June 15, 2021

CSI Communication

Monthly Newsletter of Catalysis Society of India

Circulated to all CSI Members

Commercial & Policies

- **India Brings Forward by 2 years 20% Ethanol Blend to Gasoline**

India's government will bring forward to 2023 from 2025 the possibility of fuel companies selling gasoline containing up to 20% of ethanol (E20), according to brokers and a publication in the country's official gazette. The move from India towards higher production and use of ethanol is expected to cut the country's exportable surplus of sugar, potentially leading to higher international prices for the sweetener. India has been giving soft loans to sugar mills to increase ethanol production capacity by adding distillation infrastructure to existing plants. Large volumes of E20 by 2023, however, will depend on how quick car manufacturers can adapt, since it will require new engine specifications. Source: Reuters, 6/2/2021.

- **Bangalore Start-up Receives Award for Developing Solution for Conversion of CO_2 to Chemicals, Fuels**

The Ministry of Science and Technology informed that a Bangalore based startup has received the National Award 2021 from the Technology Development Board (TDB) for developing a commercial solution for the conversion of CO_2 to chemicals and fuels. According to a press release issued by the Ministry, Breathe Applied Sciences, a startup incubated at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) developed efficient catalysts and methodologies for the conversion of CO_2 to methanol and other chemicals. It has led to improvisation of process engineering to enhance the production of chemicals and fuels from anthropogenic CO_2 generated from various sources including coal and natural gas power generation sectors, steel industry, cement industry, and chemical industries, and integrating multiple components involved in the CCUS. The research was carried out by Professor Sebastian C Peter and his group from the New Chemistry Unit at JNCASR. He is also a co-founder and director of Breathe Applied Sciences. The start-up signed an agreement with JNCASR, an autonomous institute of the Department of Science and Technology for the transfer of technology based on lab-scale research on reducing CO_2 to methanol and other useful chemicals and fuels. Source: ANI News, 5/25, 2021.

- **India's Natural Gas output Rises 23% as RIL-BP fields Start Production**

India's natural gas production jumped 22.7 per cent in April after Reliance Industries Ltd and its partner BP Plc ramped up output from their eastern offshore KG-D6 block, government data released on Friday showed.

India produced 2.65 billion cubic meters of natural gas in April, up from 2.16 bcm in the same month last year, as per the data released by the Ministry of Petroleum and Natural Gas. Source: https://energy.economictimes.indiatimes.com/news/oil-and-gas/indias-gas-output-rises-23-pc-as-ril-bp-fields-start-production/82830992

- **Numaligarh Refinery Ltd to use Honeywell Technology to Produce Cleaner-Burning Diesel and Increase Crude Oil Conversion**

Honeywell announced Numaligarh Refinery Limited NRL, a public sector undertaking under the Indian Ministry of Petroleum and Natural Gas, will use UOP technology to produce cleaner-burning diesel fuel in compliance with India's BS-VI emission standards and increase crude oil conversion. The Numaligarh Refinery Expansion Project (NREP) will facilitate economic development in the north-eastern states of India by expanding the region's crude processing capacity from the present 3.0 million metric tonne per annum (MMTPA) to 9.0 MMTPA in Numaligarh, located in the Indian state of Assam.
The UOP Distillate Unionfining™ process will enable NRL to produce diesel that complies with India's BS-VI emission standards, which were implemented last year. The process removes impurities to improve the quality of middle distillate feedstocks that meet increasingly stringent regulations for fuels such as diesel. "This project with Numaligarh marks the first-ever UOP licensed process unit in an NRL refinery, and it's the first grassroots diesel hydrotreating unit in India using a latest-generation UOP catalyst," said Mike Banach, Managing Director, UOP India.
Source: https://www.digitalrefining.com/news/1006479/numaligarh-refinery-selects-unionfining-technology-from-honeywell-uop#.YMWjs6Yz

- **Praj Industries Develop Technology to produce Lignin-based Bio-Bitumen**

Praj Industries has achieved yet another milestone by developing innovative technology to produce Bio-bitumen based on lignin. The Netherlands-based Circular Biobased Delta, one of Europe's premier consortia to promote bioeconomy, has approved Praj's Bio-bitumen samples processed from Purified Lignin, as a part of their flagship CHAPLIN program. Lignin is one of the co-products resulting from the 2nd generation Ethanol plants, paper making and from Compressed Bio-Gas plants. Bitumen is a black viscous mixture of hydrocarbons produced by fractionation of crude oil and has wide applications in road construction and roofing as binder. Praj has now developed a proprietary process (under patenting) to convert the crude lignin into Bio-bitumen which has potential to replace this fossil-based bitumen and offer eco-friendly green bitumen. The binding and viscoelastic property of Bio-bitumen makes it useful for applications in asphalt. Circular Biobased Delta (CBBD) facilitates cooperation between knowledge centers, public authorities, and industry to grow usage of biomass as a raw material in the chemical, construction, and packaging industries. Under its flagship program CHAPLIN, it aims at stimulating the development and commercialization of Bio-bitumen as binder for use in asphalt to improve the greening approach in road construction while reducing CO_2 intensity. Praj had provided Bio-bitumen samples processed from Rice and Wheat Straw as feedstock in their 2G Biorefinery Demo plant in India to CBBD for testing and

evaluation. After thorough evaluation and studies in their advanced laboratories, CBBD has approved Praj's Bio-bitumen sample for scale up in Asphalt on a Dutch test strip on the road. Source:https://www.business-standard.com/article/news-cm/praj-develops-bio-bitumen-samples-using-proprietary-process-121051800339_1.html

- **India: BASF Ships Molecular Sieves to Support Oxygen Production**

Chemical company BASF is supplying molecular sieves to various companies in India that are ramping up oxygen supply through the conversion of nitrogen generation units. BASF said the molecular sieves are integral to the units as they help enrich atmospheric oxygen from 21% to medical-grade oxygen, ranging from 90%-95%. To help distribution of the molecular sieves, the Government of India is supporting BASF in airlifting the products to augment the oxygen capacity.

The first shipment of sieves arrived from Frankfurt in Mumbai on 8th May. As a reciprocal gesture, BASF is donating the next batch of 70 tonnes of molecular sieves. Commenting on the company's efforts, Narayan Krishnamohan, Managing Director of BASF India, said, "The need of the hour is to support the demands for medical infrastructure." "BASF has therefore leveraged its global and local network to supply chemistry that enables additional oxygen generation as well as much needed medical equipment." "Proactive and timely support from the Government of India enabled quick shipment of our product to address the critical medical oxygen need in the country." BASF said it will continue to monitor the situation and explore additional ways to support the government's and local organisations' relief efforts in India. Source: https://www.gasworld.com/india-basf-ships-molecular-sieves-to-support-oxygen-production/2020898.article

- **Net Zero by 2050: A Roadmap for the Global Energy System**

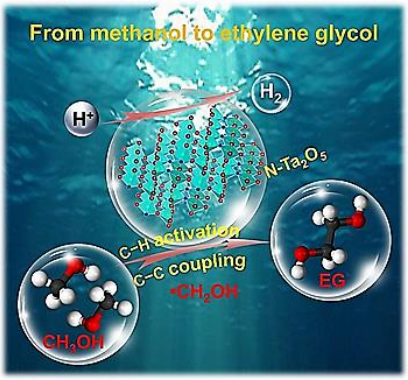
The number of countries announcing pledges to achieve net-zero greenhouse gas emissions over the coming decades continues to grow. At the same time, questions are being asked about whether net-zero emissions can be achieved globally by 2050 with a view to limiting global warming to 1.5°C, and in particular what it would mean for the energy sector. In line with an official request by the COP26 Presidency, the IEA has developed a new special report providing the first comprehensive energy-sector pathway towards global net-zero emissions by 2050. The IEA special report assesses the policy requirements, the deployment and innovation needs, the necessary investments, the economic benefits, and the wider implications for the world. Source: International Energy Agency (IEA), 5/18/2021.

Scientific Updates

- **A Solar Energy-driven Sustainable Process for Synthesis of Ethylene Glycol from Methanol**

Direct photocatalytic coupling of methanol to ethylene glycol (EG) is highly attractive. The first metal oxide photocatalyst, a tantalum-based semiconductor, is reported for preferential

activation of C-H bonds within methanol to form hydroxymethyl radical (*CH_2OH) and subsequent C-C coupling to EG.



The nitrogen doped tantalum oxide (N-Ta_2O_5) photocatalyst is an environmentally friendly and highly stable candidate for photocatalytic coupling of methanol to EG. It is of great interests that a 'dream catalytic reaction' of direct coupling of methanol to ethylene glycol ($2CH_3OH—HOCH_2CH_2OH + H_2$, denoted as MTEG) could be achieved through the solar energy-driven C-H activation and C-C coupling processes, and this MTEG reaction has not been achieved through thermocatalysis yet.

Recently, a research team led by Prof. Ye Wang from Xiamen University and Yanshan University, China, reported the first metal oxide photocatalyst, tantalum-based semiconductor, for preferential activation of C-H bond within methanol to form hydroxymethyl radical (*CH_2OH) and subsequent C-C coupling to EG. Compared with other metal oxide photocatalysts, such as TNO_2, ZnO, NO_3, Nb_2O_5, tantalum oxide (Ta_2O_5) is unique in that it can realize the selective photocatalytic coupling of methanol to EG. The co-catalyst free nitrogen doped tantalum oxide (2%N-Ta_2O_5) shows an EG formation rate as high as 4.0 mmol/g/h, about 9 times higher than that of Ta_2O_5, with a selectivity higher than 70%. The high charge separation ability of nitrogen doped tantalum oxide plays a key role in its high activity for EG production. This catalyst also shows excellent stability longer than 160 h, which has not been achieved over the reported metal sulfide photocatalysts. Tantalum-based photocatalyst is an environmentally friendly and highly stable candidate for photocatalytic coupling of methanol to EG. The results were published in *Chinese Journal of Catalysis*. Source: Chinese Journal of Catalysis 42 (2021) 1459–1467

- **Using Carbon Dioxide to Make Greener Plastics**

Six percent (6%) of the oil produced worldwide is used in the production of plastics, which means that finding an alternative source of carbon is a priority, both for the plastic industry and for the environment. The solution, initiated and developed by Christoph Gürtler, Head of Catalysis and Technology Incubation at plastic polymer manufacturer Covestro, and Walter Leitner, Director at the Max Planck Institute for Chemical Energy Conversion and Professor for Chemical Technology at RWTH Aachen University, facilitates an up to 20% reduction in the amount of fossil feedstocks required to make a polyurethane precursor, while also providing a use for waste CO_2 from other industries. With 50 years of combined experience in the fields of chemistry, petrochemistry and catalyst research, Gürtler and Leitner saw this obstacle as a challenge. Empowered by the industry-academia collaboration between Covestro (at the time still known as Bayer Material Science), Gürtler's employer, and RWTH Aachen University, where Leitner is Professor, the pair and their teams began

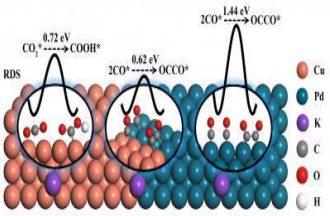
investigating the potential of previously examined catalysts, assessing their effectiveness in converting CO_2 into useful materials.

Gürtler and Leitner found that a reaction involving chemical compounds derived from crude oil, CO_2 and other starting materials in the presence of a suitable catalyst would have the desired effect. The resulting material was developed and later brought to market by Covestro as cardyon®, a chain-like molecule with two or more hydroxyl groups, otherwise known as a polyol. As a chemical precursor, cardyon can be applied in exactly the same way as other high-quality polymer intermediates. It is used, for example, in the production of flexible foams for mattresses and as a binder for padded sports floorings. In 2019, Covestro announced that the material can also be made into stretchy textile fibres used in clothing, such as in socks. If further research continues to show that Gürtler and Leitner's innovation can be applied to a wider range of polyurethane-based production processes, then there is hope that their invention could lead to a much greater reduction in crude oil use, in parallel to the utilization of vast quantities of waste CO_2, ultimately playing a significant role in closing the carbon loop. Source: Chem Europe, 5/7/2021.

Technique is accelerating the shift to circular economy by enabling commercially viable re-use of CO_2. A product of collaboration between industry and academic.

- **Tuning the Intermediate Reaction Barriers by a CuPd Catalyst for CO_2 Electroreduction To C2 Products**

Recently, a research team led by Prof. Min Liu from Central South University, China designed a Cu-Pd bimetallic electrocatalyst possessing CuPd(100) interface which can lower the energy barrier of C2 product generation. The electrocatalyst was obtained using an in-situ growth method based on thermal reduction to afford Pd nanoparticles as nucleated seeds. The density functional theory (DFT) calculation shows that the CuPd (100) interface enhanced the adsorption of CO_2 and reduced the energy barrier of CO_2* hydrogenation step, thus sufficient CO* participated in the C-C coupling reaction. In addition, the energy barrier of rate-determining step for C2 product generation on CuPd (100) interface is 0.61 eV, which is lower than that on Cu(100) surface (0.72 eV). Then the target CuPd (100) interface catalyst was prepared by a simple wet chemical method and proved by different characterization methods. The temperature programmed desorption and gas sensor experiment results

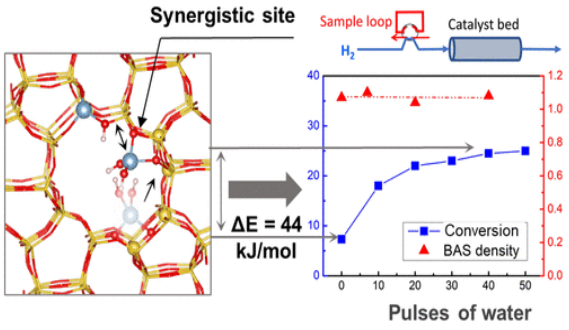


An intimate CuPd(100) interface was designed to lower the energy barriers of intermediate reaction (CO_2 hydrogenation and C-C coupling) and improve the efficiency of C2 products. The optimal CuPd(100) interface catalyst exhibited a C2 Faradaic efficiency*

proved the enhanced CO_2 adsorption and CO_2* hydrogenation ability on CuPd(100) interface, respectively. As a result, the CuPd(100) interface catalyst exhibited a C2 Faradaic efficiency of 50.3%, which was 2.1 times higher than that of Cu catalyst (23.6%) at -1.4 VRHE in 0.1 M KHCO3. This work provides a reference for the rational design of Cu-based electrocatalyst for CO_2 electroreduction by adjusting the intermediate reaction energy barrier. Source: EurekAlert!, 5/25/2021.

- **Quantifying the Influence of Water on the Mobility of Aluminum Species and Their Effects on Alkane Cracking in Zeolites**

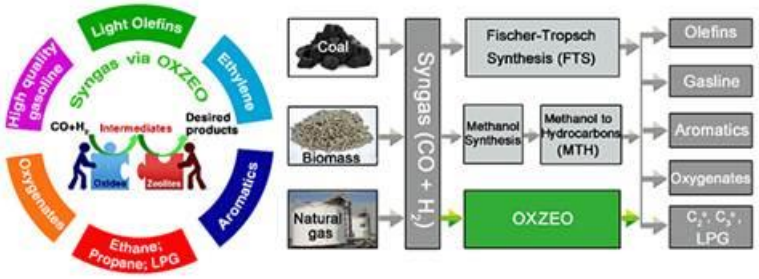
The role of extra-framework Al (EFAL) species on industrially important reactions such as alkane cracking has been extensively discussed and debated. It has long been known that water treatments influence the framework aluminum sites and, in some cases, can modify activity. What is less understood, however, is the direct relationship between the structural modifications and reactivity of important reactions such as alkane cracking and isomerization. The collective understanding of the multiple roles that water plays in the modification of zeolites and influence on reaction rates is continuously evolving. Extra-lattice Al species in close proximity to a framework Brønsted acid sites (BAS) have been proposed to modify the energies associated with surface intermediates and kinetically relevant transition states, which results in an enhancement in the rates of alkane cracking reactions.



However, the kinetic role of water on the migration of these extra-framework alumina species to generate highly active sites is less understood and is the focus of this study. Water is introduced in controlled pulses to ZSM-5 zeolites with various Si/Al ratios and EFAL densities, with responses in n-hexane cracking activity used to investigate the generation of new active sites. A pulse technique allows decoupling of water dosing, lattice rearrangement, and drying, thereby enabling the quantification of activation energies associated with the generation of new active sites without losses in crystallinity or total BAS density. Further, by subtraction of the contributions to the reaction rate associated with isolated BAS, the reaction rate associated with the newly created sites is estimated. The results show that the energy barrier required for cracking on highly active sites is much lower than that observed on traditional Brønsted sites (75 vs 110 kJ/mol). The temperature dependence for the generation of these new sites reveals a 44 kJ/mol activation energy for the kinetically relevant step associated with their generation in the presence of water vapor, which to the best of our knowledge has not been previously quantified. It is reported that, while water vapor is essential for the generation of these new active sites, it also binds to these sites and strongly inhibits the cracking rate. These findings clarify some of the conflicting reports regarding the role of water in activity enhancement. Source: ACS Catal. 2021, 11, XXX, 6982–6994

- **Oxide-zeolite-based Composite Catalyst Concept Enables Syngas Chemistry Beyond Fischer-Tropsch Synthesis**

A group led by Prof. Pan Xiulian and Prof. Bao Xinhe from the Dalian Institute of Chemical Physics of the Chinese Academy of Sciences (CAS) proposed an oxide-zeolite-based composite (OXZEO) catalysis concept, which can separate activation of reactants CO and H_2, and C-C coupling onto two different types of active sites. The researchers summarized the state-of-the-art, opportunities and challenges of the OXZEO catalysis concept in the field of C1 chemistry. The concept turned syngas conversion into a tandem reaction and allowed the product selectivity to be manipulated by shape-selective zeolites. It enabled direct conversion of syngas to a variety of chemicals and fuels with their selectivity surpassing the limit predicted by Anderson-Schultz-Flory model via the conventional FTS route. However, the selectivity control mechanism is far from being understood. Therefore, further studies should focus on the selectivity control mechanism of the OXZEO concept in order to understand the challenges and prospects for future development of much more active and more selective catalysts. This work was supported by CAS, the Ministry of Science and Technology of China, and National Natural Science Foundation of China. The study was published in *Chemical Reviews* on May 25. Source: Dalian Institute of Chemical Physics (DICP), 6/4/2021.



Oxide–zeolite-based composite catalyst concept that enables syngas chemistry beyond Fischer–Tropsch synthesis (Image by Jiao Feng and Miao Dengyun)

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Research Oppourinities

- Recruitment of Scientific Positions in CSIR-National Metallurgical Laboratory, Jamshedpur. The details are available on https://lnkd.in/g_wvhQK & last date for application is 28-06-2021.

Announcements

- CSI welcome the following newly joined life members in the Month of May 2021

Sr. No.	Member Name	Life Membership Number
1	**Kum. Aditi Sugha,** Guru Nanak Dev University Amritsar, Punjab	LM1070
2	**Ms. Laveena Gulabchandani,** Department of Chemistry, Sophia Girls' College (Autonomous), Ajmer	LM1071
3	**Dr. Aparna Yeddala,** Asst. Professor, Matrusri Engg College Hyderabad, Telangana	LM1072

4	**Dr. Prakash Chandra,** Department of Chemistry, Bundelkhand University Jhansi	LM1073
5	**Dr. Anand G. Chakinala,** Associate Professor & Head, Department of Chemical Engineering, School of Civil & Chemical Engineering, Manipal University, Jaipur.	LM1074
6	**Dr. Neha Rani Kumar,** Research Scholar, IISER Kolkata	LM1075
7	**Dr. Kiran D. Patil,** Professor of Chemical Engineering, Dr. Vishwanath Karad MIT World Peace University, Pune	LM1076

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

Name	Achievement
Dr. Kiran Patil Professor of Chemical Engineering, School of Chemical Engineering, Dr. Vishwanath Karad MIT World Peace University, Pune, Maharashtra, India 	Recipient of National Award **"Shiksha Bharati Award-2020-21",** in recognition of outstanding professional achievements & contributions in nation building from Indian Achiever's forum, New Delhi.

Quote of the Month

"The future depends on what you do today" – Mahatma Gandhi

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