November 2022

CSI Communication

Monthly Newsletter of Catalysis Society of India

Circulated to all CSI Members

Important Announcement:

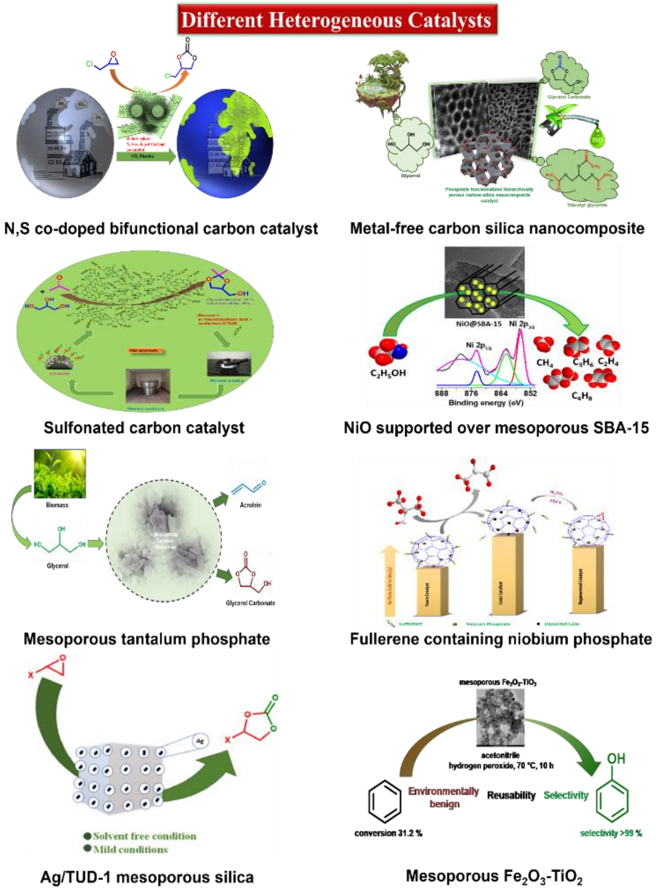
CSI newsletter shall be pleased to publish half a page write-up under the title, Centre of Excellence in Catalysis Research in India from any Indian Academics, Research laboratories or Industrial organizations. You may send your brief write-up on your research activities to us which will be published in coming issues of CSI.

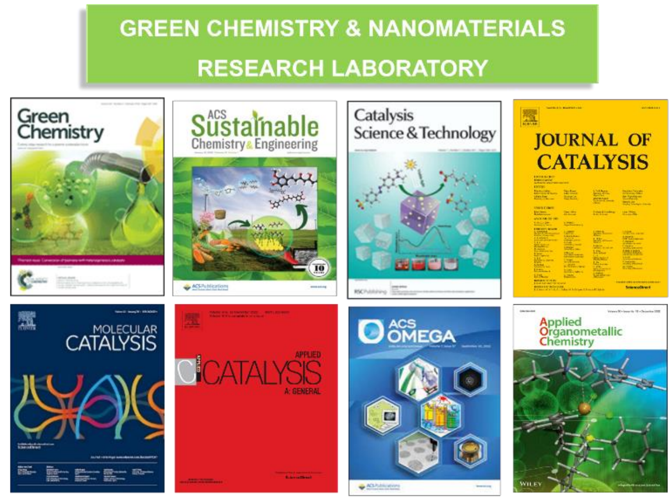
You can also share your recent happy moments like publications, granted patents, technology commercialization, fellowship, awards, etc. to highlight in the CSI communication.

We request all CSI members listed among top 2% scientists in the World in this year's list published by Stanford University so that we can display the list in next issue of Communication.

- ### Green Chemistry and Nanomaterials Laboratory @Prof. Biswajit Chowdhury; IIT (ISM) Dhanbad

Prof Biswajit Chowdhury's research focused on the synthesis of nanostructured material, its characterization and application towards CO_2 mitigation, biomass conversion, green hydrogen generation, photocatalysis and toxic pollutant removal from industrial wastewater. The group recently developed several carbon, phosphate and oxide-based catalysts for CO_2 fixation in epoxide, production of lower olefin and alcohols from CO_2, photocatalytic CO_2 fixation. Our work extended to synthesis of fine chemicals and fuels from biomass, C-H activation and epoxidation reactions. The group has successfully synthesized N, S doped carbon material for the synthesis of cyclic carbonates using CO_2 at ambient condition (***Green Chemistry*** 24***,*** **2022*,****1673*). Also, we have prepared metal free porous carbon-silica nanocomposite catalyst for glycerol carbonylation which is also active towards glycerol esterification reaction ***(ACS Sustainable Chemistry & Engineering*** 10*,* **2022***, 11242)*. The group synthesized surfactant embedded carbon catalyst towards glycerol acetalization reaction (***Catalysis Science and Technology*** 10,**2020**,4827). Another novel catalyst developed was Fullerene containing niobium phosphate catalyst useful for dehydration reaction (***Molecular Catalysis*** 475, ***2019*** 110470). The reduction of nitroaromatics (***ACS Omega***, 4 (2), ***2019***,4071) is one of the industrially important reactions carried by the group members. The dehydration of glycerol to acrolein (***Molecular Catalysis*** *518* ***(2022)*** *112074*). The effect of silylation on gold-titania catalyst towards propylene epoxidation reaction is a successful outcome of Indo-Netherland project which were published in (***Catalysis Science and Technology*** *8* ***(2018)*** *3052* ***; Journal of Catalysis*** 344,***2016***,434-444). Prof Chowdhury completed several national and international projects successfully.





Research publication: 83 journal articles; 3 Book chapter; 1 conference proceedings, 5 review article, 4 patents

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Commercial & Policies

- **Government Identifies 10 states for Green Hydrogen Manufacturing**

The government has identified 10 potential states (Karnataka, Odisha, Gujarat, Rajasthan, Maharashtra, Tamil Nadu, Andhra Pradesh, Kerala, Madhya Pradesh and West Bengal) that could be the key enablers in manufacturing green hydrogen in the country. The states are likely to have green hydrogen or ammonia manufacturing zones or clusters, helping India kickstart its National Green Hydrogen Mission in its initial years. These states have been identified based on the existing steel and fertilizer industries, refineries and ports located there, along with the operational and potential renewable energy generation capacity in the regions.

Source: https://www.constructionworld.in/energy-infrastructure/power-and-renewable-energy/government-identifies-10-states-for-green-hydrogen-manufacturing/37290

- **World's Largest CO_2-to-Methanol Plant Starts Production**

The world's first commercial scale CO_2 to Methanol plant has started production in Anyang, Henan Province, China. The cutting-edge facility is the first of its type in the world to produce methanol a valuable fuel and chemical feedstock at this scale from captured waste carbon dioxide and hydrogen gases. The plant's production process is based on the Emissions to Liquids (ETL) technology developed by Carbon Recycling International (CRI) and first demonstrated in Iceland. The new facility can capture 160,000 tonnes of carbon dioxide emissions a year, which is equivalent to taking more than 60,000 cars off the road. The captured carbon dioxide is then reacted with the recovered hydrogen in CRI's proprietary ETL reactor system with the capacity to produce 110,000 tonnes of methanol per year.

Source: Carbon Recycling International, 10/26/2022.

- **Kerala to invest $575 million to Build a Green Hydrogen hub in Kochi**

India Hydrogen Alliance (IH2A), a business organization with headquarters in Delhi, and the Keralan government announced that they are jointly assessing a proposal for the construction of the Kochi green hydrogen (KGH2) hub with a potential capital expenditure of $575 million. According to the official press release, the plant will have a 150 MW electrolyser, storage facility, and infrastructure hub, a capacity of 60 tonnes per day (TPD), with the potential to reach gigawatt-scale capacity.

Source: https://powerline.net.in/2022/11/15/india-hydrogen-alliance-and-kerala-government-to-build-kochi-green-hydrogen-hub/

- **20 million PET Bottles to be Recycled Annually by Indian Oil Corporation Ltd.**

PET waste is PET packaging that has been used but discarded by the consumer. The IOCL will set up a team to take 20 million of these bottles each year and turn them into yarn that can be used to weave or knit fabric. After that, this will be provided to a textile company to produce uniforms for the LPG gas agency employees and IOCL's petrol pump attendants.

Source: https://www.chemanalyst.com/NewsAndDeals/NewsDetails/20-million-pet-bottles-to-be-recycled-annually-by-indian-oil-corporation-ltd-11812

- **HPCL-Mittal Energy to start 100,000-tpy bio-ethanol plant in 2023**

India's HPCL-Mittal Energy Ltd will start up a bio-ethanol plant at its Bathinda refinery in northern India in 2023 as part of measures to reduce its carbon emissions. It in the process of constructing 100,000 tonnes per annum ethanol plant based on agricultural inputs like waste food.
Source: https://www.business-standard.com/article/companies/hpcl-mittal-energy-to-start-100-000-tpy-bio-ethanol-plant-in-2023-122092800543_1.html

- **LyondellBasell and Shakti Plastic Industries collaborating to advance mechanical recycling in India**

LyondellBasell Industries N.V. (Rotterdam, the Netherlands) and Shakti Plastic Industries, India's largest plastic scrap recycler and waste collection company, have signed MoU to form a joint venture to build and operate a fully automated, mechanical recycling plant in India. The plant is intended to process rigid packaging post-consumer waste and produce 50,000 tons of recycled polyethylene (PE) and polypropylene (PP) per year, equivalent to the single-use plastic waste produced by 12.5 million citizens. It is envisaged that the new facility will become the largest mechanical recycling plant in India and is estimated to start at the end of 2024. LyondellBasell will market the recycled products produced by this joint venture adding volume to its *Circulen* Recover range of existing PE and PP materials to help meet increasing demand by converters and brand owners in India for recycled polymer materials.
Source: https://www.recyclingtoday.com/article/lyondellbasell-shakti-plastic-partner-to-buiild-mechanical-recycling-plant-in-india/

- **Epsilon Carbon arm seeks funding to boost lithium-ion battery material business**

Epsilon Carbon, India's leading coal tar derivates company, is diversifying into battery material business to develop and manufacture high performance and quality carbon products for anode components of Lithium-Ion Batteries (LiB). The battery materials business will be housed under a new subsidiary Epsilon Advanced Materials formed with the purpose of becoming a preferred supplier of synthetic graphite material to cell manufacturers and energy storage device companies across the globe. Graphite Anode's consist of 25% volume of LiB cells and are the highest single material in a cell chemistry.
Source: https://www.epsiloncarbon.com/press/press-release/epsilon-advanced-materials-forays-into-battery-material-business

Scientific Updates

- **Top Ten Emerging Technologies in Chemistry**

IUPAC has released the 2022 Top Ten Emerging Technologies in Chemistry. The goal of this initiative is to showcase the transformative value of chemistry and to inform the general public about the potential of chemical sciences to foster the well-being of Society and the sustainability of our planet. These technologies are defined as transformative innovations in between a discovery and a fully commercialized technology, having outstanding potential to open new opportunities in chemistry, sustainability, and beyond. The catalysis play an important role in few technologies out of them.

The 2022 finalists are (in alphabetical order):

1. Aerogels
2. Fibre batteries
3. Film-based fluorescent sensors
4. Liquid solar fuel synthesis
5. Nanoparticle mega libraries
6. Nanozymes
7. Rational vaccines with SNA
8. Sodium-ion batteries
9. Textile displays
10. VR-enable interactive modelling

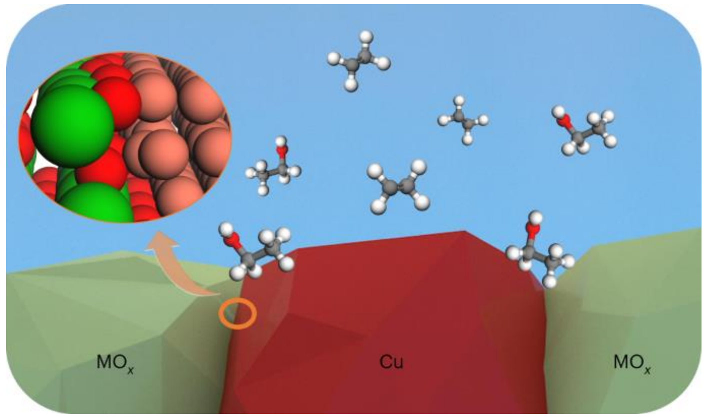
- **Half-Sandwich Complexes of Magnesium as Catalysts**

The use of alkaline earth metals in catalysis is an emerging research field. Magnesium is a particularly interesting candidate, as it exhibits high biocompatibility and low toxicity.

In general, hydroelementation and dehydrocoupling reactions are highly atom-economic processes, providing access to a variety of compounds.
Bringing together these two aspects, André Schäfer and colleagues, Saarland University, Saarbrücken, Germany, have developed a series of structurally constrained magnesium complexes, which can act as potent catalysts in hydroelementation and dehydrocoupling reactions. The team prepared four different *ansa*-half-sandwich complexes of magnesium (pictured, R = H, Me; R′ = Me, Ph; R″ = ^{t}Bu, Ph) via reactions of the corresponding ligands with dibutylmagnesium. The system, thus, represents an interesting advancement in the field of homogeneous magnesium catalysis.
Source: ChemCatChem 2022, https://doi.org/10.1002/cctc.202201007

- **Copper/alkaline earth metal oxide interfaces for electrochemical CO2-to-alcohol conversion by selective hydrogenation**

Multicarbon alcohols produced by electrochemical CO_2 reduction (CO_2RR) are attractive alternatives to fossil fuels; however, the selectivity towards alcohols in CO_2RR remains low, a result of competing hydrocarbon (that is, ethylene) production. Here we report on Cu catalysts decorated with different alkaline earth metal oxides (MOs). We found that BaO delivers a Faradaic efficiency of 61% towards C_{2+} alcohols.

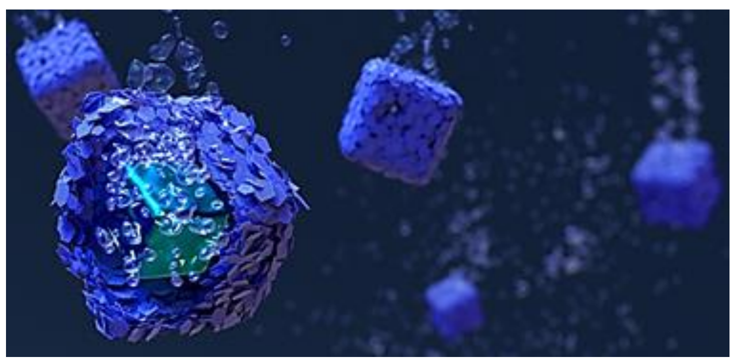


At an industry-relevant current density of 400 mA cm^{-2}, the ratio of alcohols to hydrocarbon reached 3:1. Mechanistic studies, including in operando X-ray absorption spectroscopy, in situ Raman spectroscopy and density functional theory calculations, suggested that the increased selectivity towards alcohols originates from sites at the MO/Cu interface. Furthermore, computational studies indicated that the incorporation of MOs favours a hydroxy-containing C_2 intermediate (*HCCHOH) over the hydrocarbon intermediate (*HCC) at interfacial Cu sites on the path to alcohol products. We also propose that the relative bond strengths of Cu–COH and C–OH correlate with the selectivity for alcohol over hydrocarbon.

Source: Nature Catalysis 202 https://www.nature.com/articles/s41929-022-00880-6

- **Clean Hydrogen Fuel is Easier to Produce from Seawater with Stable Hierarchical Electrocatalysts**

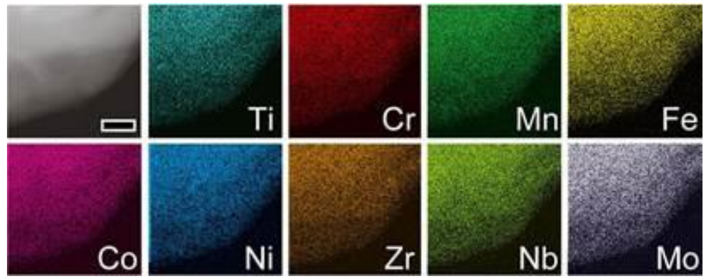
Seawater, which comprises more than 95% of the Earth's water, could become a key resource in the sustainable production of clean hydrogen fuel with use of water-splitting catalysts developed by a KAUST-led team. Chemist Huabin Zhang's team devised an approach that provides high-efficiency and stable hydrogen evolution



KAUST scientists are exploring ways to produce hydrogen fuel from seawater, which is much more abundant than precious fresh water. Credit: © 2022 KAUST; Thom Leach

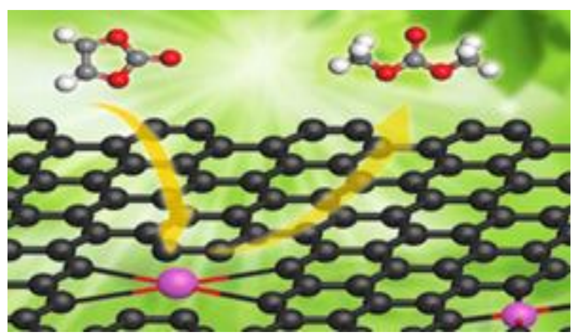
electrocatalysts for seawater splitting. The researchers created tiny cubic reactors, in which the catalyst was encased in a molybdenum sulfide protective shell. The catalyst core consisted of a carbon-supported molybdenum-based redox active compound and featured a zeolite-like ordered nanoporous structure. Using a metal organic framework (MOF)-based approach, the researchers combined metal complex precursors with the linker imidazole in the presence of surfactant to generate zeolite-like zinc–molybdenum cubes. They mixed the resulting structures with thioacetamide in ethanol under reflux to form a cubic molybdenum oxide phase confined in a thin zinc sulfide shell. The nanoreactors exhibited high electrocatalytic activity and stability in both fresh water and seawater. The core displayed numerous active sites that boosted hydrogen production and the shell presented several defects within its layers, especially subnanometer-sized holes that allowed water molecules to permeate and access the internal active sites. Source: phys.org, 11/1/2022.

- **Researchers Develop a Non-noble Catalyst for Hydrogen Production**



Researchers from the University of Tsukuba and collaborating partners have developed catalysts that can overcome the limitations of noble metals. Professor Yoshikazu Ito and co-workers use numerous non-noble metals all at once. The team used high-entropy alloys, which are mixtures consisting of many elements. While some of these alloys can be used to generate large quantities of hydrogen, others undergo a process called oxidation which gives the alloys some corrosion resistance ability. The study offers novel possibilities and new approaches toward replacing the highly scarce noble metals, especially iridium, with a worldwide production of only 7 tons per year. With the increase in the use of water electrolyzers globally, the demand for iridium is expected to be 700 kilograms per gigawatt. Source: Inceptive Mind, 11/15/2022.

- **Highly Active and Stable Superbasic Catalysts**



Solid superbases can act as heterogeneous catalysts for a variety of reactions, e.g., transesterifications, alkylations, or isomerizations, under mild conditions. However, available solid superbases suffer from limitations such as aggregation and the leaching of active sites. This results in a low utilization of active sites and poor stability during recycling.

Researchers have developed new solid superbases that feature potassium single atoms on graphene. These superbases were prepared via a tandem redox strategy. An initial redox reaction between KNO_3 as a potassium source and the graphene support at around 200–400 °C gives K_2O, as well as NO and CO_2 as gaseous products. In a second redox reaction at about 800 °C, the graphene further reduces K_2O to form potassium single atoms on graphene (K1/G). According to the researchers, K1/G is highly active in the synthesis of dimethyl carbonate via transesterification (pictured) because of the high dispersion of such superbasic sites. The turnover frequency of the catalyst is much higher than that for other reported catalysts, and it is stable when recycled.

Sourec: *Angew. Chem. Int. Ed.* **2022**. https://doi.org/10.1002/anie.202215157

Catalysis Research out of India

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/

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2. Ravi Ranjan, Nitin B Mhamane, Sadhu K Kolekar, Chinnakonda S Gopinath, "Electronic Structure Evolution from Metallic Vanadium to Metallic V_xO_y: A NAPPES Study for O_2 + V Gas–Solid Interaction", **J. Phys. Chem. C** 2022, 126, 45, 19136–19146
3. Ganesan Raman, Jagannath Das, Kshudiram Mantri, Jakkidi Krishna Reddy, Rakshvir Jasra "Highly efficient mesoporous ZSM-5 for trace olefin removal from aromatic stream", **Inorganica Chimica Acta,** 2023, 544, 121201.
4. Suraj Prakash Tripathy, Satyabrata Subudhi, Asheli Ray, Pragyandeepti Behera, Jayashree Panda, Srabani Dash, Kulamani Parida, "Hydrolytically stable mixed ditopic linker-based zirconium metal organic framework as a robust photocatalyst towards Tetracycline Hydrochloride degradation and hydrogen evolution", **Journal of Colloid and Interface Science,** 2023, 629, 705-718.
5. "Defect Control via Compositional Engineering of Zn-Cu-In-S Alloyed QDs for Photocatalytic H_2O_2 Generation and Micropollutant Degradation: Affecting Parameters, Kinetics, and Insightful Mechanism" **Inorganic Chemistry,** 2022 https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.2c02977
6. Pragyandeepti Behera, Asheli Ray, Suraj Prakash Tripathy, Lopamudra Acharya, Satyabrata Subudhi, Kulamani Parida, "ZIF-8 derived porous C, N co-doped ZnO modified Bg-C_3N_4: A Z-Scheme charge dynamics approach operative towards photocatalytic Hydrogen evolution and Ciprofloxacin degradation" **Journal of Photochemistry and Photobiology A: Chemistry,** 2022, https://www.sciencedirect.com/science/article/abs/pii/S1010603022006384

Webinar Organized by CSI, Baroda Chapter on 15th November 2022

The Catalysis Society of India, Baroda Chapter organized Webinar on **" Towards the Refinery of the Future: Advances in Operando Spectroscopy & Microscopy of Heterogeneous Catalysts" by Prof. Bert Weckhuysen** on 15th November 2022. The webinar was very informative, well appreciated & received huge response from academia and industries.

3. International Conference on Recent Advances in Material Chemistry & Catalysis from March 1-3, 2022 at Dibrugarh, Assam (India) https://ramccdu2023.com
4. 75th Annual Session of Indian Institute of Chemical Engineers (CHEMCON-2022), Harcourt Butler Technical University, Kanpur 27-30 December 2022. www.chemcon2022.com
5. 59th Annual Convention of Chemists 2022, of the Indian Chemical Society, is being organized from December 16–18, 2022 in the Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM), Dhanbad, Jharkhand.

Announcements

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

Name	Achievement
 **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	First Bharat Ratna Dr. APJ Abdul Kalam award for Science and Technology by MIT Art Design & Technology University, Pune on 9th November 2022

Quote of the Month

"Progress is impossible without change, and those who cannot change their minds cannot change anything."

— **George Bernard Shaw**

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