February 2024

CSI Communication

Monthly Newsletter of Catalysis Society of India

Circulated to all CSI Members

Important Announcement:

CSI newsletter shall be pleased to publish a page write-up under the title, Centre of Excellence in Catalysis Research in India from any Indian Academics, Research laboratories, or Industrial organizations. You may send your brief write-up on your research activities to us which will be published in the coming issues of CSI.
You can also share your recent happy moments like publications, granted patents, technology commercialization, fellowship, awards, etc. to highlight in the CSI communication.

▪ Functional Nanomaterials for Renewable Energy @ Dr. Aditi Halder Group, IIT Mandi

Dr. Aditi Halder's group at IIT Mandi works on developing functional nanomaterials for renewable energy. The group focuses on designing those nanomaterials that will be utilized as electrocatalysts for hydrogen generation in the electrolyzer, layered materials for energy storage (especially for the metal-air battery application), electrocatalysts for the selective conversion of CO_2 to value-added products like ethanol, photocatalysts and photoelectrocatalysts for environmental remediation. The research group under the supervision of Dr. Halder aims to address certain issues which are critical for the well-being of future generations. With the help of various advanced tools and technologies and the strategic development of multi-component catalyst systems including heterojunctions, inter-metallic alloys, near-surface alloys, and high entropy alloys, it is possible to provide an affordable solution to address the pressing issues of energy demand and environmental remediation.

Development of Next-Generation Batteries Beyond Lithium:

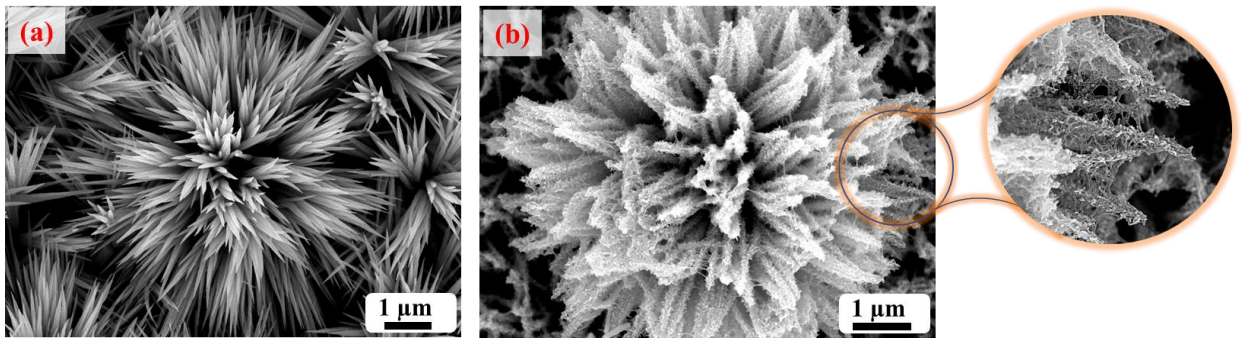
The stochastic nature of renewable energy resources along with fluctuation in their continuous supply creates obstacles in their effective utilization. To address this intermittency issue in the energy supply, studies are undergoing to develop strategies to store renewable energy in different forms like electrochemical energy storage. In the last few years, the group worked continuously to design newer electrode materials for the next generation metal-air battery like the Zn-air battery to replace the usage of Li-battery. Zn is safer, less costly, and more environmentally friendly. The group also develops flexible Zn-air batteries for personal health care

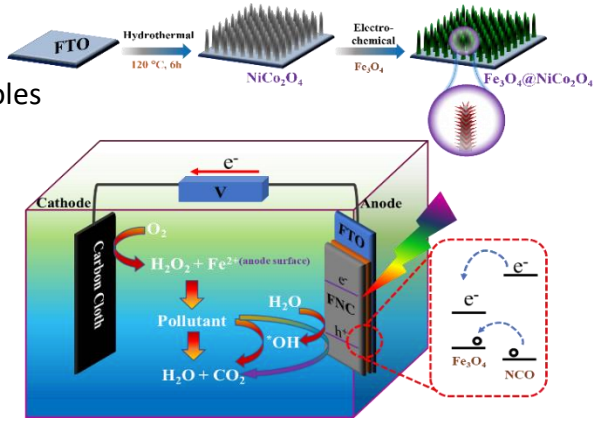
For further information of CSI please visit, http://www.catalysisindia.org, https://www.begellhouse.com/journals/catalysis-in-greenchemistry-and-engineering.html & https://www.linkedin.com/groups/13923122/

devices (Nanoscale 16 (8), 4157-4169,2024). The researchers from the group have developed excellent layered materials of MnO2 and doped with various metal ions like Ni, Co, and Fe and studied their performance as oxygen electrodes for rechargeable zinc-air batteries (Journal of Energy Storage 74, 109350,2023). The group is one of the very few groups in India who are working on the photo-enhanced performance of batteries (Materials Today Energy 19, 100612,2021).

Simultaneous Pollutant degradation and hydrogen generation:

The group designs materials with multi-functional properties where photoelectrode can degrade the pollutants and simultaneously will generate hydrogen. E.g. a bifunctional self-standing photoelectrode could degrade the water pollutant molecules at the anode with simultaneous production of molecular hydrogen at the cathode using Bi_2O_3 coated over the surface of self-standing TiO_2 nanorods (ACS Applied Nano Materials 6 (6), 4297-4308,2023).





Thus, prepared photoelectrodes show high degradation efficiency for rhodamine molecules, where direct oxidation of rhodamine by the holes generated under solar light illumination was detrimental to its activity. During simultaneous pollutant removal and energy production experiments, the anode shows 100% degradation of pollutant molecules while the cathode shows high hydrogen gas production. For these purposes, the catalyst should be easy to prepare and robust in activity. Its robust activity, high stability, and durability open a new avenue for wastewater treatment with simultaneous renewable energy production technologies. The group has also developed photoelectrodes which are good for hydrogen peroxide synthesis and useful for environmental degradation (Chemical Engineering Journal 479, 147575,2024).

Electrochemical CO_2 Reduction

The Paris Agreement sets a target of a decline in the usage of greenhouse gas emissions to 43% by 2030 to combat climate change. However, the progress towards this target is still plodding. For example, CO_2 concentrations in the atmosphere for the year 2021 itself reached 415.7 parts per million (ppm) which was 149 percent of pre-industrial levels before human activities started disrupting the natural balance of these gases in the atmosphere. Thus, it is essential to utilize this anthropogenic CO2 in value-added products. Electrochemical conversion of CO_2 to value-added

products is a very effective way to mitigate the concentration of CO2. The group is designing many materials for electrochemical conversion of CO2 to value-added products (Journal of Nanoparticle Research,20,46,2018).

Electrochemical Hydrogen Generation using non-platinum group elements

The group has expertise in synthesizing various defect-enriched nanostructures which can be used for water electrolyzer. They have used high entropy alloys to generate the hydrogen (NanoResearch 15, 4799–4806, (2022). The defect-enriched alloys and heterojunction materials played indeed important for enhancing the performance of hydrogen evolution (ACS Applied Energy Materials 3 (6), 5333-5342,2020). Details about these have been tabulated also as a book chapter on defect-enriched transition metal oxides toward photoelectrochemical water splitting.

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https://sites.google.com/site/renewableenergyforgreenerearth/home?authuser=0

Commercial & Policies

- **L&T commissions indigenously built hydrogen electrolyser at Hazira**

Larsen & Toubro (L&T) has commissioned its first indigenously manufactured electrolyzer at the green hydrogen plant at A M Naik Heavy Engineering Complex in Hazira, Gujarat, the company said in a regulatory filing. The electrolyzer, featuring a rated power capacity of 1 MW (expandable to 2 MW), can produce hydrogen of 200 Nm^3/hr. The electrolyser will now undergo rigorous testing to optimize its performance, and in turn, pave the way for full-fledged manufacturing of electrolysers.

Source: https://www.thehindubusinessline.com/companies/lt-commissions-first-indigenously-built-hydrogen-electrolyser-at-hazira/article67903111.ece

- **PM Modi laid the foundation stone of Digboi and Guwahati refineries capacity expansion**

The Prime Minister laid the foundation stone for important projects in the oil and gas sector including the capacity expansion of Digboi Refinery from 0.65 to 1 MMTPA (million metric tonnes per annum); Guwahati Refinery Expansion (1.0 to 1.2 MMTPA) along with installation of Catalytic Reforming Unit (CRU); and augmentation of Facilities at Betkutchi (Guwahati) Terminal: Indian Oil Corporation Limited, among others.

Prime Minister will also dedicate to the nation the 718 Km long Barauni - Guwahati Pipeline to supply natural gas to nine geographical areas covering 31 districts across these three states through authorized city gas distribution (CGD) entities along its route.

PM also inaugurated the Indian Oil Corporation Limited Mono Ethylene Glycol project in Paradip Refinery which will bring a revolutionary change in the polyester industry of eastern India. This will also provide raw materials to the textile park in Bhadrak and Paradip.

Source: https://pib.gov.in/PressReleaseIframePage.aspx?PRID=2012973

- **CSIR-NIIST Transfers Technology for Single-use Biodegradable Tableware**

The National Institute for Interdisciplinary Science and Technology (NIIST) has signed an agreement with East Corridor Consultant India Pvt. Ltd, a Lucknow-based clean-tech startup, for transferring its technology for manufacturing single-use biodegradable tableware from rice and wheat waste. This is the 16th company acquiring the same technology from CSIR-NIIST. The developed cutlery is shelf-stable for up to 10 to 12 months and can serve hot/boiled solid and liquid food. It has enough tensile strength to hold the food item according to its shape and can resist microbial growth for up to 12 months in India's humid atmospheric conditions.

Source: https://www.newsexperts.in/csir-niist-transfers-technology-for-single-use-biodegradable-tableware/

- **NTPC Green Energy to set up India's largest green hydrogen production facility near Vizag**

NTPC Limited has signed a Land Lease Agreement to realize its green energy and green hydrogen objectives, thus also contributing to the Government of India's efforts towards energy transition. The hub will come up on 1,200 acres of land near Pudimadaka village of Atchutapuram Mandal in Visakhapatnam, Andhra Pradesh. The Pudimadaka Green Hydrogen Hub aims to create a world-class ecosystem for technologies in the new energy paradigm, such as electrolyzer and fuel cell manufacturing, related ancillary industries, and start-up, incubation, testing facilities, production and export of green hydrogen and its derivatives such as green ammonia and green methanol. The project includes the construction of India's largest green hydrogen production facility (1,200 tons per day), which will enable further conversion of green hydrogen to derivatives such as green ammonia and green methanol, primarily catering to various export markets.

Source: https://pib.gov.in/PressReleaseIframePage.aspx?PRID=2007793

- **Reliance Industries to establish 50 compressed biogas plants**

Reliance Industries (RIL) is embarking on an ambitious initiative to establish more than 50 compressed biogas (CBG) plants within the next two years, with a projected expenditure exceeding Rs 5,000 crore. These plants will diversify CBG utilization across automotive, industrial, and commercial sectors. Each plant is designed to process 250–500 tonne per day (tpd) of feedstock, yielding CBG output ranging from 10 to 20 tonnes per day. RIL's dedicated team will oversee feedstock procurement, engaging with various sugar mills for sugarcane press mud and feedstock to support CBG production. The company has already operationalized two CBG demo units at its Jamnagar refinery in Gujarat and commissioned the first commercial-scale CBG plant in Barabanki, Uttar Pradesh. Through these ventures, RIL aims to utilize 5.5 million tonnes of

agro-residue and organic waste, mitigating nearly two million tons of carbon emissions annually while generating 2.5 million tons of organic manure. Additionally, it anticipates reducing imported LNG by approximately 0.7 million tonnes per year. These CBG facilities will also facilitate the expansion of CBG and bio-CNG retailing at Jio-BP fuel outlets.
Source: https://www.manufacturingtodayindia.com/reliance-industries-to-establish-50-compressed-biogas-plants-rs-5000-crore-allocated/

- **LyondellBasell's Joint Venture Starts Operations at Chemical Recycling Feedstock Facility**

Source One Plastics, a collaboration between 23 Oaks Investments and LyondellBasell, has achieved a successful startup of its plastic waste sorting and recycling facility situated in Eicklingen, Germany. This cutting-edge unit is designed to process challenging-to-recycle post-consumer plastic waste, including mixed plastic packaging and flexible polyolefins materials that are typically destined for incineration. With an anticipated annual processing capacity of 70,000 metric tons, the facility aims to address plastic waste equivalent to that generated by approximately 1.5 million German citizens annually.
Source: https://www.chemanalyst.com/NewsAndDeals/NewsDetails/lyondellbasell-joint-venture-starts-operations-at-chemical-recycling-feedstock-facility-25535

- **Aether Industries to commission 15 MW solar power plant in Gujarat's Bharuch**

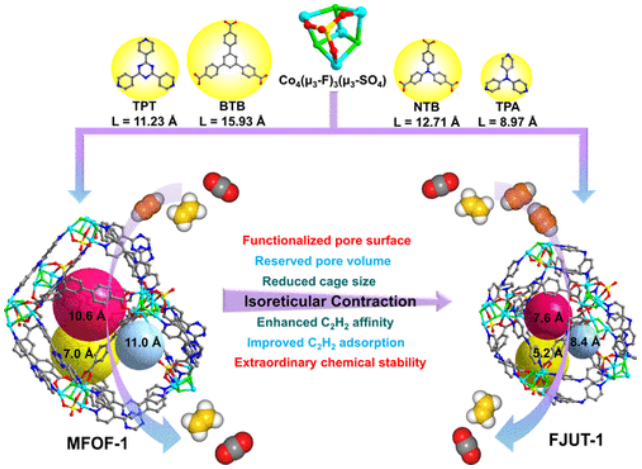
Aether Industries has taken significant stride towards sustainability with the initiation of 15 MW Solar Power Project (Auto-Tracker Modules) under the Captive Power Producer (CPP) segment. This order has been entrusted to KPIG Energia, a Wholly owned subsidiary of KPI Green Energy. Aether Industries had in past, commissioned a 16MW Solar Power Project (Fixed Modules) under the Captive Power Producer (CPP) segment, in July 2022 and this new Solar Power Plant under CPP, will add to its renewable energy sources and further move towards the sustainability. The solar power farm will be in Gujarat's Bharuch District and spread across 60 acres. The captive solar power plant is one of the most important initiatives in the specialty chemicals industry. The phase-wise commissioning of the solar power plant is set to begin as early as during the coming FY.
Source: https://www.epcworld.in/p/post/aether-industries-to-commission-15mw-solar-power-plant-at-bharuch-gujarat

- **BASF and Envision Energy enter a collaboration to drive sustainable energy solutions**

Backed by their respective expertise, the two companies aim to optimize the process of producing e-methanol from green hydrogen and CO_2, paving the way for a more sustainable energy landscape. This collaboration will see BASF provide its cutting-edge SYNSPIRETM catalyst technology, which Envision Energy will integrate with its innovative energy management system. The two organizations plan to demonstrate the viability of the advanced process design next year, at Envision Energy's Chifeng site in Inner Mongolia, China. The new catalyst developed by BASF represents a significant breakthrough in sustainable energy solutions. It enables the efficient conversion of green hydrogen and CO_2 into e-methanol.
Source: https://www.basf.com/global/en/media/news-releases/2024/01/p-24-113.html

Scientific Updates

- **Isoreticular Contraction of Cage-like Metal–Organic Frameworks with Optimized Pore Space for Enhanced C_2H_2/CO_2 and C_2H_2/C_2H_4 Separations**

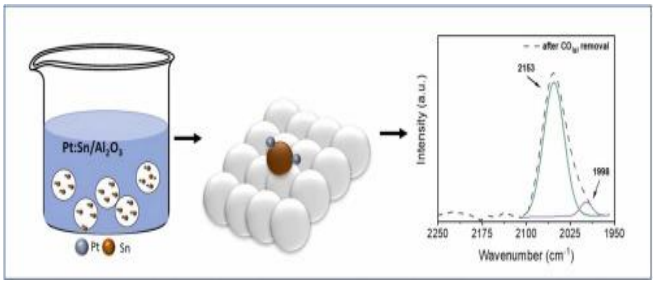


The C_2H_2 separation from CO_2 and C_2H_4 is of great importance yet highly challenging in the petrochemical industry, owing to their similar physical and chemical properties. The pore nanospace engineering of cage-like mixed-ligand MFOF-1 has been accomplished via contracting the size of the pyridine- and carboxylic acid-functionalized linkers and introducing a fluoride- and sulfate-bridging cobalt cluster, based on a reticular chemistry strategy. Compared with the prototypical MFOF-1, the constructed FJUT-1 with the same topology presents significantly improved C_2H_2 adsorption capacity, and selective C_2H_2 separation performance due to the reduced cage cavity size, functionalized pore surface, and appropriate pore volume. The introduction of fluoride- and sulfate-bridging cubane-type tetranuclear cobalt clusters bestows FJUT-1 with exceptional chemical stability under harsh conditions while providing multiple potential C_2H_2 binding sites, thus rendering the adequate ability for practical C_2H_2 separation application as confirmed by the dynamic breakthrough experiments under dry and humid conditions.

Source: J. Am. Chem. Soc. 2024, https://doi.org/10.1021/jacs.3c12032

- **Tuning the interfacial interactions between alumina support and pseudo-single atom platinum-tin catalytic sites for heavy naphtha reforming**

Heavy naphtha reforming, a crucial downstream process in oil refineries for improving the octane number of the gasoline feedstock, requires expensive Pt metal catalysts and it accounts for 60% of the catalyst cost. These conventional Pt nanoparticle sizes range between 1 – 2 nm and thus, only ≈ 80% of the Pt atoms of the particle are available for the catalytic reactions. In this work, we hypothesized that it might be possible to achieve 100% atom utilization if the Pt atoms are distributed as single or pseudo-single atom clusters, where all the atoms are exposed to the reactant molecules and by tuning their Interfacial Interactions.

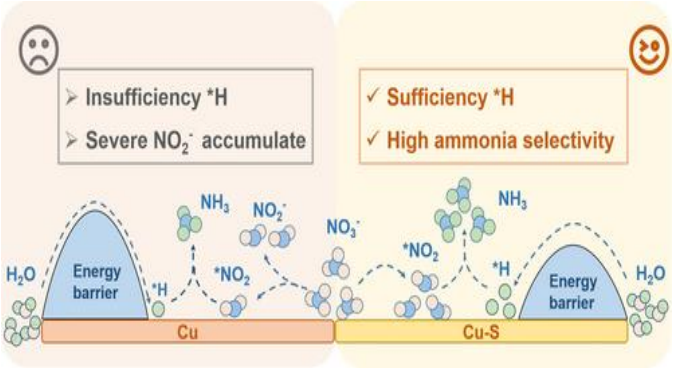


We aimed to significantly reduce the Pt contents by dispersing the active Pt sites as pseudo-single atoms on industrially relevant γ-Al2O3 support. Interfacial Interactions and stability of Pt sites were then tuned by using tin (Sn) as a promoter. These catalysts were then evaluated for heavy naphtha reforming in a fixed-bed reactor. The catalyst with

Sn/Pt mole ratio of 1.68 showed excellent performance with aromatics of 83 wt% and research octane number (RON) of ≈ 103. These results indicated our catalyst preparation methodologies and interfacial interaction tuning successfully disperse Pt on the spherical alumina support leading to better atom economy. With 30–50% less Pt content when compared to the industrially used catalyst, made the heavy naphtha reforming process was economical and sustainable.
Source: Catalysis Today, 2024, https://doi.org/10.1016/j.cattod.2024.114606

- **Sulphur-Boosted Active Hydrogen on Copper for Enhanced Electrocatalytic Nitrate-to-Ammonia Selectivity**

Electrocatalytic nitrate reduction to ammonia is a promising approach in term of pollutant appreciation. Cu-based catalysts performs a leading-edge advantage for nitrate reduction due to its favorable adsorption with $*NO_3$. However, the formation of active hydrogen (*H) on Cu surface is difficult and insufficient, leading to the significant generation of by-product NO_2^-. Herein, sulphur doped Cu (Cu−S) is prepared via an electrochemical conversion strategy and used for nitrate electroreduction.

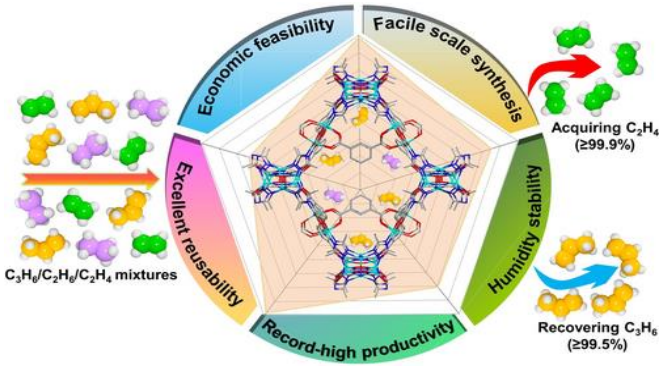


The high Faradaic efficiency (FE) of ammonia (~98.3 %) and an extremely low FE of nitrite (~1.4 %) are achieved on Cu−S, obviously superior to its counterpart of Cu (FE_{NH3}: 70.4 %, FE_{NO2}^-: 18.8 %). Electrochemical in situ characterizations and theoretical calculations indicate that a small amount of S doping on Cu surface can promote the kinetics of H_2O dissociation to active hydrogen. The optimized hydrogen affinity validly decreases the hydrogenation kinetic energy barrier of $*NO_2$, leading to an enhanced NH_3 selectivity.
Source: Angewantdte Chemie, 2024, https://doi.org/10.1002/anie.202400289

- **Scalable Synthesis of Robust MOF for Challenging Ethylene Purification and Propylene Recovery with Record Productivity**

Ethylene (C_2H_4) purification and propylene (C_3H_6) recovery are highly relevant in polymer synthesis, yet developing physisorbents for these industrial separation faces the challenges of merging easy scalability, economic feasibility, and high moisture stability with great separation efficiency.

Author reported a robust and scalable MOF (MAC-4) for the simultaneous recovery of C_3H_6 and C_2H_4. Through creating nonpolar pores decorated by accessible N/O sites, MAC-4 displays top-tier uptakes and selectivities for C_2H_6 and C_3H_6 over C_2H_4 at ambient conditions. Molecular modelling combined with infrared spectroscopy revealed that C_2H_6 and C_3H_6 molecules were trapped in the framework with stronger contacts relative to C_2H_4. Breakthrough experiments demonstrated exceptional separation performance for binary C_2H_6/C_2H_4 and C_3H_6/C_2H_4 as well as ternary $C_3H_6/C_2H_6/C_2H_4$ mixtures, simultaneously affording record productivities of 27.4 and 36.2 L kg^{-1} for high-purity C_2H_4 (≥99.9 %) and C_3H_6 (≥99.5 %). MAC-4 was facilely prepared at deckgram-scale under reflux condition within 3 hours, making it as a smart MOF to address challenging gas separations.



Source: Angewantdte Chemie, 2024, https://doi.org/10.1002/anie.202319978

Industrial Conclave on Sustainable Chemical Processes for API and Key Intermediates: Affordable and Recyclable Catalytic Options

The Indian Society of Chemists and Biologists, Lucknow, The Catalysis Society of India (CSI) & Environment Research Foundation of India, Rajkot jointly organized an **"Industrial Conclave on Sustainable Chemical Processes for API and Key Intermediates: Affordable and Recyclable Catalytic Options"** on 8th March 2024 at Seasons Hotel, Rajkot, Gujarat.

Padma Vibhushan Prof. (Dr.) M. M. Sharma and Dr. Raksh Vir Jasra were esteemed speakers followed by panel discussion. The event was organized by Prof. (Dr.) Anamik Shah President, Indian Society of Chemists and Biologists and supported by Rhodium Master. The conclave is attended very well by researchers from academia and various industries.

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Catalysis Research out of India

1. Aayushi Lodhi, Kalpana C Maheria "Zeolite-catalysed esterification of biomass-derived acids into high-value esters products: Towards sustainable chemistry", **Catalysis Communication, 2024** https://doi.org/10.1016/j.catcom.2024.106883
2. PP Neethu, B Kunjumon, P Aswin, NJ Venkatesha, A Sakthivel, "Hexanol conversion over mixed metal oxides derived from hydrotalcite: Influence of molybdate species on catalytic activity", **Molecular Catalysis, 2024, 558, 114000** ; https://doi.org/10.1016/j.jcis.2023.12.136
3. Niharika Tanwar, Himani Narjinari, Harsh Sharma, Sunil Dhole, Raksh Vir Jasra, Akshai Kumar "Electrocatalytic Oxidation of Methanol and Ethanol with 3d-Metal Based Anodic Electrocatalysts in Alkaline Media Using Carbon Based Electrode Assembly" ***Inorg. Chem.* 2024**, 63, 6, 3005–3018
4. Hanumant B Kale, Arun D Kute, Rahul P Gaikwad, Paolo Fornasiero, Radek Zbořil, Manoj B Gawande "Synthesis and energy applications of copper-based single-atom electrocatalysts" **Coordination Chemistry Reviews, 2024** https://doi.org/10.1016/j.ccr.2023.215602
5. Ganapati D Yadav, "The Net Zero Goal and Sustainability: Significance of Green Hydrogen Economy in Valorization of CO2, Biomass and Plastic Waste into Chemicals and Materials" **Climate Action and Hydrogen Economy: Technologies Shaping the Energy Transition, 2024,** 61-90, Springer Nature Singapore
6. Rohit B Meshram, Ganapati D Yadav, Kumudini V Marathe, KL Sahoo, "Evaluating the carbon footprint of sulphur recovery unit: A comprehensive analysis" **Journal of Environmental Chemical Engineering, 2024, 12(2), 111916**
7. Harmitkumar Pandya, Chathakudath Prabhakaran Vinod, Virendra Rathod, Mannepalli Lakshmi Kantam, "Kinetic Model of Hydrogenation of Glucose to Sorbitol on a Ni/Bentonite Catalyst" **Industrial & Engineering Chemistry Research, 2024**, DOI: 10.1021/acs.iecr.3c03808
8. Rajesh Belgamwar, Kotni Santhosh, G Valavarasu, Pradip Sarawade, Vivek Polshettiwar, "Tuning the Interfacial Interactions between Alumina Support and Pseudo Single Atom Platinum-Tin Catalytic Sites for Heavy Naphtha Reforming" **Catalysis Today, 2024** https://doi.org/10.1016/j.cattod.2024.114606
9. Manas Barik, Brijesh Patel, Shilpa Dabas, Parul Rathour, Dharm S Padariya, Lakhya Jyoti Konwar, Atul Kumar, Rajendra Srivastava, Palani S Subramanian, Saravanan Subramanian "The resurgence of old material: The impact of boehmite-derived catalytic material on the formation of dihydropyran compounds and its application to access fragrant derivatives" **Chemical Engineering Journal, 2024** https://doi.org/10.1016/j.cej.2024.149798

Upcoming Symposium/Conferences/Seminars/Workshop

1. International Conference on "Catalysis for Clean Energy Technologies and Sustainable Development" Organized under the aegis of the Catalysis Society of India in association with Dr. SSB UICET Panjab University Chandigarh on 5th &6th April, 2024.
2. 18th International Congress on Catalysis from July 14-19, 2024, LYON, France.
3. XXIII International Symposium on Homogeneous Catalysis at Trieste, July 21-26, 2024.
4. "19th Edition of Global Conference on Catalysis, Chemical Engineering & Technology" at Rome, Italy, from September 19th-21st, 2024.
5. Decarbonizing the chemical industry and 2nd Sustainable feedstocks for the future of chemicals and plastics, 23-24, May 2024 – Antwerp, Belgium.
6. 18th Edition of International Conference on Catalysis, Chemical Engineering, and Technology" (CCT 2024) during June 17-19, 2024 at Paris.
7. 19th Edition of Global Conference on Catalysis, Chemical Engineering & Technology, September 19-21, 2024 | Rome, Italy | Hybrid Event

Announcements

- **CSI Congratulates the following CSI members on the recognition they received recently.**

Name	Achievements
Padma Shri Professor Ganapati D. Yadav, *FTWAS, FNA, FNASc, FRSC (UK), FIChemE (UK), FIIChE* Emeritus Professor of Eminence & Former Vice Chancellor & R.T. Mody Distinguished Professor J.C. Bose National Fellow (Govt. of India), ICT Mumbai 	Received SASTRA-CNR Rao Award 2024 for Chemistry and Materials Sciences on National Science Day
Dr. Priyanka Verma Assistant Professor, Department of Chemistry, Indian Institute of Technology Delhi 	Selected for International Association of Catalysis Societies (IACS) Young Researcher Award 2024

Quote of the Month

"No matter what people tell you, words and ideas can change the world."

— Robin Williams

Editorial Team

Dr. Sharad Lande

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