October 15, 2021

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 on Centre of Excellence in Catalysis Research in different Indian academics, Research laboratories or industrial R&D organizations. You may send your brief write-up to us which will be published in coming issues of CSI.

Commercial & Policies

- **Manali Petrochemicals Partners with Econic for Production of CO_2 Containing Polyols**

Manali Petrochemicals (MPL) and Econic Technologies have entered a Memorandum of Understanding (MoU) with the aim to introduce more environmentally friendly, CO_2 containing polyols, into the $28Bn global polyols market. Manali Petrochemical signed an MoU with Econic Technologies to scale their catalyst technology that allows for the substitution of fossil based raw materials with captured waste CO_2 in the production of polyols. The partnership involves MPL and Econic collaborating to scale the technology at MPL's pilot plant in India. On successful completion, this will be followed by the introduction of the process to one of the production trains in MPL's main plant. The shared intent is to bring CO_2 containing polyols to MPL's customers. Source: Econic Technologies, 9/27/2021.

- **India Targets Alternate Fuels, EVs in Clean Transport Push**

India is framing policies to promote the use of clean fuels, including electric vehicles (EVs), and tightening emission norms to meet its carbon reduction targets, transport minister Nitin Gadkari told the Reuters Impact conference. India is the third-largest user of transport automobiles in the world but 70% of its transport energy need is fulfilled by importing fossil fuels. "The aim is to gradually shift to fuels, which are import substitutes, cost effective, indigenous and pollution free," Gadkari said, adding that this includes biofuels, ethanol blends as well as hybrid EVs and hydrogen fuel cells. India is targeting reducing carbon emissions by 33%-35% by 2030 as part of its commitment under the Paris Climate Agreement, Gadkari said, and it is looking at sustainable mobility and clean energy to achieve its goal. Source: Reuters, 10/4/2021.

Advent of Electric Vehicles in the country, catalytic convertors used presently in gasoline /diesel run vehicles will be redundant. Excellent catalysis R&D that resulted into convertors can be explored for VOC mitigation form different situations. --------- CSI comments

Reliance Signs Agreement with Indian Government on Plastic Recycling

The Council of Scientific & Industrial Research-National Chemical Laboratory (CSIR-NCL, Pune, and Reliance Industries (RIL), and other companies can produce useful molded plastic components from COVID-19 personal protection equipment (PPE) waste. CSIR says that the pilot project has the potential to scale up and replicate throughout India to convert PPE waste into useful and safe products. CSIR and RIL have now signed a memorandum of understanding (MOU) to scale up the production to pilot scale, laying a path to take the concept to the national level. CSIR adds that the project involved converting the decontaminated PPE waste into an easily processable and upcycled agglomerated form (pellets or granules). Source: Chemical Week, 9/24/2021.

This is good start to reuse spent polymeric materials at the first level. However, there is need to carry out vigorous catalytic R&D for developing technologies to convert spent polymers which are rich carbon source to valuable chemicals to achieve circular polymer production. --------- CSI comments

Carbon Clean Provides India's First Blast Furnace Carbon Capture Plant for Tata Steel

India's first carbon capture plant for a blast furnace is successfully designed and commissioned for Tata Steel by Carbon Clean, a leader in cost-effective carbon dioxide captures and separation technology at Tata Steel's Jamshedpur steel plant in India, capturing 5 tonnes of CO_2 per day. The modular skid mounted unit captures CO_2 directly from the blast furnace gas and makes it available for onsite reuse in a variety of applications. The depleted CO_2 gas is then sent back to the gas network with an increased calorific value. The 5 tonnes per day carbon capture plant along with its semi commercial use within the steel value chain, makes the Tata Steel Jamshedpur plant the first-of-its-kind in the world within the steel industry. Source: Carbon Clean, 9/14/2021.

Shell Qualifies BASF Sorbead® Adsorption Technology for Carbon Capture and Storage Applications

Shell and BASF are collaborating to accelerate the transition to a world of net-zero emissions. The Sorbead Adsorption Technology is used to dehydrate CO_2 gas after it has been captured by Shell's carbon capture technologies such as ADIP Ultra or CANSOLV. The Adsorption Technology has several advantages for CCS applications: Sorbead, an aluminosilicate gel material, is acid resistant, has high capacity for water, and regenerates at a lower temperature compared to activated alumina or molecular sieves. Source: BASF, 9/29/2021.

BASF Announces Innovations in its Catalysts Portfolio

BASF introduced a range of new catalysts listed below which will be presented during the upcoming European Petrochemical Associations Conference (EPCA).

- High performance oxo alcohol catalyst Ni 3354 E to produce IPA through hydrogenation of acetone.

- Chromium-free copper extrudate catalysts as Cu 0560 E to further broaden its hydrogenation catalyst offering.
- O4-204, a new catalyst for n-butane based maleic anhydride production. Compared to previous product generations, allowing a longer catalyst on-stream time, which makes the process more cost-effective.
- Next generation of its selective hydrogenation catalysts by the end of 2021. These new E 15x light catalysts complete BASF's selective hydrogenation portfolio with the well-established E 15x series and the recently launched sulfur resistant E 15x S, being installed in two world-scale units in the upcoming months. Source: BASF, 9/27/2021.

Scientific Updates

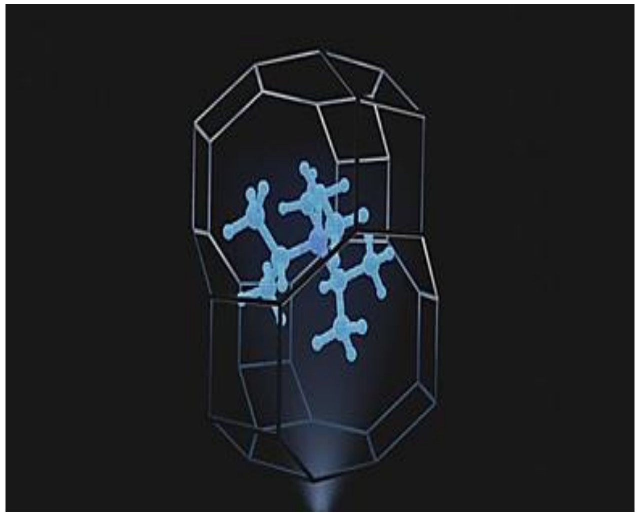
Fibrous Catalyst Support Boosts Yields and Reduces Coke Build up

A new fibrous catalyst support material can enhance a wide range of industrial catalytic reactions, allowing higher yields and reduced coke buildup compared to pellet supports. Unifrax leveraged its expertise in ceramic materials to develop the high-alumina fiber catalyst support (photo) that can accommodate several different types of catalyst payloads, the company says. The company developed a proprietary process for coating different catalytic metals onto the fibrous surface in a way that prevents the metals from migrating when in use. Unifrax has also developed a way to customize the support for different processes.
In recently completed testing at high-throughput testing company hte GmbH, the fiber-supported catalyst has shown to increase product output by 20% compared to the conventional substrate in a model propane dehydrogenation reaction, while also generating 50% less side products per cycle. Another advantage of the fibrous catalyst support is its light weight one-tenth the weight of conventional supports which allows faster loading and unloading and less downtime. Unifrax has partnered with various catalyst makers to deliver process ready products, on which several users are currently conducting commercial validation testing.
Source: Chemical Engineering, 9/2021.

A Strategy to Control Phase Selectivity in Templated Zeolite Synthesis

Researchers at Massachusetts Institute of Technology (MIT), in collaboration with researchers at Polytechnic University of Valencia and Stockholm University, have recently proposed a new strategy to control phase selectivity during templated zeolite synthesis processes. This strategy, presented in a paper published in *Science*, is based on the combined use of atomistic simulations, literature mining, human computer interactions, synthesis, and material characterization techniques.

Researchers used high-throughput simulations based on molecular mechanics to quantify the affinity of different molecular templates to both the zeolite they were trying to create and those that were unsuitable for a given application. The team drew information from over 586,000 zeolite-molecule simulations that were aligned with existing literature in materials design. The results of the simulations led to the identification of several possible designs for zeolites that could potentially be realized in the future. While there is no certainty that all the designs, they identified would be ideal, the work by Gomez-Bombarelli, Daniel Schwalbe-Koda, another researcher involved in the study and their colleagues could help to narrow down the search for promising zeolite designs and speed up zeolite synthesis processes. This recent study confirms that high performing computational tools and algorithms could play a key role in the identification of new promising materials. The new computational strategy for controlling zeolite synthesis and structure composition presented by Gómez-Bombarelli, Schwalbe-Koda, Moliner and their colleagues could soon aid the discovery of new promising zeolite templates. The researchers have thus decided to make their data publicly available through an online interactive website. Source: Phys.Org, 9/24/2021.



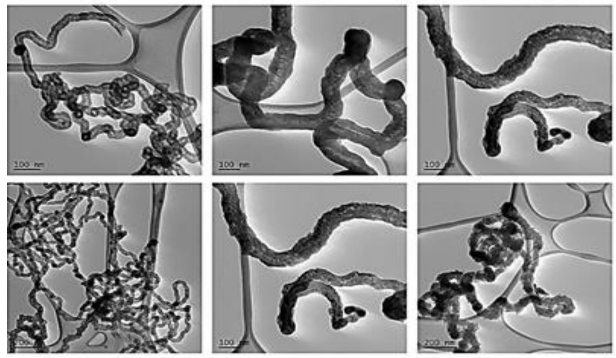
Computational methods enable the design of templates for zeolite cavities. Credit: Schwalbe-Koda et al.

- **From Recycling to Upcycling: A Smarter Way of Dealing with Plastic**

A new method from researchers at RMIT University can produce high value products from plastic carbon nanotubes and clean liquid fuel while simultaneously upcycling agricultural and organic waste. The team's two-step process, revealed in the *Journal of Environmental Management*, converts organic waste into a carbon rich and high-value form of charcoal, then uses this as a catalyst to upcycle the plastic. The new plastic upcycling approach offers a sustainable alternative to produce carbon nanotubes (CNTs). These hollow, cylindrical structures have exceptional electronic and mechanical properties, with applications across a broad range of sectors including hydrogen storage, composite materials, electronics, fuel cells and biomedical technologies. The new method starts with converting agricultural or organic waste to biochar a carbon-rich form of charcoal often used for improving soil health. The biochar is used to eliminate toxic contaminants such as Poly-cyclic Aromatic

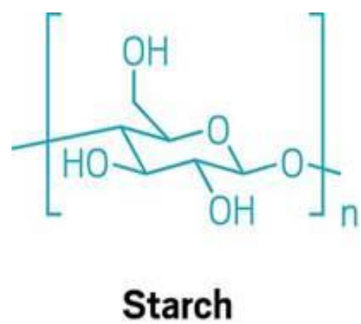
Hydrocarbons, known as PAHs as the waste plastic is broken down into its components of gas and oil. The process eliminates those contaminants and convert plastics into high quality liquid fuel. At the same time, the carbon in the plastic is converted into carbon nanotubes, which coat the biochar.

The study is the first to use low cost and widely available biochar as a catalyst for making contaminant free fuel and carbon nanomaterials from plastic.
Source: RMIT University, 9/29/2021.



Examples of carbon nanotubes produced with the new approach, at different magnifications.

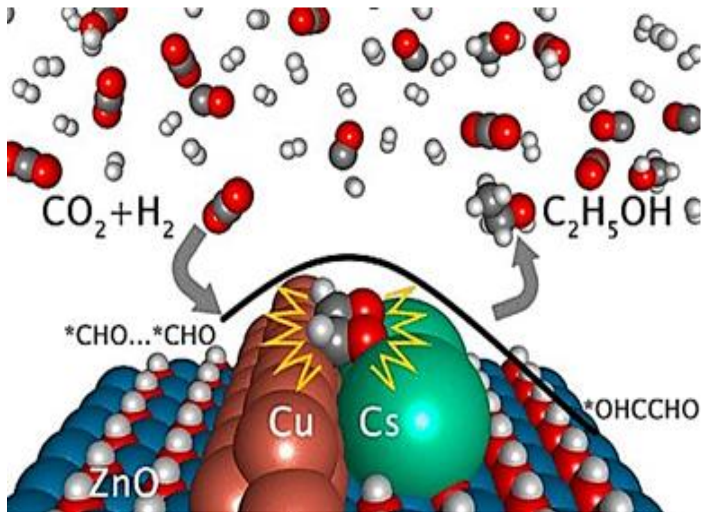
- **New Method Makes Starch from CO_2 Faster than Plants Can**



The new technique, which relies on chemical catalysts and a curated combination of natural and engineered enzymes, converts CO_2 to starch 8.5 times as efficiently as corn plants can. To use CO_2, Yanhe Ma, a microbiologist at the Tianjin Institute of Industrial Biotechnology, and his colleagues use a zinc and zirconium-based catalyst to reduce CO_2 to methanol, which serves as the building block for the rest of the process. They use enzymes to turn the methanol into three carbon sugar molecules. And then again using enzymes, they polymerize those sugars into six-C sugars, and finally into long-chain starch molecules. The process involves 11 core reactions and originally took 10 h, the researchers report. To speed it up, they systematically studied the efficiency of each step. They identified bottlenecks caused by natural enzymes and made better enzyme variants with the help of computational design. This was key to making the process more efficient, leading to a final run time of 4 h, says Ma. Corn plants require 120 days to make starch. The new technique converts CO_2 into starch at a rate of 22 nanomoles per min, 8.5 times as efficiently as corn. Source: Chemical & Engineering News (C&EN), 9/24/2021.

- **Catalyst Study Advances Carbon-Dioxide-to-Ethanol Conversion**

Led by the U.S. Department of Energy's (DOE) Brookhaven National Laboratory, a group of international scientists determined that bringing cesium, copper, and zinc oxide together into a close-contact configuration catalyzes a reaction pathway that transforms carbon dioxide (CO_2) into ethanol (C_2H_6O). Such processes will lead to technologies that are able to recycle CO_2 emitted from combustion and convert it into usable chemicals or fuels. None of the three components examined in the study can individually catalyze the CO_2 to ethanol conversion, nor can they in pairs. But when the trio is brought together in a certain configuration, the region where they meet opens a new route for the carbon carbon bond formation that makes the conversion of CO_2 to ethanol possible.



The key to this is the well-tuned interplay between the cesium, copper, and zinc oxide sites. The interface is formed by depositing tiny amounts of copper and cesium onto a surface of zinc oxide. One of the things they learned from modeling is that the cesium is a vital component of the active system. Without its presence, ethanol cannot be made. In addition, good coordination with copper and zinc oxide is also important. But there is much more to learn. Source: Brookhaven National Laboratory (BNL), 9/10/2021.

Catalysis Research out of India

1. Santosh Agrawal, Kshudiram Mantri, Vipul Sharma, Raksh Vir Jasra & Pradip Munshi, "Catalytic Dehydrogenation of Cyclohexanone to Phenol Over the Ru, Rh, Pd and Pt Surfaces in Sub-critical Water" **Catalysis Letters 2021** https://doi.org/10.1007/s10562-021-03789-0
2. Sumit, Devesh Chandra, Ankita Thakur, Ankit Kumar Dhiman, and Upendra Sharma, "Cp*Rh(III)-Catalyzed Regioselective C(sp3)-H Electrophilic Trifluoromethylthiolation of 8-Methylquinolines" **The Journal of Organic Chemistry,** 2021, doi.org/10.1021/acs.joc.1c01938.
3. Inder Kumar, Ankita Thakur, Manisha, and Upendra Sharma, "α-Oxygenation of N-Aryl/Alky Heterocyclic Compounds via Ruthenium-Photocatalysis" **Reaction Chemistry & Engineering**, 2021, doi.org/10.1039/D1RE00200G.
4. Manisha, Shiv Shankar Gupta, Ankit Kumar Dhiman, and Upendra Sharma "Rh (III)-Catalyzed Selective C7 Halogenation of Indolines" **European Journal of Organic Chemistry,** 2021, doi.10.1002/ejoc.202100964.
5. Ankit Kumar Dhiman, Rohit Kumar, and Upendra Sharma "Catalyst and Additive-Free Synthesis of Fluoroalkoxyquinolines" **Synthesis,** 2021, DOI: 10.1055/a-1531-2248.
6. Debarati Das, Bhalchandra M Bhanage, "Nickel-Catalyzed Carbonylations" **Carbon Monoxide in Organic Synthesis: Carbonylation Chemistry,** 51-81, 2021.
7. Pooja Rana, Rashmi Gaur, Bhawna Kaushik, Sneha Yadav, Priya Yadav, Priti Sharma, Manoj B Gawande, Rakesh K Sharma, "Surface engineered Iridium-based magnetic photocatalyst

paving a path towards visible light driven CH arylation and cyanation reaction" **Journal of Catalysis,** 401, 297-308, 2021

8. Deepak S Desai, Ganapati D Yadav, "Friedel-Crafts acylation of furan using chromium-exchanged dodecatungstophosphoric acid: effect of support, mechanism and kinetic modelling" **Clean Technologies and Environmental Policy,** 23 (8), 2429-2441, 2021.
9. Dnyanesh Vernekar, Mohammad Dayyan, Satyajit Ratha, C. V Rode, M Ali Haider, Tuhin Suvra Khan, Dinesh Jagadeesan, "Direct Oxidation of Cyclohexane to Adipic Acid by a WFeCoO (OH) Catalyst: Role of Brønsted Acidity and Oxygen Vacancies" **ACS Catalysis,** 10754-10766, 2021.
10. Bijoy Tudu, Naresh Nalajala, Kasala Prabhakar Reddy, Pranjal Saikia, Chinnakonda S Gopinath, "Rationally Designed, Efficient, and Earth-Abundant Ni–Fe Cocatalysts for Solar Hydrogen Generation" **ACS Sustainable Chemistry & Engineering,** 2021, DOI: 10.1021/acssuschemeng.1c05158

M/s Hindustan Platinum Ltd. is publishing Catalysts and Chemicals newsletter series explores the intricacies behind the processes, including salient features like catalyst preparation, activity, selectivity, and recyclability. The details are available on https://www.hp.co.in/download.php

Upcoming Symposium/ Conferences/Seminars

1. Refining India 2021 October 20-21, 2021 | Online Event https://refiningindia.com
2. CHEMCON-2021, December 27-30, 2021, Bhubaneswar, India https://www.chemcon2021.com
3. 6th International Conference on New Energy and Future Energy System (NEFES 2021), November 1-4, 2021. Xi'an, China http://www.intergridconf.org
4. XVth International Symposium on Environment, Catalysis and Process Engineering (ECGP-2021) November 23-25, 2021 Marrakech, Morocco. https://ecgpmorocco.com
5. Webinar on New Approaches and Strategies in Main Group Catalysis organized by Chem, Chem Catalysis & Trends in Chemistry on 02nd November 2021. Free registration on https://www.brighttalk.com/webcast/16651/510107?utm_campaign=Webinars&utm_medium=email&_hsmi=170382198&_hsenc=p2ANqtzqgDURYI638Qo9LHlBmjSW1icAsLihZ7RRZk0q0lj6rKDOIMywZWqEP83CQc5KTDU9BUb7Bl0sSY2qTZfeq6Mt168qA&utm_content=170380357&utm_source=hs_email

Quote of the Month

"To succeed in your mission, you must have single minded devotion to your goal."
— APJ Abdul Kalam

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