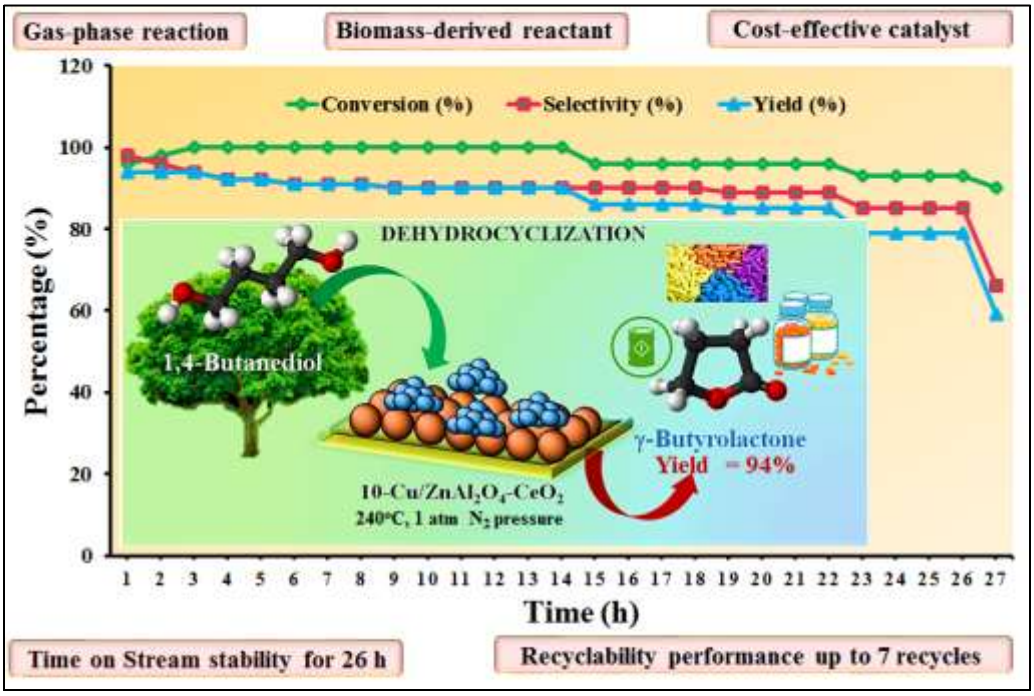

Figure 1. Catalytic activity of Cu/ZnAl$_2$O$_4$-CeO$_2$ towards dehydrogenation of 1,4-butanediol during time on stream study.

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P-024

DES-Modified Silica Catalyst for Chemical Fixation of CO_2 Conversion into Styrene Carbonate

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Abstract:

The substantial increase in the CO_2 emission in the last decades has urged researchers to utilize this inexpensive and abundant raw material in the synthesis of several important chemicals such as cyclic carbonates. In this context, we synthesized fibrous silica and then modified it with deep eutectic solvent (DES) to incorporate both acidic and basic sites in the final catalyst. The physicochemical properties of the catalyst were studied with the assistance of several characterization techniques such as XRD, FT-IR, FE-SEM, NH_3-TPD and BET. The catalyst was then tested for its activity towards synthesis of cyclic carbonates from epoxides in the presence of CO_2. Additionally, the effect of temperature, effect of different bases, effect of reaction time and effect of catalyst loading towards the synthesis of cyclic carbonate were studied and discussed in detail. In combination with TBAI as a base, the DES-modified fibrous silica catalyst effectively led to the 100% conversion with 96% yield towards the desired cyclic carbonates under atmospheric pressure of CO_2. Both the acidic and basic sites showed synergistic effect in epoxide ring opening under mild reaction conditions which has also been proposed in the plausible reaction mechanism. Further, the catalyst also demonstrated decent tolerance for different substituted epoxides along with substantial recyclability performance up to several cycles without significant loss in its catalytic activity. Therefore, the DES-modified fibrous silica can be considered as highly active and stable catalyst making the present approach of CO_2 conversion green and sustainable.

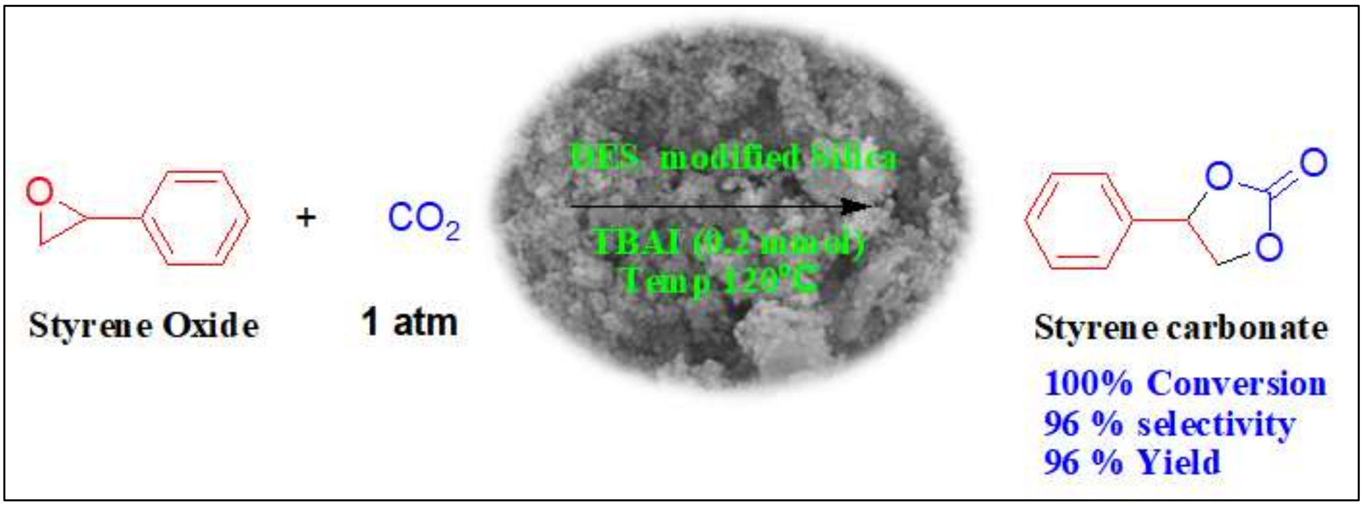

Figure 1. CO_2 conversion into styrene carbonate.

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P-027

Synthesis and characterization of mesozeolite H-BEA and its catalytic application in n-pentyl levulinate synthesis

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Abstract:

Amongst the several microporous materials, zeolites are gaining increasing attention due to their wide use as solid acid catalysts in varied catalysed organic transformations, gas storage materials in gas separation and sorbents/ion-exchangers in water softening. Salient features of zeolites include their composition, tuneable acidity and well-defined uniform pore structure of their cavities and channel system. These framework types belong to small, medium- and largepore zeolites and possess free dimensions of the pore opening in the range 0.5–0.8 nm. However, the accessibility to the pores is tough and is limited only to small molecules due to small pore size. Trends in the development of solid acid catalysts with less hindered and more active sites have led to the development of multiple porosities within zeolites, often termed mesozeolites, hierarchical zeolites, or micro-mesoporous composites. The mesozeolites are promising materials due to their enhanced accessibility generated from the hierarchical interconnected pore networks, high surface area and high acidity [1].

In this work, an attempt has been made to prepare micro-mesoporous zeolite BEA (MTYK) with bimodal porosity via sol-gel route from alkali treated zeolite BEA precursor using tetradecyltrimethyl ammonium bromide (TTAB) surfactant as mesotemplate and additional ingredient, yeast. The resultant micro-meso composite of zeolite material (MTYK) has been characterized by several characterization methods such as SEM, small-angle XRD, wide-angle XRD, FT-IR, NH3-TPD, ICP-OES and BET surface area. The alkali treated zeolite H-BEA material was found to exhibit bimodal porosity (microporosity and mesoporosity). Fig.1(a) and 1(b) depict small and wide angle XRD (WXRD) of micro-meso composite of H-BEA zeolite. The major characteristic peak of parent microporous H-BEA is observed between 2θ range, 7° - 10° and 23° – 25° [2]. These are also observed in MTYK catalyst, suggesting preservation of zeolite H-BEA crystallinity, even after post modification. The presence of a highly intense peak in the 2θ range ~ 0.5°–1° in small angle (SXRD) pattern of MTYK catalyst indicates the formation of highly ordered mesostructure which is resulted due to post treatment [3]

Further, the catalytic activity of MTYK is investigated in n-pentyl levulinate synthesis via esterification reaction between biomass derived levulinic acid and n-pentanol. n-Pentyl levulinate has a wide usage as a plastifying agent, odorous substance and an important industrial chemical intermediate. The reaction has been optimized by varying several reaction parameters such as molar ratio (LA:n-pentanol), catalyst amount (%), and reaction time (h). In nutshell, a promising catalyst is developed using environmentally benign synthetic approach for the green synthesis of value-added chemical from biomass derived scaffold.

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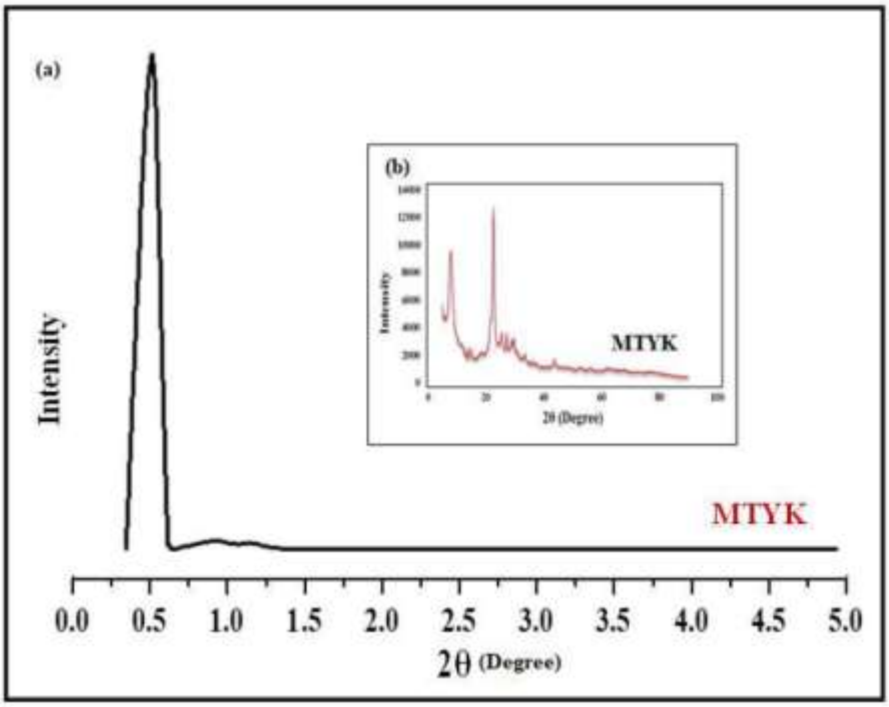

Figure 1 SXRD (a) of WXRD (b) patterns of MTYK catalyst

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P-028

Sustainable utilization of bio-derived furfuryl alcohol to yield alkyl levulinate over zeolite catalyst

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Introduction

A bio-derived furfuryl alcohol transformation into various high-value chemicals is a growing field of interest among researchers[1,2] Alkyl levulinates obtained from furfuryl alcohol have potential applications like biofuel and as additives in flavor and fragrance products [3]. This reaction utilizing furfuryl alcohol is challenging as the intermediate 2-(alkoxy methyl) furan (AMF), an ether, needs to be converted into alkyl levulinate (keto ester) which is difficult compared to traditional carboxylic acid route (levulinic acid). This study reports an exclusive investigation of the porosity and active sites responsible for the efficient alcoholysis of furfuryl alcohol to alkyl levulinate by the aid of zeolite catalyst. Screening of different microporous materials and conventional solid acid catalysts showed that H-ZSM-5 is the most efficient catalyst. Further, the influence of acidity of H-ZSM-5 zeolite on activity and product selectivity was studied by varying silica to alumina ratio (SAR) of the catalyst.

Materials and Methods

HZSM-5 catalyst was synthesized from the procedure similar to the reported one [4] For a better understanding of the catalytic activity, various physicochemical properties of the catalyst were investigated using techniques such as XRD, NH_3-TPD, N_2-sorption, XRF and SEM. The samples of the reaction mixture were quantitatively analyzed by gas chromatography (GC) and the products were confirmed by Gas chromatography–mass spectrometry (GCMS).

Results and Discussion

Butanolysis of furfuryl alcohol to yield butyl levulinate was carried over various solid acid catalysts such as HZSM-5, H-Beta, Y-zeolite, mordenite, sulfated zirconia, amberlyst-15, SAPO-34 and Al-SBA-15. Among them, amberlyst-15, a pure Brönsted acidic catalyst, gave the highest selectivity (92%) for butyl levulinate followed by HZSM-5 (66%) with conversions for both the catalysts near to completion. The better catalytic performance of amberlyst-15 catalyst can be attributed to the high number of Brönsted acidity present in it compared to other catalysts. However, due to its low thermal stability, the calcination cannot be employed for the removal of the adsorbed substrate/product species. Therefore, there was a drastic decrease in activity to 22% upon recycling. For HZSM-5, its unique uniform medium-sized micropore structure as well as its strong Brönsted acid character might have helped in getting good performance for this reaction. The rest of the catalysts exhibited lower catalytic activity (< 20 %) as shown in Fig. 1. Hence, HZSM-5 with high thermal stability was opted for further studies which gave almost complete conversion and fairly high selectivity for butyl levulinate. HZSM-5 with different SAR ranging from 22 to 160 was investigated to understand the role of acidity in the reaction. Though the conversion of all the HZSM-5 catalysts was above 95%, interestingly, the selectivity towards butyl levulinate did not show any linearity. However, the strong acidity had less influence on the selectivity

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though the trend of the catalytic performance was a volcanic peak (Fig. 2). The order of the catalytic performance of the SARs in HZSM-5 with respect to selectivity (%) is SAR95 > SAR117 >SAR160 > SAR57 > SAR22. This trend may be due to the competing reactions leading to pore/ active site blockage making the reaction slower with time for HZSM-5 with lower SAR. Oligomerization is more prone in lower SAR catalysts due to the higher Brönsted acidity. In the case of higher SARs, low acid site density leads to low catalytic activity. Further, ZSM-5 was modified with different post–synthesis treatments to vary acidity and porosity to understand the physico-chemical properties needed in the catalyst to get best activity and selectivity for this reaction. Therefore, SAR95 was the best catalyst that favored efficient production of butyl levulinate compared to the rest with the highest catalytic selectivity of 85%.

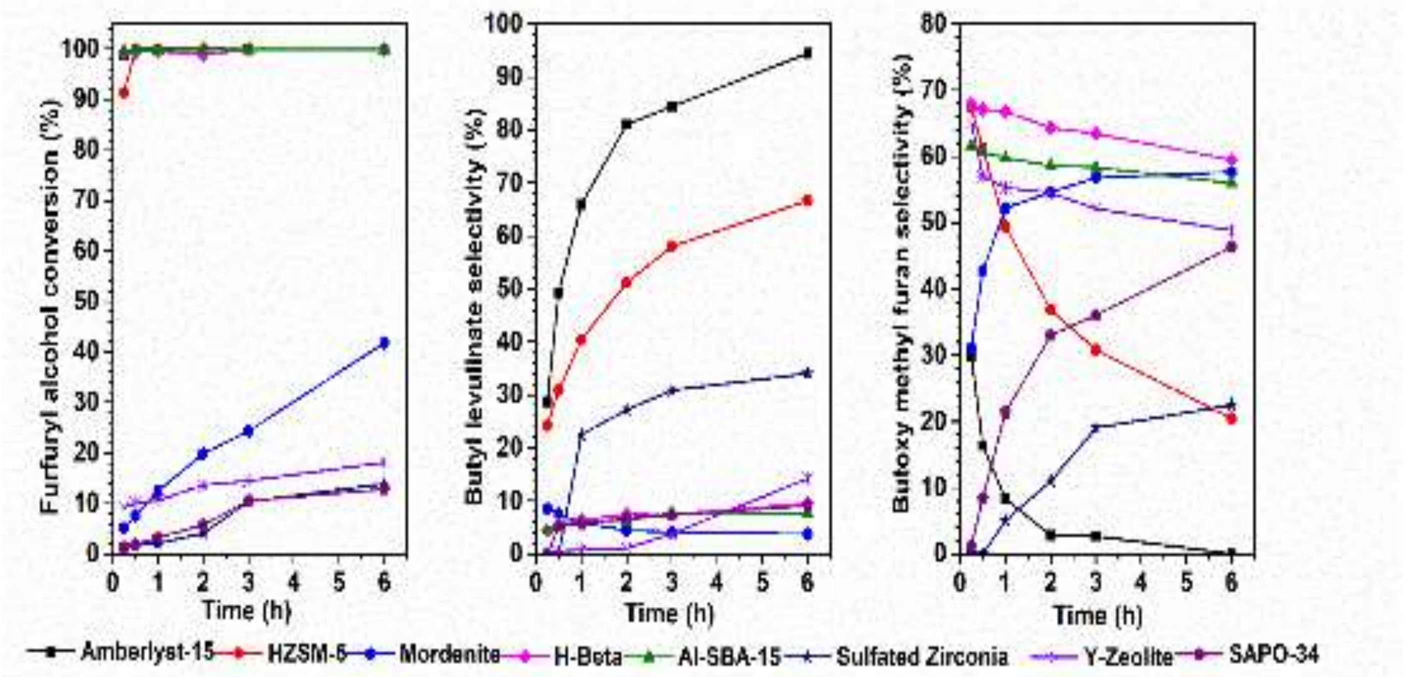

Figure 1. Catalyst screening. Reaction conditions: catalyst concentration-3wt%, temperature-110 °C, mole ratio- 1:10 (furfuryl alcohol: butanol), time- 6 h.

Significance:

Zeolites being one of the classic materials are still startling the scientists by its flexible material properties and promising catalytic activities in many important and challenging transformations. In alcoholysis of furfuryl alcohol which was efficiently converted into butyl levulinate with the aid of HZSM-5 (SAR95) in a batch regime proved the exclusive requirement of the uniform medium size micropore structure, high surface area, strong Brönsted acidity, optimal number of acid sites and good thermal stability for this reaction. The combination of the properties inherited by the HZSM-5 with the tuning of acidity makes it different from the other catalysts. Considering the green chemistry principles such as moderate experimental conditions, excellent reusability, low reactants mole ratio and catalyst concentration, HZSM-5 (SAR95) proves to be the best candidate for this transformation as it addresses all the drawbacks of the reported catalysts.

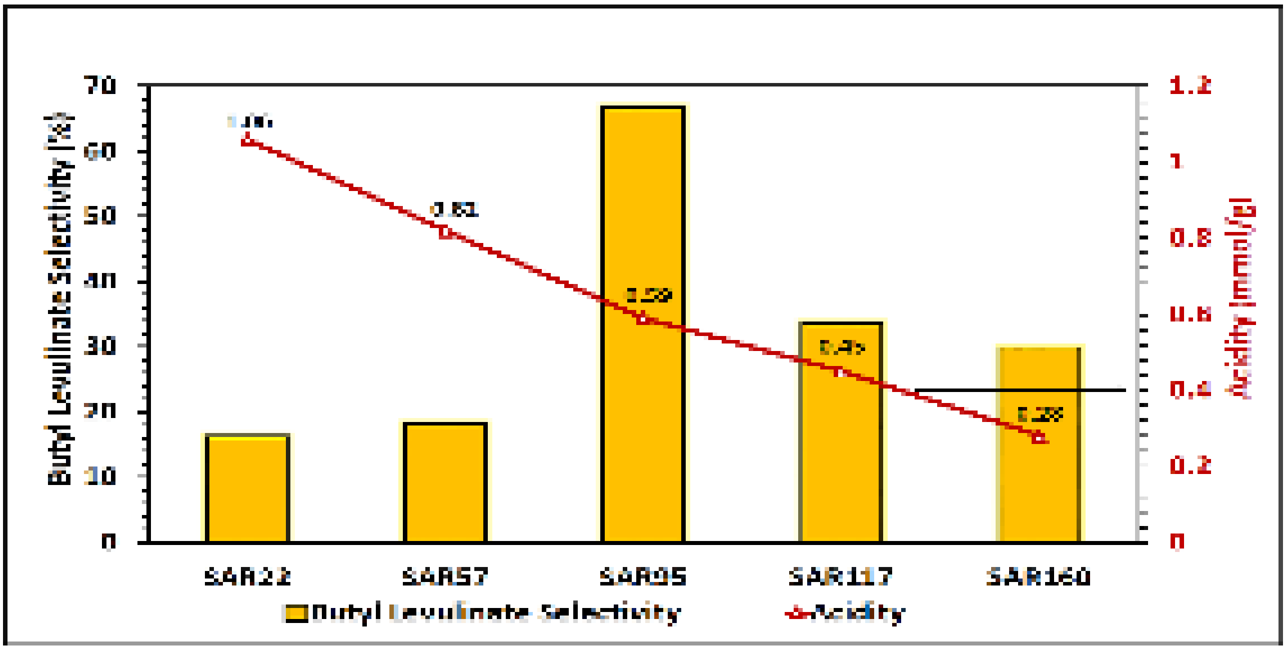

Figure2. **Butyl levulinate selectivity for different SAR of HZSM-5 correlating with with acidity. Reaction conditions: Catalyst concentration- 3wt%, temperature- 110 °C, reactant mole ratio- 1:10, time- 6 h. furfuryl alcohol conversion ≥ 99%.**

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P-029

Green route for carbonylation of amines by CO_2 with Sn-Ni bifunctional catalyst: How to predict the best active sites?

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Abstract:

Reaction between n-alkylamine and CO_2 has gained interest due to the demand for the dialkylurea for various applications. For the first time, the tool *Mathematica* was used to analyze the experimental data with an idea to derive an equation which determines the best suited active sites for any given input set of dependent parameters. The equation can further be used to predict the product yield with the known values of active sites for a reaction. Among several Sn containing mixed oxides, Sn-Ni oxide (Sn-Ni-O) was found to be the better performing catalyst. The studies indicate that the formation of new defect sites when NiO and SnO_2 are in the mixed state and possibly a solid solution enhances the catalytic efficiency. There are two main reasons for improved catalytic performance; one, mixing of SnO_2 into NiO which reduces the number of holes (h^+) localized on lattice oxygen ($O^{2-} + h^+ \rightarrow O^{\bullet -}$) and two, smaller SnO_2 particles are dispersed on the bigger particle NiO which alters the acidic and basic active sites in the catalyst. The characterization results indicate that the formation of new defect sites when NiO and SnO_2 are in the mixed state and possibly a solid solution enhances the catalytic efficiency. The occurrence of Sn^{2+} is attributed to the solubilization of tin in NiO matrix along with the creation of oxygen vacancy. The increase in the Sn content of Sn-Ni-O-600 increased both acidity and basicity which could be due to an increase in the distribution of SnO_2 on the surface of NiO. TPR confirms the interaction of NiO and SnO_2 in the mixed phase which could be responsible for the creation of acid and base sites. Also, molar ratio of metals in the catalyst and calcination temperature play a vital role in creating active sites, and hence, influence the catalytic activity. The better catalytic activity of Sn1.1-Ni-O-600 could be due to the appropriate amount and strength of acid-base sites. The reactions of various amines with CO_2 showed that the catalyst performed well with aliphatic amines, diamine and amino alcohol, whereas trace yields were obtained for aromatic and secondary amines. Under optimized reaction condition, Sn1.1-Ni-O-600 gave 77.3 % of n-butylamine conversion and 75.7% of yield for 1,3-dibutylurea. The versatility of the catalyst was tested for carbonylation of different aliphatic and aromatic amines, diamine and hydroxy amine with CO_2.

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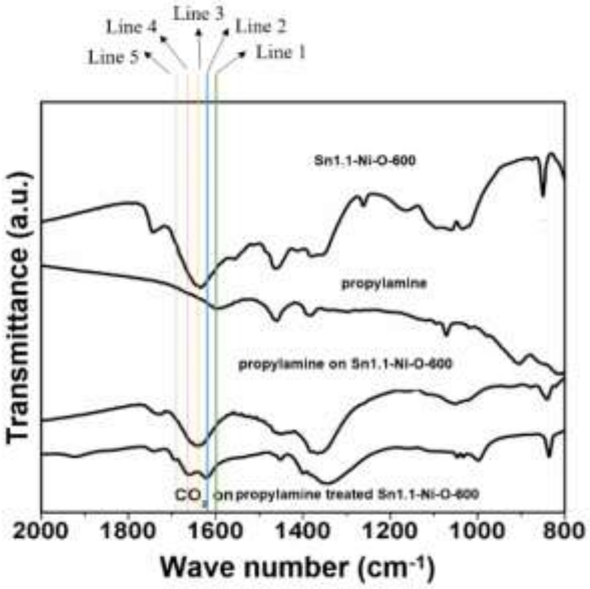


Figure 1. FT-IR study on reaction of propylamine and CO_2 on surface of Sn1.1-Ni-O-600 catalyst

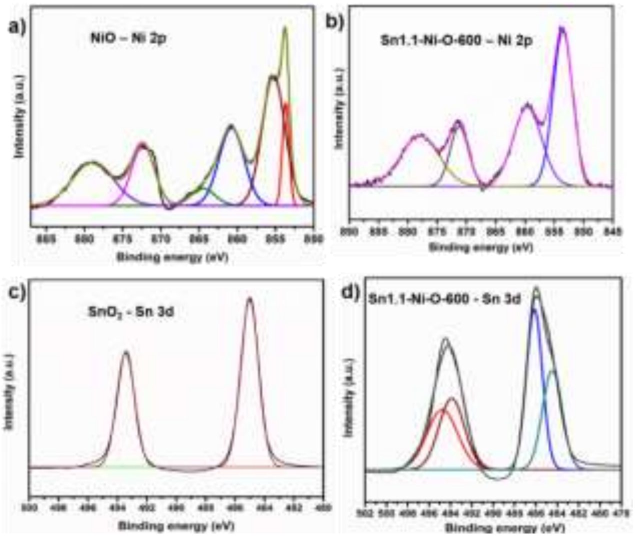
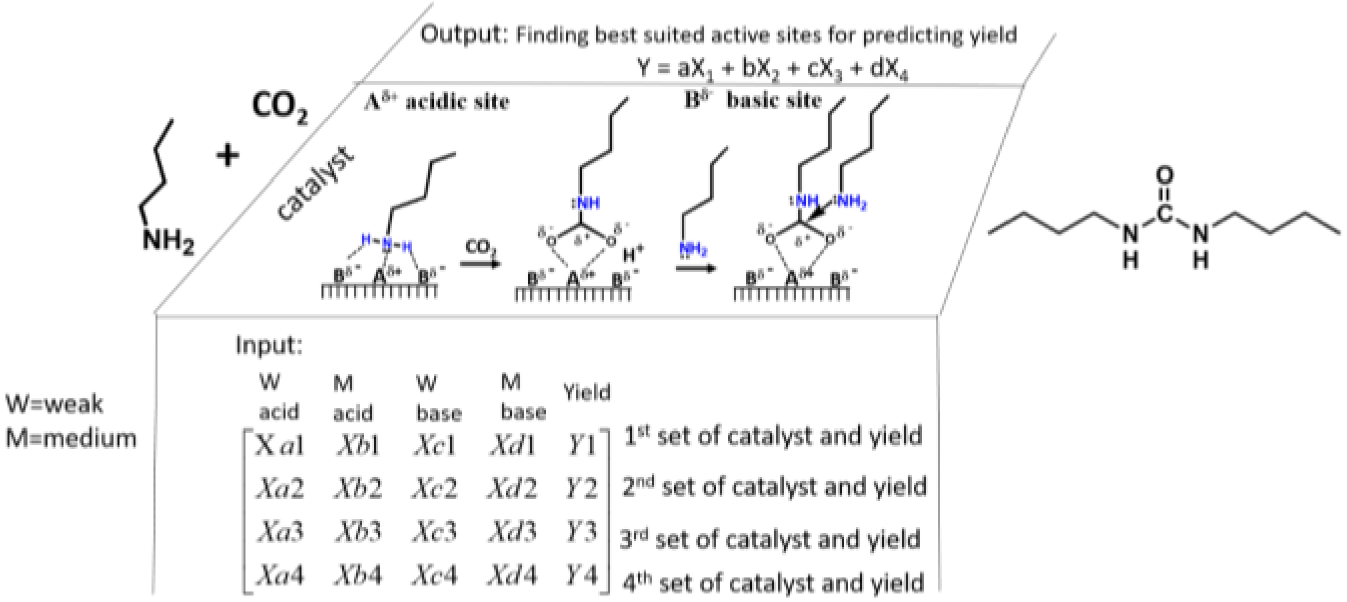


Figure 2. XPS spectrum of Ni 2p for a) NiO, b) Sn1.1-Ni-O-600, and Sn 3d for a) SnO_2, b) Sn1.1-Ni-O-600 catalyst.



Scheme 1. The mechanistic representation of acidic and basic sites for carbonylation of amine with CO_2 and the use of Mathematica to derive the best active sites

P-030

Fischer-Tropsch synthesis over noble metal (Ag, Pt, and Ru) and Mn promoted cobalt catalysts

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Abstract:

Fischer-Tropsch synthesis (FTS) is a viable technology for the production of fuel-grade hydrocarbons from feedstocks like coal, natural gas, and biomass. Cobalt-based catalysts are widely used for this process due their high activity and selectivity towards C_5+ compounds. In this work, titanosilicate supports were synthesized using a surfactant-free templating process and impregnated with 15 wt.% cobalt. The catalysts were promoted with 1 mol.% noble metal (Ag, Pt, and Ru) as well as different concentrations of Mn (5, 10, 20 mol.%) using coimpregnation. The synthesized materials were extensively characterized using BET, H_2-chemisorption, XRD, TPR, XPS, and XAS. The materials exhibited a type-IV hysteresis and possessed pore sized in the range of 12-14 nm. The surface area of the catalysts reduced by ~20 % after the addition of metals to the support. The dispersion of cobalt increased from 4.9% to 6.6-7.1 % with the addition of promoters. Furthermore, the addition of Ag decreased the temperature required for reduction by 34 °C. The extent of reduction of the catalysts was found to be similar for all the catalysts when reduced under flowing hydrogen at 400 °C for 18 h. The FTS activities of the catalysts were studied in a fixed bed reactor at industrially relevant conditions- 220 °C, 250 psig, 2000 $mL_{syngas}/mL_{catalyst}/h$ with a syngas composition of CO:H_2:Ar = 30:60:10. Catalysts promoted by noble metals exhibited increases in conversion by 10-15 % with increases in selectivity for CH_4 (4-12%) and CO_2 (3-9 %). Pt-promoted catalyst exhibited the highest CO conversion (95±2%), highest CH_4 selectivity (24.6 %), and greatest rate of deactivation (0.07 %/h). Among the noble metal promoters tested, Ag had the lowest rate of deactivation (0.03 %/h). The addition of Mn to the catalyst increased the C_5+ selectivity of the catalyst by ~5% while suppressing the CH_4 selectivity by ~6%. The optimal composition of the catalyst was found to be Co:Mn:Ag = 100:10:1. Box-Behnken method was used to optimize the reaction parameters (temperature, pressure, GHSV) and was found to be 219 °C, 300 psi and 1800 h^{-1}. The time-on-stream activity of the catalyst was tested for 400 h under these reaction conditions. The catalyst showed a starting CO conversion of 87 % with a deactivation rate of 0.02 °C/h. The catalyst was regenerated at 500 °C under flowing air and reduced in situ before testing. The regenerated catalyst showed a CO conversion of 85.6 %.

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P-031

ZSM-5 / Sodium Alginate Based Mixed Matrix Membranes for Pervaporation Dehydration of Ethanol

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Abstract:

Ethanol is an important industrial chemical, used as a solvent in the synthesis of other organic chemicals, and as an additive to automotive gasoline (forming a mixture known as a gasohol) as directed by the Indian government. But ethanol forms azeotrope with water at 97.2% (by volume) and the separation by conventional separation processes like extractive or azeotropic distillation has they are energy intensive. Pervaporation, a potential industrial process is a promising alternative as it is economical, safe and ecofriendly. The key to the success of pervaporation process is synthesis of suitable membranes yielding high permeability, good selectivity and sufficient mechanical strength. So the major focus of the present study is preparation of Sodium Alginate (NaAlg) based Mixed Matrix Membranes (MMM’s) by solution casting process incorporating varying wt. % of ZSM-5 zeolite particles. The membranes thus prepared were cross-linked with glutaraldehyde. The MMM’s were characterized by Fourier transform infrared spectroscopy (FTIR), Thermo-gravimetric analysis (TGA) and Scanning electron microscopy (SEM), respectively. Further Sorption studies with varying composition of ethanol-water mixture were correlated with the PV results. The 10 wt. % zeolite loaded NaAlg membrane exhibited lower permeate flux and enrichment factor but greater selectivity.

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P-032

Simulation Studies For Continuous Production Of Butyl Levulinate By Esterification Of Levulinic Acid And Butanol

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Abstract:

With the diminishing fossil fuel resources and the apprehension of them exhausting in a few decades has led to escalating studies in the field of renewable energy, especially biofuels. Levulinic acid is produced abundantly from biomass processing; it serves as an eminent precursor for the synthesis of a variety of levulinate esters as fuel additives. The excellent fuel blending properties of levulinates has led to research in this field. Various catalysts have already been studied for manufacturing levulinate based value added products. One such product is Butyl Levulinate which possess excellent fuel blending properties.

The present work focuses on the production Butyl Levulinate continuously at a large scale. The simulation studies have been performed on ASPEN PLUS V10 using nano composite as the catalyst to check the feasibility of the process. The unit operations and unit processes employed were a packed bed reactor followed by distillation columns for separation of the product, along with auxiliary equipment's like pumps and heaters. The process variables were optimized by carrying out a sensitivity analysis to maximize the yield and separation. In order to achieve a continuous production of BL, a simulation was performed on Aspen Plus, and the performance of the unit operations is optimized individually. The process gave a purity of the product Butyl Levulinate (95.9 %) at a flowrate of 91.343 mol/s. The present works presents an eco-friendly route to scale up the production of butyl levulinate.

Keywords: Biomass, Biofuels, Levulinic acid, Simulation, Butyl levulinate

POSTER PRESENTATION

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P-008

An Eco-friendly approach for synthesizing TiO_2/ZnO Nanocomposites for removal of organic pollutants from water

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Abstract:

In contemporary research, it is challenging to remove organic pollutants which are chemically active compounds discharged from industries, such as dyes, pesticides, fuels and etc from aqueous streams. These pollutants not only affect the human life but aquatic life is also disturbed. The current research is aimed to remove organic pollutants present in water using TiO_2/ZnO nanocomposites synthesized via green synthesis approach. Green synthesis is simple, affordable and prominent method of synthesizing the nanoparticles. Here in, we propose to synthesize TiO_2 and ZnO nanoparticles using "ALTERNANTHERA SESSILIS" plant extracts. The synthesized nanoparticles were characterized by using XRD, FTIR, UV, SEM, and TEM. The synthesized nanocomposites were used for degradation of Methylene Blue dye. The chosen plant extract has good amount of flavanoids and phenols which will act as reducing species in converting the precursor solution to metals/metal oxides.

Key words: ALTERNANTHERA SESSILIS, TiO_2, ZnO, Methylene Blue

Experimental Methodology:

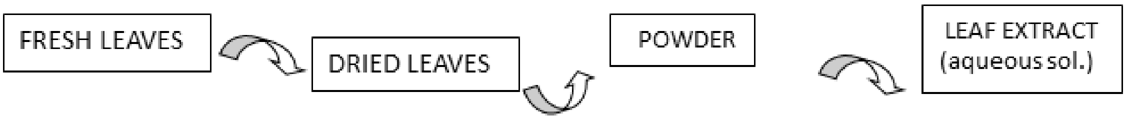

Figure.1: Block diagram representation of Plant extract prepartion

Fresh leaves were taken and dried in a room temperature and make into a powder form. Take 2g of dry leaves powder was added into 100ml of distilled water with tempartuer 60^{0}C for 1hr. The extract was filtered using Whatman filter paper then the condensed liquid seperates .It can be used for further synthesis process. The precursor solution of TTIP and ZnO were dissolved seperately. In the 500ml beaker 20ml of leaf extract and 80ml double distilled water and add the precursor solution one by one under the stirring. The solution was kept for stirring with 60^{0}C temparature for 4hrs. The samples undergoes for centrifugation process and the collected samples were kept in hot air owen for 3hrs the final obtained particles were kept in muffle furnace for calcination with temparature for 400^{0}C with 2hr.

This process is performed for synthesized nanocomposite of TiO_2/ZnO. Take a required conical flask to prepare ppm's of methylene blue solution for reference. Then take a beaker and add some ppm with distilled water and add catalyst TiO_2/ZnO nanocomposite then the solution kept in stirrer it continues up to the pale blue color changes to colorless.

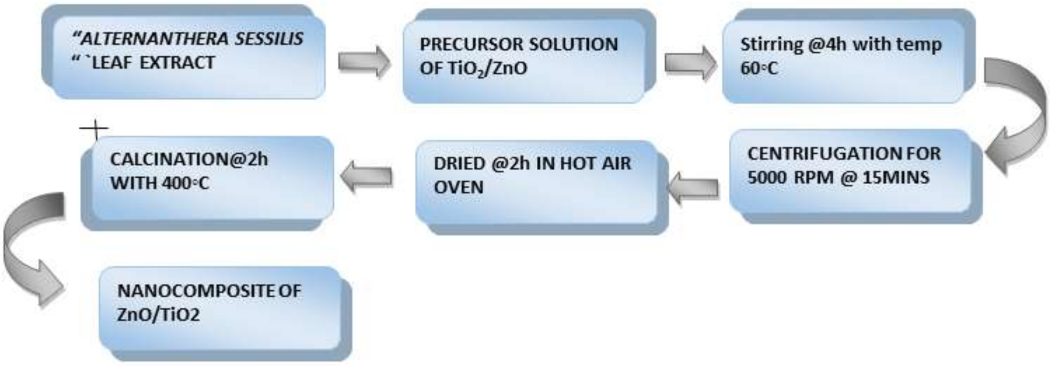

Figure 2: Block diagram of synthesis process Degradation studies of organic pollutants

Results:

The preliminary characterization technique for the synthesized nanoparticles was confirmed with XRD Results. The TiO_2 XRD peaks for the synthesized nanoparticles with diffraction angles 25.28°, 37.5°, 47.5°, 55°, 62.4°, 70° and 76.5° respectively. Further, ZnO nanoparticles show diffraction peaks located at 31.84°, 34.52°, 36.33°, 47.63°, 56.71°, 62.96°, 68.13° and 69.18°. The XRD patterns confirm the presence of both TiO_2 and ZnO nanoparticles and composite assembly XRD pattern is about to analyze.

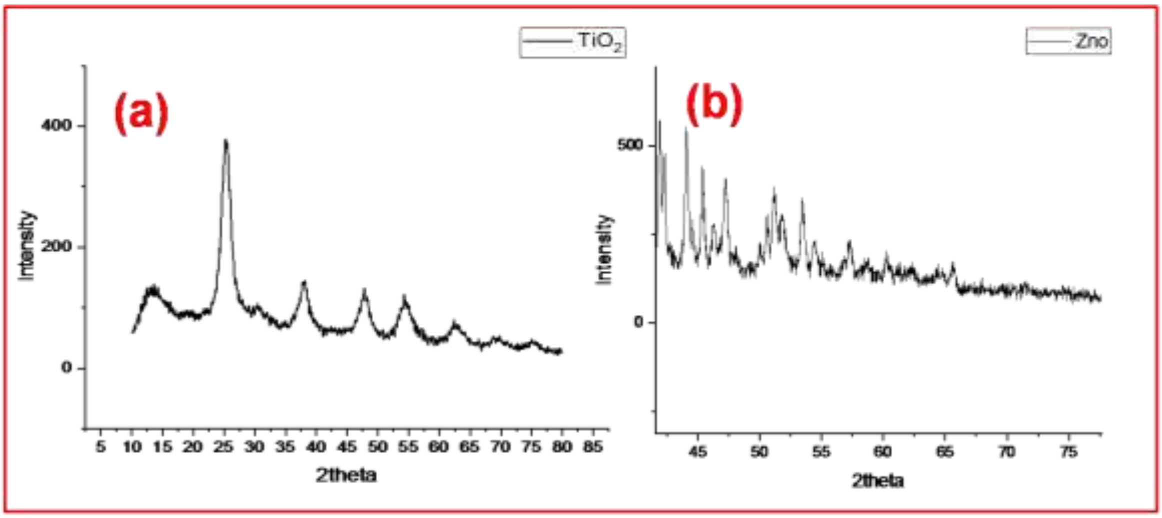

Figure 3 a) XRD Pattern of TiO_2 Nanoparticles; **3b)** XRD Pattern of ZnO nanoparticles

Conclusions:

The TiO_2/ZnO nanocomposite was synthesized by using the plant extracts of “Alternanthera Sessilis” leaves. Green synthesis is a simple and eco friendly approach without involving any usage of chemicals. The synthesized samples were characterized by using XRD and matched with JCPDS data. All the samples (TiO_2, ZnO) show good crystalline nature and were in good agreement with existing literature. SEM, TEM, UV-Vis spectroscopy, and FTIR is pending for analysis. The nanocomposite assembly was used for various applications such as the organic pollutants like methylene blue degradation. It can be predicted that TiO_2/ZnO nanocomposite assembly to be having maximum degradation efficiency in comparison to individual assemblies.

P-009

Methylene Blue Dye removal studies using Activated Carbon prepared from Tamarindus Indica seeds

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Abstract:

The direct release of Industrial Effluents results in the release of toxic pollutants to the aquatic environment. The presence of dyes in waste water is a major concern for toxicological reasons. Textile Industries are the main source of water pollution which affects the aquatic flora and fauna. Waste water releasing from textile industries contain more toxic dyes that causes aquatic pollution and soil pollution. Hence, before releasing the industrial outlet into water bodies the dye has to be degraded. Adsorption, coagulation, ion exchange, membrane filtration etc., are the physical dye removal methods in which adsorption have more advantages. Adsorption is one the effective and economical method among other dye degradation methods. Activated carbon is a good adsorbent which is eco friendly, economical and easy to prepare. Activated carbon is produced from carbonaceous sources materials such as coconut, peat, tamarind seed etc.,
Tamarind seeds are one of the most commonly available carbonaceous material. As Tamarind seeds are economical and eco-friendly they can be used as adsorbent after converting them into Activated carbon. The prepared samples will be characterized using XRD, FT-IR Spectroscopy, and SEM. The Batch and Continuous Column studies were carried out to observe the effect of various parameters such as contact time, pH and adsorbent dosage.

Key words: Methylene Blue, Tamarindus Indica seeds, Adsorption, Activated Carbon

Experimental methodology:

Tamarind seeds (with & without peel in equal quantities) are initially weighted, oven dried at 110° for 2hours, cooled to room temperature & then weighted. Dried tamarind seeds are heated in a heating mantle at 60° for 1hour, burned in muffle furnace at 500° for 2hrs, cooled to room temperature and weighed. Obtained coal is powdered. Sieved on 420 μm and collect the char retained on 250 μm sieve. Char is weighted, NAOH is used as an activation agent. Equal ratios of char and NAOH are combined with distilled water and stirred for 1 hr then oven dried at 130°c to obtain Activated carbon as shown in Figure 1.

Dye degradation was carried out in both Batch and Continuous modes as shown in Fig 2. The samples were collected at every 15 minutes and UV-Vis spectra were taken for all samples in order to understand the absorption spectra of dye.

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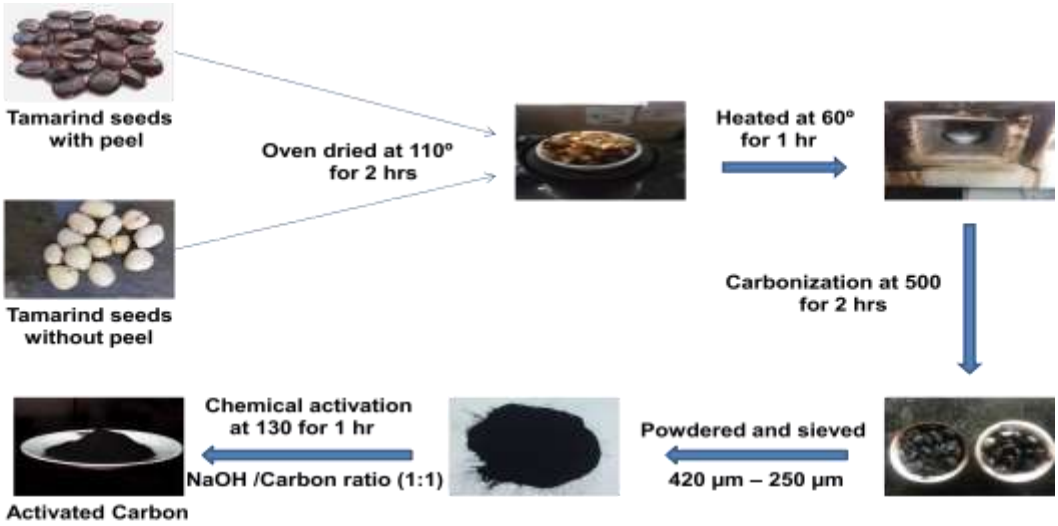

Figure 1 - Preparation of Activated carbon

Experimental setup:

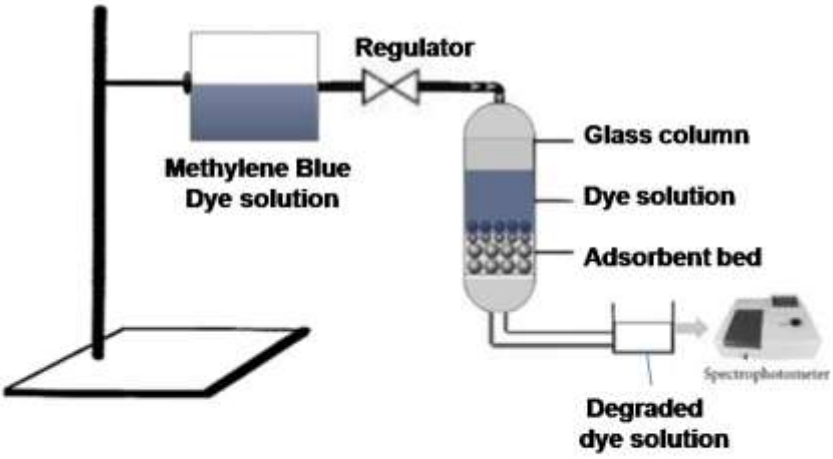

Figure 2 – Batch and Continuous column studies

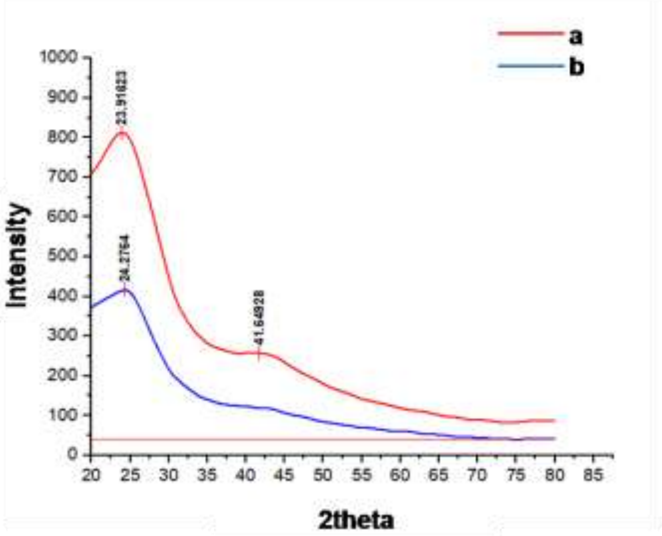

Figure 3 - XRD results of Activated carbon (a) With peel (b) Without peel

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Results:

The preliminary characterization technique X-ray Diffraction (XRD) confirms the Activated carbon with the 2 theta angles of AC 23.97°, 40.83° (for with peel seeds) and AC 24.32° (for without peel seeds) as shown in Fig 3 and was consistent with reported literature [1]. The characterized samples were studied in batch and continuous column studies and complete degradation was observed after 2 hours as shown in Fig 4.

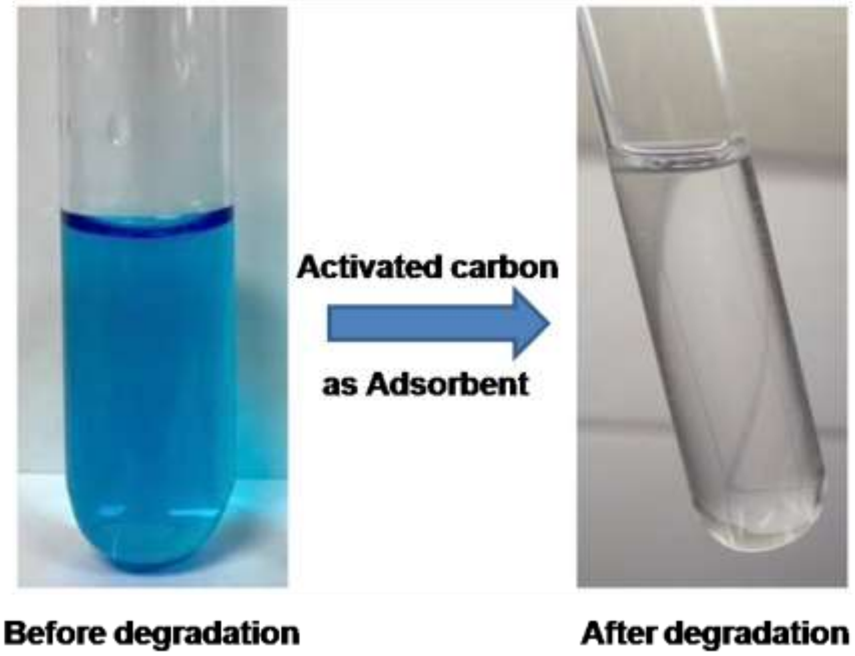

Figure 4 – Degradation process

Conclusions:

Activated carbon is prepared by using tamarind seeds. Synthesized Activated carbon is characterized using XRD and the results confirm the Activated carbon. Further characterization techniques like FT-IR Spectroscopy, SEM and BET analysis were needed to be done for the obtained Activated carbon. Degradation of Methylene blue dye is observed in continuous column adsorption studies. Batch adsorption studies have to be carried out and the samples of degraded dye will be analyzed using UV-VIS Spectroscopy to study the effect of various parameters such as contact time, adsorbent dosage and pH.

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P-011

Synthesis of Zinc oxide Nanoparticles using Acacia Catechu Leaf Extract

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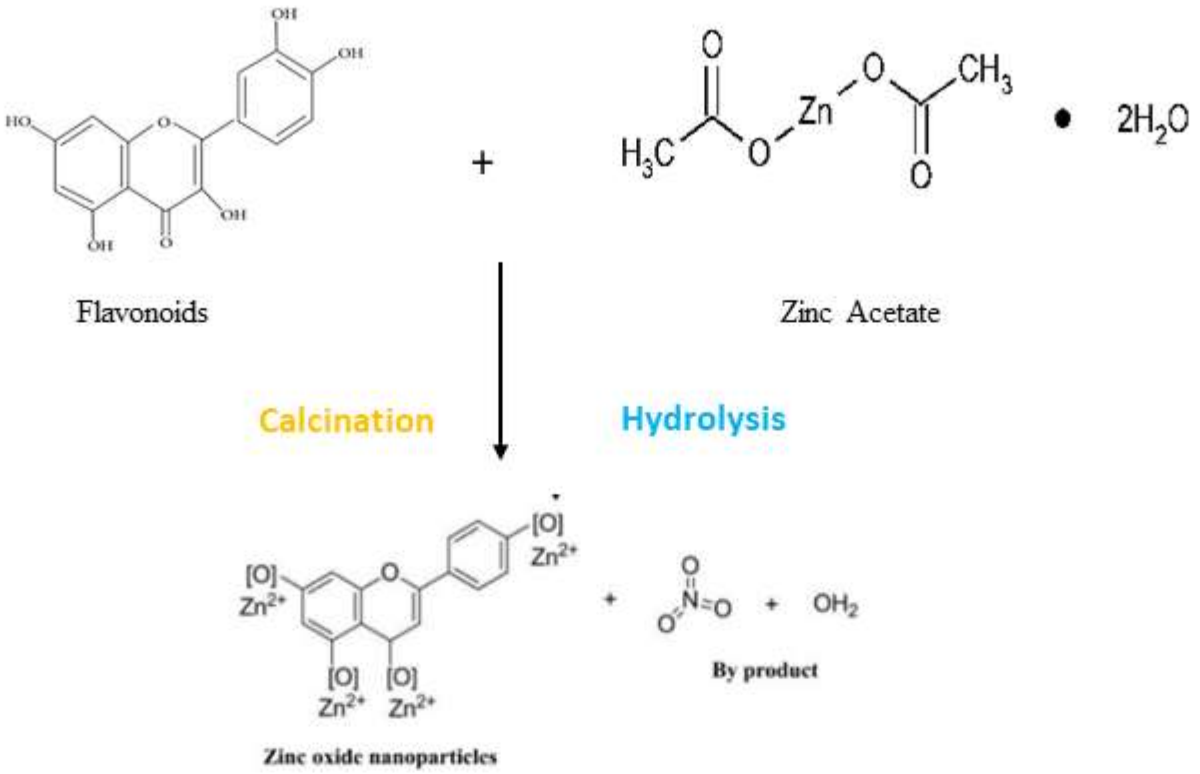
Abstract:

Nanotechnology, as one of the most advanced technologies, has demonstrated its impact on various fields by implementing and improving product rates in their respective fields such as Agriculture, Chemical, Construction, Mechanical, Medical, Electronics, and so on. In the current study it focuses on the synthesis of Zinc oxide nanoparticles via a green route using *Acacia Catechu* plant. The leaf extract of the Acacia Catechu acts as a reducing agent to reduce their respective precursor and help synthesize the metal oxide nanoparticles. The leaves of Acacia Catechu plant were chosen as it consists huge amount of Flavonoids and Phenols which are mainly responsible for reducing the precursor. Thus, synthesized nanoparticles were characterized using UV-Vis Spectroscopy to determine the concentration, FT-IR to know the functional groups present in the sample, DLS to attain the average particle size, XRD and SEM.

Synthesis Mechanism



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XRD Results

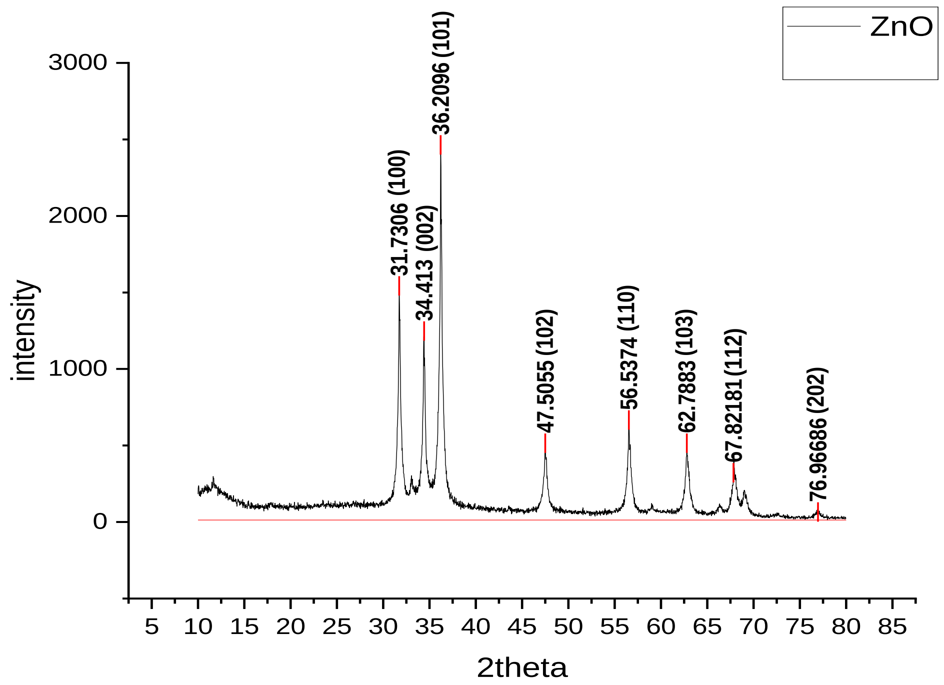

Figure 1: XRD of ZnO oxide Nanoparticles.

The XRD result has obtained peaks at 31.73, 34.41, 36.20, 47.50, 56.53, 62.78, 67.82, and 76.96 which confirms the Zinc Oxide nanoparticles according to JCPDS data. From the previous literature it can be predicted that the synthesized nanoparticles can be used for different applications such as removal of organic pollutants, heavy metals from waste water and antibacterial studies.

Keywords: synthesis, Acacia Catechu, Zinc oxide nanoparticles, XRD, Green route synthesis.

P-013

Graphitic Carbon Nitride Supported Palladium Nanocatalyst for Treating Environmental Contaminants

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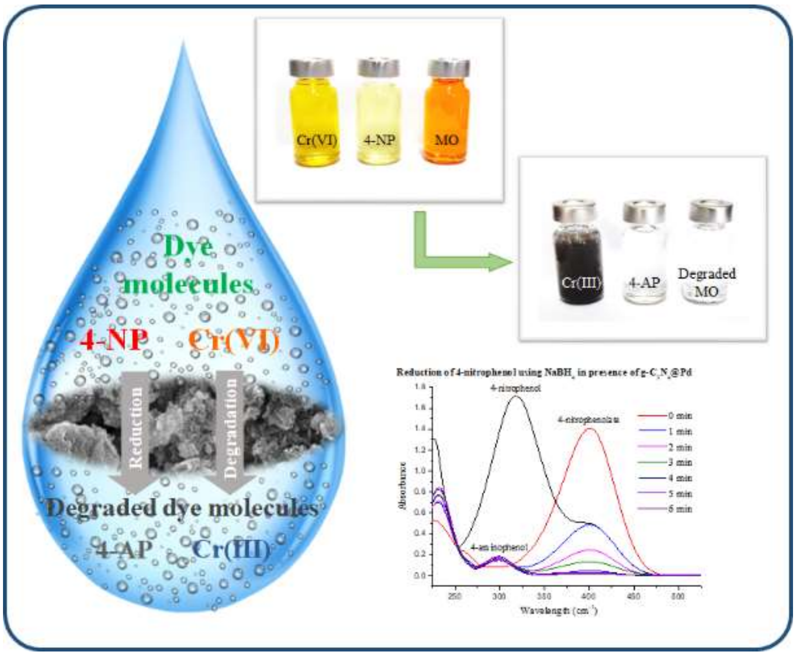
Abstract:

The stability and safety of our ecosystem determines the well-being of the human race. Regrettably, environmental pollution has jeopardized the health of human beings, including the flora and fauna that define nature. A leading contributor to contaminating our planet is the discharge of untreated hazardous and toxic chemical effluents like heavy metal ions, synthetic organic dyes, and nitrogenous compounds from various industries mainly into our water sources altering the quality of water. In continuation of our recent investigations of the application of heterogeneous catalytic systems in treating environmental contaminants, herein we report design and synthesis of palladium nanoparticles embedded on graphitic carbon nitride (g-C_3N_4@Pd) as nanocatalyst from melamine in a facile four-step synthesis. The nanocatalyst was characterized by various spectroscopic and microscopic techniques such as such as Fourier transform-infrared spectroscopy (FT-IR), energy-dispersive X-ray spectroscopy (EDS), field-emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), X-ray powder diffraction (XRD), thermogravimetric analysis (TGA) and Brunauer-Emmett-Teller surface area analysis (BET) to confirm its structure and morphology. It was then successfully explored for its catalytic activity in the treatment (reduction or degradation) of various water contaminants, such as chromium (VI), 4-nitrophenol and methyl orange. Being heterogeneous in nature, the nanocatalyst could be easily recovered from the reaction mass by simple filtration or centrifugation. The nanocatalyst showed very good performance and the method is economical, facile, requires mild reaction conditions and produce non-toxic byproducts.

Keywords: graphitic carbon nitride, palladium nanoparticles, nanocatalyst, water contaminants, reduction, degradation



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P014

Challenges and Opportunities of Waste Management for Sustainable Development

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ABSTRACT:

Arising quality of life and high rates of resource consumption patterns have had a unintended and negative impact on the environment - generation of wastes far beyond the handling capacities of governments and agencies. India generates about 68 million tonnes of food waste every year. This number shoots up to 350 million tonnes in the case of agricultural waste. The world needs eco-friendly products which minimises the current damage to the environment. Hence, using residues to make useful products, not only helps in waste management, but also is a way of greener production. Producing paper from agricultural wastes promotes afforestation. On the other hand, production of bioplastics from food wastes notonly saves the land from pollution, but also helps in protecting the atmosphere from toxic chemicals which are released from burning plastic products. At last, production of essential oils from dry leaves is an innovative initiative to make the best out of waste. Therefore the current review summarizes research and studies on sustainable waste management with emphasis on challenges and opportunities. Various methods have been described to manage the waste from dry leaves, food and agricultural residues to essential oils, bioplastics and paper. This ensures saving theenvironment and moving towards a world of sustainable development and minimal wastage.

Keywords: Waste management, Bioplastic, Paper, Essential oils, Sustainability

I. INTRODUCTION

The world generates 2.01 billion tons of municipal solid waste annually, and at least 33 percent of that is extremely conservative and not managed in an environmentally safe manner. Looking forward, global waste is expected to grow to 3.40 billion tons by 2050. Managing this waste comes at a high cost both economically and environmentally. The major constituents of the municipal wastes are agricultural wastes and food wastes. Over the years, the importance of reusing and recycling waste has been understood. Thewastes which are predominantly present across the globeare solid municipal wastes (food waste, agricultural by products, grass clippings etc.) and plastic wastes. Therefore, it is our moral duty, as the humans of this generation, to start a sustainable movement for the betterment of this world. In this paper, we intend toreview the various methods and technologies used toconvert the following waste into sustainable productsthrough eco-friendly techniques:

a. Agricultural waste to paper
b. Food waste to bioplastics
c. Dry leaves to oil

II. MATERIALS & METHODS

Agricultural residue to paper: Bagasse, Wheat straw, Cotton and Corn stalks etc are found to be the best alternative of wood for papermaking because of its low cost, longer fiber, low refining energy

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consumption and good sheet formation and paper smoothness, enabling to meet the quality requirements for newsprint and fine paper manufacture using Chemical, Mechanical and Chemical Thermal mechanical pulping (CTMP) methods.

Figure 1: Potential non-wood fibre sources for paper making (a.bagasse, b. wheat straw, c. cotton stalks, d. corn stalks)

Food waste to bioplastics: The tremendous amount of food waste from diverse sources is an environmental burden if disposed of inappropriately. To resolve FW problems, implementation of a biorefinery platform is essential. The adoption of such a process (eg: Volarization) can produce value-added products while reducing the waste. Production of bioplastics from food waste (Cassava Peel, Banana Peel, Jackfruit Seed, Orange peel etc) was found to be more prospective and offer a wide scope of applications (packaging, agriculture, gastronomy, consumer electronics and automotive).

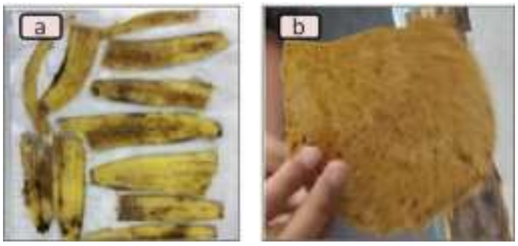

Figure 2: Bioplastic from banana peels

Dry leaves to oil: One of the dominant constituents of municipal wastes is dry leaves. Its disposal is a recurringissue as the world consists of almost 400 billion trees. Burning of leaves results in harmful toxins being released which are the cause of major health problems. These leaves have various properties that can be put into good use like extraction of essential oils through maceration, steam and hydo distillation techniques.

III. CHALLENGES

World faces major environmental challenges associated with waste generation and inadequate waste collection, transport, treatment and disposal. Current systems are unable to cope with the volumes of waste generated by an increasing urban population and this impacts on the environment and public health.

IV. FUTURE SCOPE

Dry leaves, Agricultural & Food waste are zero-value and non-consumable resources. In this context employing well-structured and efficient technologies such as distillation of dry leaves to extract oil, pulping of agricultural residues for paper making and valorization of food waste for making bioplastic can be an attractive and viable approach to counter the current global energy crisis and in establishing a sustainablebioeconomy.

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IV. CONCLUSION

This paper focuses on sustainable development and making the best out of waste. Extensive waste products are seeing the light of day because of industrialization, increase in population and increased production of goods. This has led to overfilling of landfills, and pollution that is caused by wrong disposal of waste materials. Hence, using residues to make products that are useful not only helps in proper use of waste, but is also a way of greener production.

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P-015

New Urea Derivatives as Potential Antimicrobial Agents: Synthesis, Biological Evaluation, and Molecular Docking Studies

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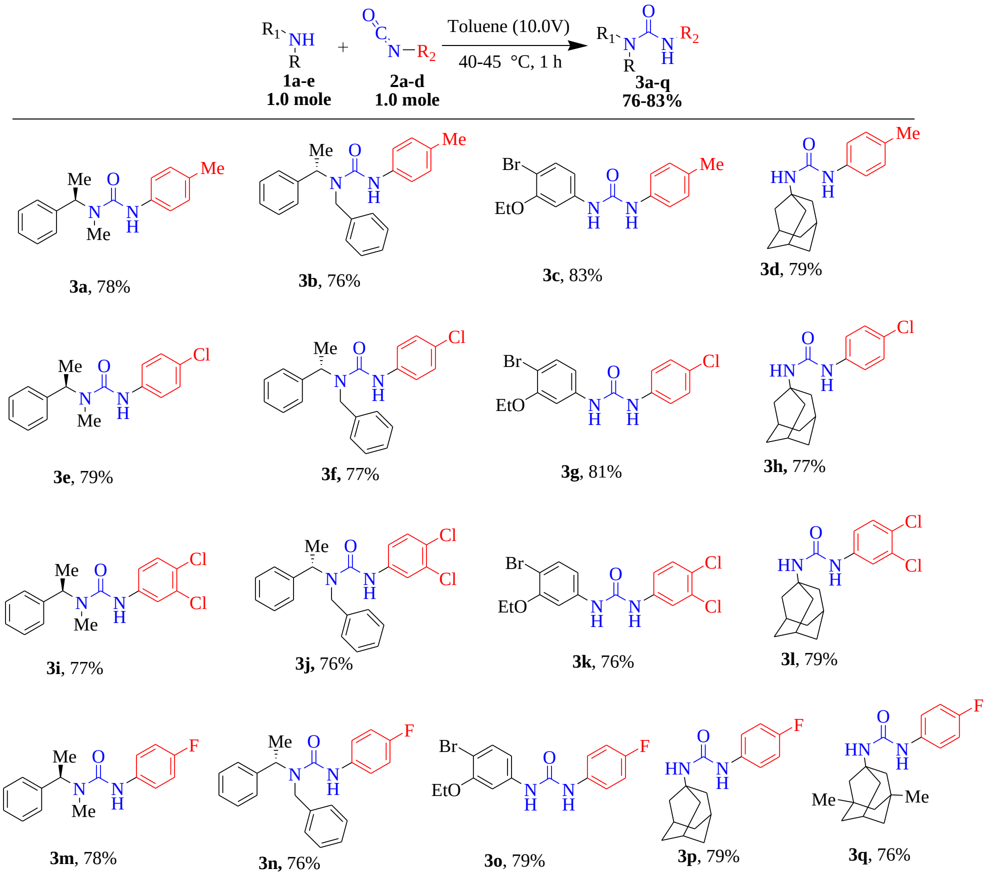
Abstract:

A series of new urea derivatives, containing aryl moieties as potential antimicrobial agents, were designed, synthesized, and characterized by ^{1}H NMR, ^{13}C NMR, FT-IR, and LCMS spectral techniques. All newly synthesized compounds were screened in vitro against five bacterial strains (*Escherichia coli*, *Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa*, and *Staphylococcus aureus*) and two fungal strains (*Candida albicans* and *Cryptococcus neoformans*). Variable levels of interaction were observed for these urea derivatives. However, and of major importance, many of these molecules exhibited promising growth inhibition against *Acinetobacter baumannii*. In particular, to our delight, the adamantyl urea adduct **3l** demonstrated outstanding growth inhibition (94.5%) towards *Acinetobacter baumannii*. In light of this discovery, molecular docking studies were performed in order to elucidate the binding interaction mechanisms of the most active compounds, as reported herein. The basic synthetic approach for preparation of the seventeen new urea derivatives, containing aryl moieties, is illustrated in Scheme 1. All compounds (**3a–q**) were successfully synthesized in a simple, one-step method, via the reaction of amines with commercially available isocyanates, at 40–45 °C for 1hr, in toluene. The attractive features of this method were, (1) simple one-pot procedure, (2) mild reaction conditions, (3) short reaction time, (4) easier work-up, and (5) high yields (76% to 83%).



Scheme 1: Synthesis of urea derivatives (**3a-q**).

P-021

UV activated Potassium Persulfate and Iron Oxide impregnated granular activated carbon for Complete removal of Arsenite from Groundwater

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Abstract:

The removal of poisonous arsenite [As(III)] from polluted surface and groundwater is significant. When compared to arsenate [As(V)], however, direct arsenite removal is more challenging. Peroxidation of arsenite to arsenate is therefore critical for its efficient removal from water. The removal effectiveness of arsenic from groundwater was studied by oxidising it with UV activated potassium persulfate (KPS) and then adsorbing it on iron oxide impregnated granular activated carbon (FeO/GAC). In one hour, a complete removal of 10 ppm of arsenic solution was obtained using UV activated KPS and FeO/GAC. The adsorption kinetics and thermodynamics were determined using a batch experiment. Also investigated the effects of adsorbent mass (FeO/GAC), C/Fe molar ratio, pH, arsenic concentration, competing anions, and humic acid on arsenic adsorption. Scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Brunauer-Emmett-Teller (BET), and zeta potential measurements were used to characterise the FeO/GAC adsorbent. Furthermore, the influence of pH indicated that the most efficient removal occurred in the pH range of 6.0-7.0, and that removal effectiveness fell substantially at higher and lower pH values. Even in the presence of natural pollutants, groundwater from Cheongyang, South Korea, was spiked with 10 ppm arsenic (III) and more than 82 percent arsenic removal was achieved in 90 minutes. As a consequence of the findings, UV activated KPS with FeO/GAC appears to be a successful approach for treating severely arsenic-contaminated water sources, and it may be a viable alternative to existing treatments.

Keywords: Arsenic removal, Arsenite Oxidation, Granular activated carbon, UV activated potassium persulfate

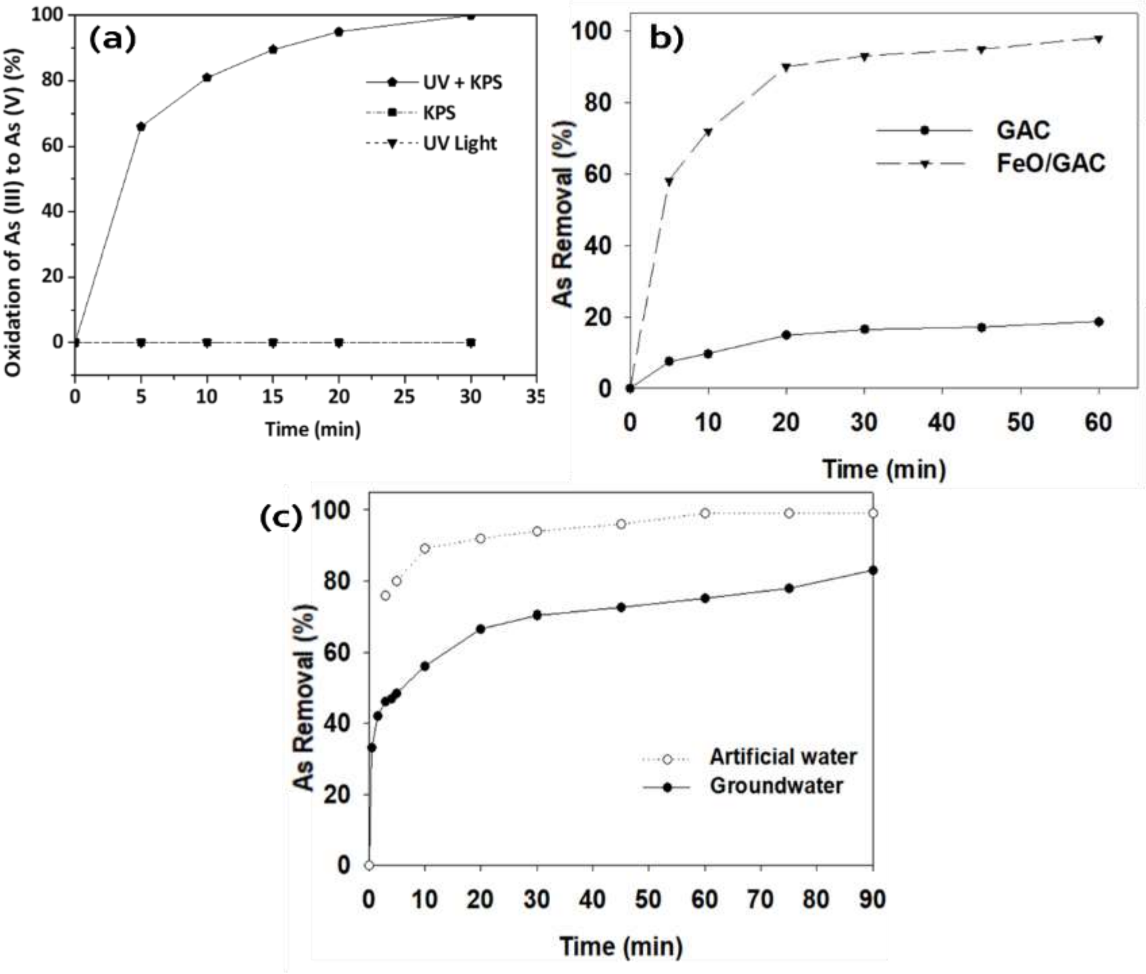

Figure.1 (a) Photochemical oxidation of As(III) to As(V), (b) Adsorption efficiency of As(V) for GAC and FeO/GAC, and (c) Arsenic removal from artificial water & groundwater collected from Cheongyang, South Korea using photochemical oxidation and FeO/GAC.

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P-026

Removal of Fluoride from Ground Water using Micellar Enhanced Ultrafiltration (MEUF)

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Abstract:

Fluoride present in drinking water is a global issue. Long term exposure to fluoride can result in fluorosis. The present study was aimed at the investigation of removal of fluoride from ground water using micellar enhanced ultrafiltration. The conventional methods for removal of fluoride were adsorption using different types of adsorbents, ion exchange process, membrane separation techniques like reverse osmosis, electrodialysis, micellar enhanced ultrafiltration (MEUF). MEUF is a process that involves the use of surfactant to form micelles, which are responsible for binding the fluoride, and hence rejected. Micelle formation and micelle characteristics are important phenomena in the entire process. In the present work Flat sheet Polyether sulphone membranes with 5 KDa MWCO is used in batch process. CPC and CTAB surfactants are chosen for formation of micelles. Further, the proposed work is aimed to study the effect of different operating parameters such as effect of time, pH, Pressure, temperature and rpm on flux and rejection. Highest fluoride removal efficiency, 89.36% (using 50 CMC of CPC) and 86.2% (using 50 CMC of CTAB) was achieved at 10 mg F^-/L and neutral pH under operating conditions of 2 kg f/cm2 pressure and 300 rpm stirrer speed. CPC has given better flux and rejection compared to CTAB.

Keywords: Micellar enhanced ultrafiltration (MEUF), Polyether sulfone (PES), Fluoride, CPC, CTAB.

Experimental Methodology:

Before each experiment, the PES membranes were soaked in distilled water for 24 hours. In the uf cell, the soaked Membrane is fixed. A gasket is positioned above the membrane to prevent leaking. The cell connections and membrane seals are verified for airtightness before and after pressurising the cell as shown in Fig. 1. Fluoride samples are made in various concentrations. The sample is dropped through the inlet with CPC or CTAB surfactant (at different CMC). Nitrogen gas is slowly released into the cell pressurising it to 2kgf/cm^2. Before applying pressure, the pressure relief valve is closed, and the safety valve is ensured to be open. The stirrer speed is set to 300 rpm and measured with a Digital Tachometer. Volumes of collected permeate and retentate are measured after a certain amount of time has passed. Ultra-filtration experiments were done by optimizing the effects of surfactant concentration (10-50 CMC), Initial fluoride concentration (10-50 mg/L), pH (2-12), Pressure (1- 4 kg f/cm^2) and Stirrer Speed (100-600 rpm). After collecting samples, Fluoride concentration is determined using ion electrode method.

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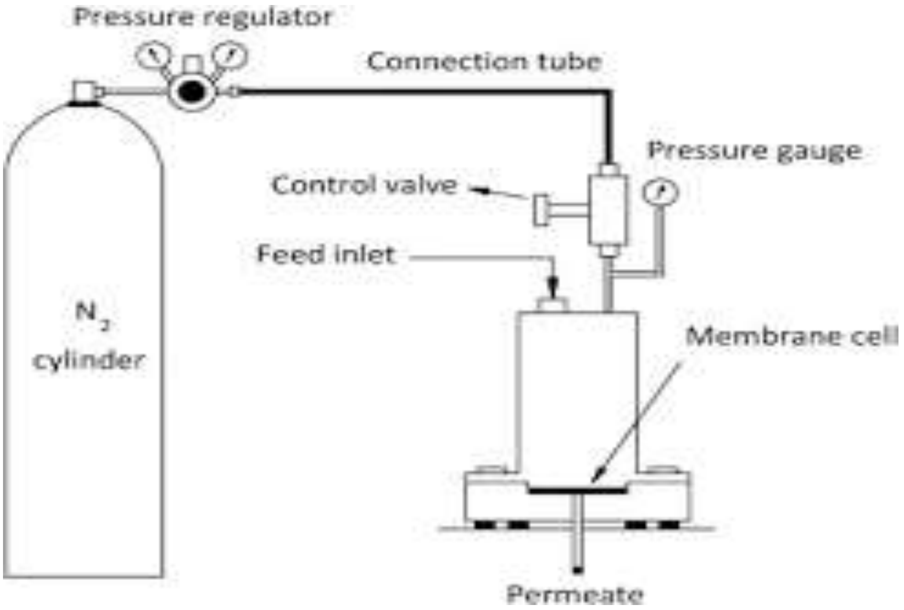

Figure 1. Schematic of the Experimental Setup Batch Concentration Mode

Results:

The experimental results obtained and presented in this study demonstrate that a PES membrane with a high Molecular Weight Cut-off (5 KDa) permitted high surfactant concentration to be used to treat fluoride content. The optimal conditions for fluoride removal were C_i=10 mg F^-/L, C_{CPC}=50 CMC, C_{CTAB}=50 CMC, pH=7.23, Pressure=2 kg f/cm^2 and stirrer speed= 300 rpm. At 10 mg F/L and neutral pH, with operating conditions of 2 kg f/cm2 pressure and 300 rpm stirrer speed, the highest fluoride removal efficiency 89.36 percent (using 50 CMC of CPC) and 86.2 percent (using 50 CMC of CTAB) was attained. The values of flux and removal efficiency determined at effects of five operating parameters is shown in **Fig 2**. and **Fig 3.**

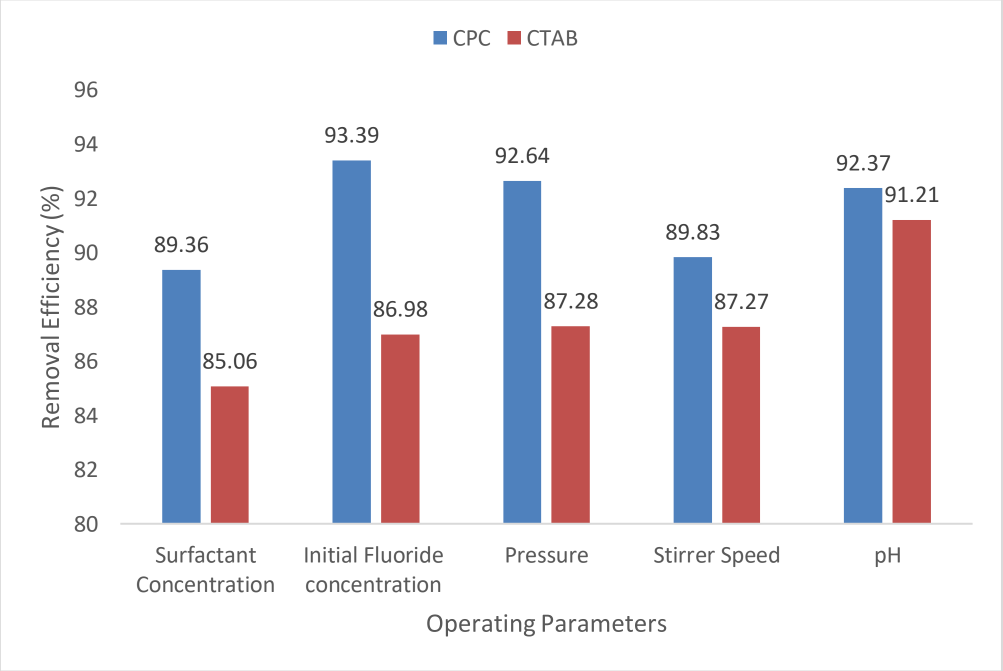

Figure 2. comparison of flux on cpc and ctab

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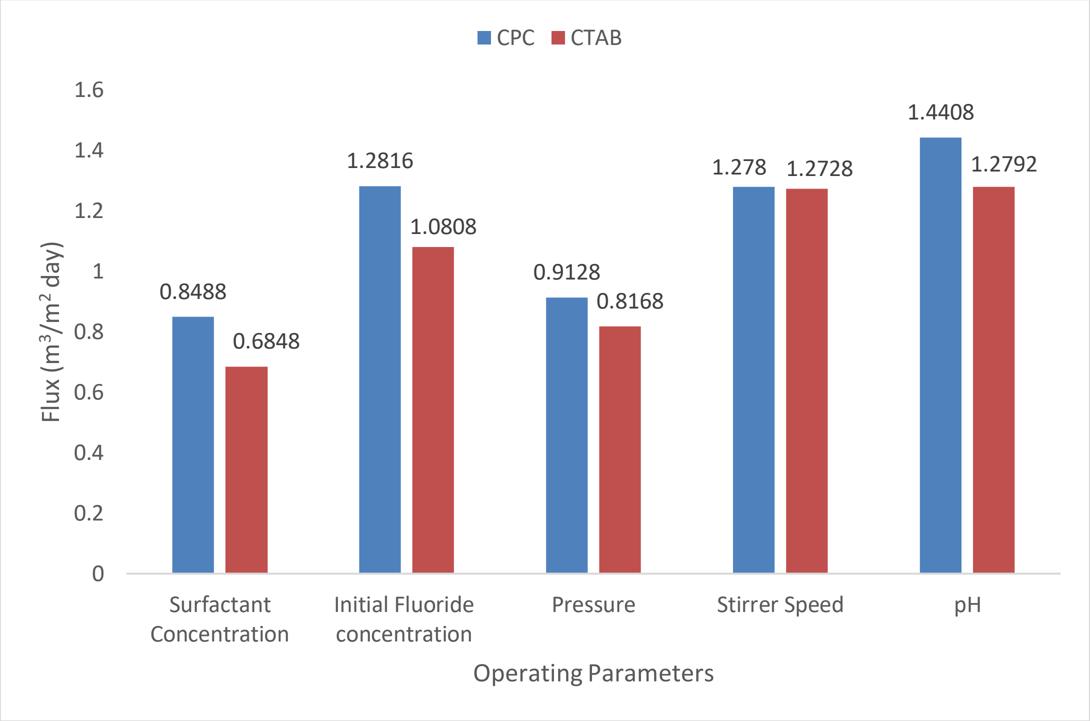

Figure 3. comparison of removal efficiency on cpc and ctab

Conclusions:

This study examined the performance of MEUF process for the removal of fluoride from aqueous solutions using a prepared PES membrane with CPC, CTAB as the cationic surfactant. PES Membranes were asymmetric porous membranes purchased from Membrane Permionics. and used in a dead-end cell. The influence of CPC and CTAB concentration, solution pH, Pressure and stirrer speed was studied on the membrane performance in terms of permeate flux and removal efficiency of Fluoride.

Glimpses of

1st Online International Conference on "Emerging Trends in Catalysis for Sustainable Chemical Processes", conducted during 26th - 28th August 2021.

Dr Archna, Chariman, BRC, IIChE

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