May 15, 2021

CSI Communication

Monthly Newsletter of Catalysis Society of India

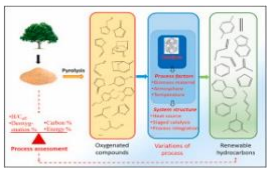
Circulated to all CSI Members

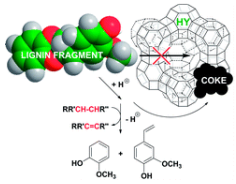
Catalysis for Bio-Fuels & Bio-Chemicals

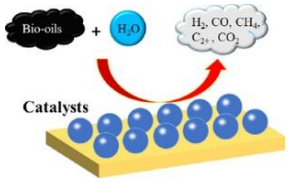
The Role of Catalysis for the Sustainable Production of Bio-fuels and Bio-chemicals describes the importance of catalysis for the sustainable production of biofuels and biochemicals, focused primarily on the state-of-the-art catalysts and catalytic processes expected to play a decisive role in the "green" production of fuels and chemicals from biomass. Various catalysts are used for the following important processes as

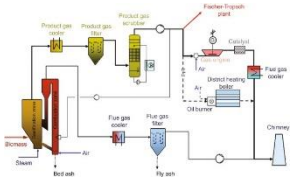
A) Catalytic pyrolysis of lignocellulosic biomass
B) Hybrid bio-gasoline by co-processing in FCC units
C) Fischer-Tropsch synthesis to biofuels (biomass-to-liquid process)
D) Steam reforming of bio-oils to hydrogen

A **B** **C** **D**









Commercial & Policies

- **Axens Selected for CPCL Cauvery Basin Refinery Project in India**
  Chennai Petroleum Corporation Limited (CPCL), a group company of Indian Oil Corporation Limited (IOCL), India, has selected Axens to supply several advanced technologies for its state-of-the-art 9 MTPA refinery to be set at Cauvery Basin at Nagapattinam in Tamil Nadu (southern part of India). CPCL's Cauvery Basin Refinery (CBR) was commissioned in November 1993, to process Narimanam crude, initially with a capacity of 0.5 MMTPA further expanded to 1.0 MMTPA in 2002. CPCL is planning to expand the capacity of CBR by adding grassroots facilities at the same location of the existing refinery in Nagapattinam. The scope of Axens' work includes the supply of process book, catalysts & adsorbents proprietary equipment, trainings and technical services. Source: Axens, 5/4/2021.

- **Maire Tecnimont Group Expands its Petrochemical Business in India with a New USD 450 Million Contract by IOCL**

  Maire Tecnimont S.p.A. announced that a consortium composed of its subsidiaries Tecnimont S.p.A. and Mumbai-based Tecnimont Private Limited has been awarded an EPCC (Engineering, Procurement, Construction and Commissioning) Lump Sum contract by Indian Oil Corporation Limited (IOCL), for the implementation of a new Para-Xylene (PX) plant and the relevant offsites facilities. The plant will be in Paradip, in the State of Odisha, in Eastern India. The scope of work entails EPCC activities up to the Performance Guarantees Test Run. Once completed, the new PX plant will have a capacity of 800,000 tons per year. The time schedule is 33 months for Mechanical Completion from the award date. The PX produced will be used to feed the adjacent PTA (Purified Terephthalic Acid) unit, thus ensuring availability of world-class feedstock that will provide a significant boost to the country's manufacturing industry. Source: Maire Tecnimont, 4/26/2021.

- **CSIR-CMERI Develops Oxygen Enrichment Technology to Optimize Medical Air Delivery**

  With the entire nation reeling under an unprecedented Covid-19 pandemic situation, oxygen shortage across the country is hitting hard the medical efforts to improve the recovery rate. Oxygen therapy is recommended for severe illness caused by Coronavirus. To meet the oxygen demand and minimize the supply chain problem of transportation and storage risks related to oxygen cylinders, CSIR-CMERI has developed an oxygen enrichment technology which has been transferred virtually to Apollo Computing Laboratories in Hyderabad last week.

  Prof. Harish Hirani, Director, CSIR-CMERI said that the unit requires easily available oil free reciprocating compressor, oxygen grade zeolite sieves and pneumatic components. It is capable of delivering medical air in the range of up to 15 LPM with oxygen purity of more than 90 percent. If required, this unit can even deliver up to 70 LPM at a purity of around 30 percent and can safely be placed in the isolation ward of the hospital for patients who are in dire need of oxygen. This will help the accessibility of oxygen in remotest places and widest points of need. The outreach factor of oxygen will be multiplied through the adoption of this in-situ and decentralised generation of oxygen.

  Source:https://government.economictimes.indiatimes.com/news/technology/csir-cmeri-develops-oxygen-enrichment-technology-to-optimize-medical-air delivery/82256736

- **IOC Awards Maire Tecnimont $ 450-mn EPCC Contract for PX Plant at Paradip**

  Maire Tecnimont S.p.A. (Rome, Italy) announced that a consortium composed of its subsidiaries Tecnimont S.p.A. and Mumbai-based Tecnimont Private Limited has been awarded an EPCC (Engineering, Procurement, Construction and Commissioning) Lump-Sum contract by Indian Oil Corporation Limited (IOCL), for the implementation of a new Para-Xylene (PX) plant and the relevant offsites facilities. The plant will be in Paradip, in the State of Odisha, in Eastern India.

  The overall value of the contract is about $450 million. The scope of work entails EPCC activities up to the Performance Guarantees Test Run. Once completed, the new PX plant will

have a capacity of 800,000 metric tons per year (m.t./yr). The PX produced will be used to feed the adjacent PTA (Purified Terephthalic Acid) unit, thus ensuring availability of world-class feedstock that will provide a significant boost to the Country's manufacturing industry. Source:https://www.chemengonline.com/maire-tecnimont-awarded-epcc-contract-for-iocls-new-para-xylene-plan

- **Indian Scientists Develop a New Cost-effective Aluminium Scrap Recycling Technology, Inspired by 'Make in India' Initiative**

  According to a recent report, a team of scientists in India has developed a new cost-effective and efficient aluminium scrap recycling technology that reduces material losses in the process. This new technology can be used by tiny & cottage industries, small-scale industries, MSME aluminium foundries, and recycling industries. The new technology is developed by Dr C. Bhagyanathan and Dr P. Karuppuswamy, Associate Professor and Professor from Sri Ramkarishna Engineering College, Coimbatore, along with Dr M. Ravi, Sr. Principal Scientist from CSIR-NIIST Trivandrum, inspired by the Government's 'Make in India' initiative and supported by the Advanced Manufacturing Technologies programme of the Department of Science & Technology (DST). The technology combines value added/ non-value added and hazardous/ non-hazardous wastes, aluminium alloys and assorted scraps for industrial applications and recycle them efficiently. Conventional aluminium recycling techniques require high investment and generate hazardous residues in form of ferrous, tin, lead, etc. But this new technology improves the purity and quality of recycled aluminium melt, equipped with advanced Aluminium Melting and Holding Furnaces, a degassing unit, filtering setup, an industrial washing machine, and Oven. While conversion rate in existing conventional technologies is 54 per cent, the new technology has increased it by 70 to 80 per cent depending on various cases of scraps dealt with.

  Source:https://www.alcircle.com/news/indian-scientists-develop-a-new-cost-effective-aluminium-scrap-recycling-technology-inspired-by-make-in-india-initiative-65084

- **Unicat Catalyst Acquires Magma Group**

  Unicat Catalyst Technologies (Unicat), a portfolio company of White Deer Energy (White Deer), has announced the acquisition of Jemmtec Limited, dba Magma Group (Magma or the Company). Magma is a UK-based leader in ceramics and catalyst manufacturing and related services. Unicat, headquartered in Alvin, TX, is a global supplier of heterogeneous catalyst products and technical services. Together, the combined businesses will offer vertically integrated global manufacturing and distribution of innovative catalyst and ceramics products and services for the refinery, syngas, chemical, steel, agriculture, and green energy industries. Source: PRWeb, 4/29/2021.

Scientific Updates

- **The Role of Hydrophobic Molecules in Catalytic Reactions**

Water molecules may appear insignificant at first glance, but they have a major influence on chemical reactions. The Franco-German team is investigating what happens at the interface between water and gold. © Elmar Weiler

Researchers from Ruhr-Universität Bochum (RUB) and Sorbonne Université in Paris have discovered how small hydrophobic molecules, such as CO_2, contribute to the energy costs of electrochemical processes by analyzing how the molecules interact in water at the interface. The water surrounding polar, i.e. hygroscopic molecules, in many electrochemical processes, behaves differently compared to the water surrounding non-polar molecules, which are also referred to as hydrophobic. Using molecular dynamic simulations, the researchers analyzed the hydrophobic hydration of small molecules such as carbon dioxide (CO_2) or nitrogen (N_2) at the interface between the gold and water. They showed that the interaction of water molecules in the vicinity of small hydrophobic molecules makes a crucial contribution to the energy costs of electrochemical reactions. The researchers implemented these findings in the Lum-Chandler-Weeks theory. This allows the energy required to form water networks to be calculated. The adapted model allows the energy costs for hydrophobic hydration to now be calculated at the interface between gold and water based on the size of the hydrophobic molecules. For instance, the model predicts that small hydrophobic molecules would tend to accumulate at the interface based on the interactions with the water, while larger molecules would remain further away in the solution. Source: Ruhr-Universität Bochum (RUB), 4/13/2021.

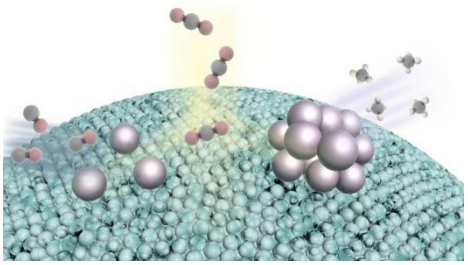
- **Study Highlights Promise of 3D Printing for Electrochemical Reactors**

3D-printed gas diffusion layer for an electrochemical reactor, printed at the Cornell NanoScale Science and Technology Facility using two-photon polymerization. Sobhani Lab/Provided

Electrochemical reactors that can capture carbon dioxide and transform it into valuable products are a relatively new and promising technology for reducing greenhouse gas emissions. Using additive manufacturing to rapidly prototype reactors with unique shapes and topologies, electrochemical reactor designs could be optimized for improved conversion rates, according to study co-author Sadaf Sobhani, assistant professor in Cornell University's Sibley School of Mechanical and Aerospace Engineering. Computationally simulating the chemical phenomena inside reactors, Sobhani was able to identify the conditions leading to mass-transport limitation, where the rate at which carbon dioxide travels to the catalyst is slower than the catalyst chemical conversion rate. Sobhani is

continuing her research into how geometry and surface properties influence overall reactor performance, leveraging the resources at the Cornell NanoScale Science and Technology Facility to print sub-micrometer surface features and advanced microstructures, and the Cornell High Energy Synchrotron Source, among other facilities, to image those features and study the internal operations of reactors. Source: Cornell University, 4/30/2021

- **Switching of Metal–oxygen Hybridization for Selective CO_2 Electrohydrogenation under Mild Temperature and Pressure**



Artificial carbon fixation contributes to closing the anthropogenic carbon cycle. However, large-scale conversion of CO_2 into selective products remains a challenge. Coupled thermal–electrochemical catalysis could offer an attractive approach to upgrading CO_2 into value-added products if selective electrocatalysts and integrated devices were developed. Here we identify a mechanistic route to selectively producing either CO or CH_4 with high selectivity (>95%) using Ir–ceria-based catalysts in an intermediate-temperature (400 °C) CO_2 electrolyser that operates at low overpotential and ambient pressure. We show that tuning of the Ir–O hybridization by controlling the Ir speciation can alter the catalyst surface chemical environment, enabling the stabilization of specific transition states to produce either CO or CH_4 during electrocatalysis. By achieving CO_2 electrohydrogenation in tandem with light-alkane electrodehydrogenation, we further demonstrate that such an advanced electrolyser could be extended to the upgrade of different carbon resources in one-step, significantly enhancing the techno-economic feasibility of the process.

Source: M. Li, Bin Hua, L. Wang, Joshua D. Sugar, W. Wu, Y. Ding, Ju Li & D. Ding, Nature Catalysis volume 4, 274–283(2021)

Catalysis Research out of India

- Ankita Thakur, Ankit Kumar Dhiman, Sumit Rakesh Kumar and Upendra Sharma, "Rh(III)-Catalyzed Regioselective C8-Alkylation of Quinoline N-Oxides with Maleimides C8-Alkylation of Quinoline N-Oxides with Maleimides and Acrylates", **J. Org.Chem.** 2021, 86,9, 6612-6621. https://pubs.acs.org/doi/10.1021/acs.joc.1c00393
- Inder Kumar , Rakesh Kumar, Shiv Shankar Gupta, Upendra Sharma**,** "C70 Fullerene Catalyzed Photoinduced Aerobic Oxidation of Benzylamines to Imines and Aldehydes" **J. Org. Chem. 2021**, 86, 9, 6449–6457. https://pubs.acs.org/doi/10.1021/acs.joc.1c00297
- Sushil Kumar, Shitanshu Pandey, Kailas L. Wasewar, Namık Ak, Hasan Uslu, "Reactive Extraction as an Intensifying Approach for the Recovery of Organic Acids from Aqueous Solution: A Comprehensive Review on Experimental and Theoretical Studies", **Journal of Chemical and Engineering Data, 2021**, 66, 4, 1557–1573

- Rohit Lade, Kailas Wasewar, Rekha Sangtyani, Arvind Kumar, Dilip Peshwe & Diwakar Shende, "Effect of aluminium nanoparticles on rheology of AP based composite propellant: experimental study and mathematical modeling", **Molecular Simulation,** Published online: 25 Feb 2021,, https://doi.org/10.1080/08927022.2021.1891305
- S. P. Tekade, A. S. Pednekar, G. R. Jadhav, S. E. Kalekar, D. Z. Shende, K. L. Wasewar, "Hydrogen generation through water splitting reaction using waste aluminum in presence of gallium", **International Journal of Hydrogen Energy** 45 (44), 23954-23965, Publication date: 2020/9/7.
- Ganapati D. Yadav, "The case for hydrogen economy" **Current Science,** 120(6), 971-972
- Dhananjay S. Doke, Mohan K. Dongare, Shubhangi B. Umbarkar, WO3/SiO2 Solid acid catalyst for synthesis of green solvent: Ethyl Lactate", **Catalysis in Green Chemistry & Engineering** 2021, DOI: 10.1615/CatalGreenChemEng.2021036141
- Kalpana C. Maheria, Aayushi Lodhi, Henilkumar Lankapati, Rishav Krishna, "Solid acid catalyzed esterification of Levulinic acid for the production of vale added chemicals" **Catalysis for Clean Energy and Environmental Sustainability,** Chapter 1, April 2021 Book Chapter Published by Springer International
- Kalpana C. Maheria, Aayushi Lodhi, Gunjan Sharma, "Microalgae oil upgrading over Zeolite-based catalysts", **Catalytic and Noncatalytic Upgrading of Oil,** ACS Symposium Series, Chapter 4, April 2021, 89-124.

Announcements

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

Name	Achievement
Dr. Sharad Lande Assistant Vice-President (R&D), Reliance Industries Ltd. Mumbai, INDIA 	Elected as a Fellow of Indian Chemical Society (ICS) May 2021

Quote of the Month

"Arise! Awake! Stop not until the goal is reached." – Swami Vivekananda

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