4th National Symposium

On

Shaping the Energy Future: Challenges & Opportunities

SEFCO-2020

(June 5, 2020)

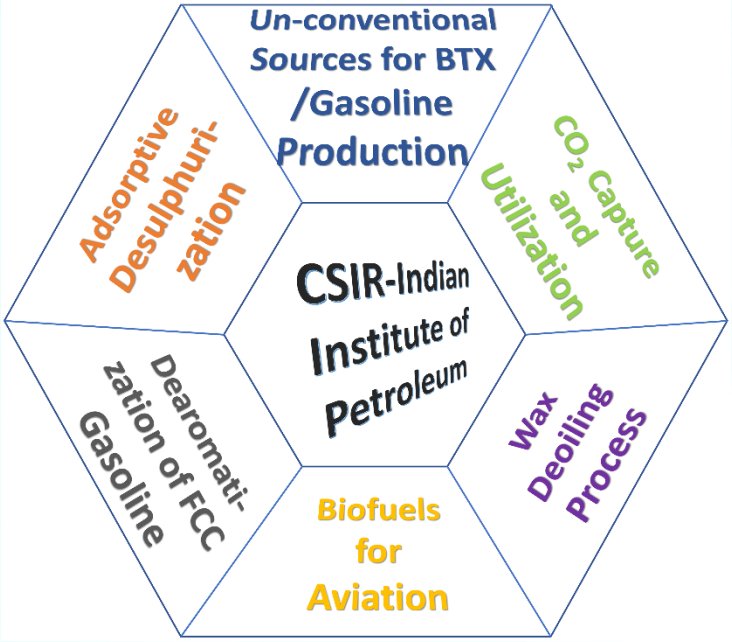
Abstract Book

Organized by

CSIR- India Institute of Petroleum,

Dehradun, Uttarakhand, India

About CSIR-IIP



Indian Institute of Petroleum (IIP) is a constituent laboratory of Council of Scientific & Industrial Research (CSIR), New Delhi. India. CSIR-IIP was established in 1959 and commenced activities at Delhi in September 1960. Later, in 1963, it was shifted to Dehradun, now the capital of the state of Uttarakhand, as a premier institute dedicated to R&D in the hydrocarbon sector. The institute works in multidisciplinary areas of R&D in the downstream sector of hydrocarbon and related industries. It acquired ISO 9001 certification in 1998.

CSIR-IIP has expertise in process & product development, scale-up, optimization, techno-economic feasibility studies, technology assessment, energy audit & conservation in chemical plants, vehicular pollution reduction, alternative fuels in IC engines, etc. Also, in petroleum refining, catalysts for refining & separation processes, solvent extraction, adsorption, lubricating oil base stocks, modified bitumen and carbon materials, modelling & simulation, bio-processing of petroleum streams, etc.

CSIR-IIP has developed a number of processes and technologies and transferred these to many industries. The institute has filed and been granted a large number of patents in India and abroad. The technology of bio-jet fuel made from non-edible oils has been successfully demonstrated for air force flight in 2018. CSIR-IIP has once again created a new paradigm by establishing the “Waste Plastic to Diesel” plant, having a capacity to produce 800-liter diesel from 1 ton of plastic wastes in its campus in August 2019. Also, a large number of research articles have been published in reputed national and international journals. The institute has been bestowed with many prestigious awards in recognition of its excellence in energy, petrochemical, and related fields.

सीएसआईआर- भारतीय पेट्रोलियम संस्थान
CSIR-Indian Institute of Petroleum

Creating Future Fuels

डॉ० अंजन रे
निदेशक
Dr. Anjan Ray
Director

Message

Dear Friends

This 4th National symposium on "Shaping the Energy Future - Challenges & Opportunities (SEFCO 2020)" at CSIR-Indian Institute of Petroleum is taking place under unique circumstances. Because of the COVID-19 pandemic, the event this year is fully digital, ironically reflecting the theme, "The Digital Future of Energy," that we had already settled upon before the lockdown happened.

This annual event has been organized since 2017 by the students and young scientists of CSIR-Indian Institute of Petroleum, India's oldest dedicated Institute in the field. We are also celebrating our Diamond Jubilee year in 2020. In these six decades, CSIR-IIP has moved beyond training and technology development into products and consulting services. Our catalysts are now in use at leading refineries in the Middle East. In partnership with other CSIR Institutes (AMPRI and NISTADS, we have recently delivered a consulting project for a second-generation ethanol plant. Our capabilities in process technology, environmental sciences, automotive engineering and energy efficiency have grown our client base beyond oil and gas to automobiles, steel, sugar and other sectors.

It is this integrated view of energy and its deep linkages with both ecological and economic sustainability that drives the annual SEFCO Symposium. In an increasingly multi-disciplinary world, we must make smarter, more agile decisions that deliver greater triple bottom lines (economic, environmental and social). The digital economy dovetails into these decisions and is part of the energy transformation that is imminent if not already upon us. As with the highly successful earlier editions of SEFCO, we are privileged to have speakers from nationally and internationally renowned scientists and technology leaders, harbingers of the future from academia and industry and a rich pool of young scientists and students having interest in Sustainable Energy.

I hope this symposium will provide you with new ideas and stimulate collaborations for an interdisciplinary, inter-institutional concerted effort for a more sustainable. The reduction in human activity during the past three months has seen significant improvements in the environment. This symposium may help identify pointers to retain these positive indicators in a favourable zone as energy consumption picks up again in a post-COVID (or perhaps a Co-COVID) future.

On behalf of Team CSIR- IIP, welcome to SEFCO Twenty and the Digital Future, web-from our eco-campus in the foothills of the Himalayas at Dehradun.

Anjan Ray

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सचिव
वैज्ञानिक और औद्योगिक अनुसंधान विभाग तथा
महानिदेशक

Dr. Shekhar C. Mande
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Secretary
Department of Scientific & Industrial Research and
Director General

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विज्ञान और प्रौद्योगिकी मंत्रालय
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वैज्ञानिक और औद्योगिक अनुसंधान विभाग

Government of India
Ministry of Science and Technology
Council of Scientific & Industrial Research
Department of Scientific & Industrial Research

Message

I am delighted to learn that the CSIR-Indian Institute of Petroleum (CSIR-IIP) Dehradun, is organizing the 4th National symposium on Shaping the Energy Future - Challenges & Opportunities (SEFCO 2020) on World Environment Day this year. With the looming climate change crisis and ever-increasing need for energy access, affordable, clean, and reliable energy is a necessary precursor to global prosperity, especially with the COVID-19 induced economic downturn. Alongside, a smart digital energy infrastructure is essential to ensure that energy systems around the world are better connected with smart producers, end consumers and agile distribution networks. Digital transformation of utilities can thus provide consumers with more capabilities and conscious choices around their energy use. All of this accelerates decarbonization and mitigates anthropogenic pollution. This symposium would provide an excellent platform to exchange ideas, views, techniques, and tools among all delegates associated with the energy field in its many facets.

CSIR is continuously pursuing national priorities in the sustainable future of energy, whether in energy efficiency, affordability, alternate energy sources, or environmental impact mitigation. I am confident this conference will be an excellent platform in identifying pathways to possible solutions for key problems faced in the energy sector. We are entering a post-COVID or co-COVID phase in the digital era and hope the researchers and industrialists throughout the nation will make the best use of the deliberations in this context during the symposium.

We look forward to an excellent virtual meeting with eminent scientists, thinkers, researchers and delegates sharing new and exciting results in energy. I wish the organizers of SEFCO-2020 all success for the event.

[Shekhar C Mande]

New Delhi
April 13, 2020

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FIPI

Dr. R.K. Malhotra
Director General

Message

I am pleased to learn that CSIR-IIP is organizing a National Symposium on 'Shaping the Energy Future-Challenges & Opportunities (SEFCO 2020)' on World Environment Day this year.

The current health crisis on account of COVID19 has been a kind of wake up call for the mankind which has been exploiting Mother Earth without worrying about any future crisis. The topic selected for this symposium is relevant in the present day context as global warming due to extensive usage of fossil fuels is causing such climate changes which can lead to even bigger destruction in future. Further the use of fossil fuels particularly for transportation has been the cause of severe pollution in our cities. We therefore need to aggressively innovate and shift to cleaner energy sources. However, till such time we continue to be dependent on fossil fuels, we have to develop and adopt the efficient and clean burning technologies besides the development and use of carbon sequestration/ conversion to useful chemicals.

The transition to any future energy source must include the assessment of the life cycle emissions and the global warming potential. Though the renewable energy sources like solar and wind would be clean and may have minimal carbon emissions in manufacturing of components but need development of energy storage systems for continued supply at all times. The bio-fuels reduce carbon emissions but should be produced from Agro or Bio waste rather than food crops. The carbon free fuel, hydrogen can be produced from various renewable sources like solar or wind based electricity, photo-electrolysis, photo-biological, Agro/ Bio-waste etc. In case of fossil sources for hydrogen production, we will need carbon capture/ sequestration technologies.

I am sure that the deliberations in the SEFCO 2020 symposium being organised by CSIR - IIP will deliberate on various opportunities and challenges for researchers in shaping the future of energy landscape which will ensure the sustainability of life on this planet.

Dr. R. K. Malhotra

New Delhi
May 28, 2020

Federation of Indian Petroleum Industry

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4th National Symposium on

Shaping the Energy Future: Challenges & Opportunities

SEFCO-2020

Schedule of SEFCO-2020	
09.30-09.35 h	About Symposium by **Ms. Neha Sharma**, Convenor SEFCO-2020
09.35-09.45 h	Welcome Address by **Dr. Anjan Ray**, Director CSIR-IIP
09.45-10.00 h	**Chief Guest: Dr. R. K. Malhotra**, DG, Federation of Indian Petroleum Industry
10.00-10.15 h	**Guest of Honour: Padma Shri Dr. T. Pradeep**, IIT Madras
Session I: Energy Efficiency and Management **Chair: Sh. Amar Kumar Jain**	
10.15-10.35 h	**K-1: Dr. Ajay Mathur**, Director General, TERI University **"Energy Efficiency: The Shape of Things to Come"**
10.35-10.50 h	**G-1: Dr. David Checkel**, University of Alberta, Canada **"Managing Future Automotive Emissions with Technology and Infrastructure"**
10.50-11.05 h	**G-2: Dr. B. M. Bhanage**. Professor, ICT Mumbai **"Mono/Bimetallic Heterogeneous Catalysts for the Conversion of Fructose to Various Value-Added Products"**
11.05-11.13 h + 0.02 h	**O-1: Dr. Ashok Kumar**, CSIR-CBRI, Roorkee, **"Energy Efficient Buildings: Qualification of Parameters"**
11.15-11.23 h + 0.02 h	**O-2: Mr. Pawan Kishore**, IIT, Jodhpur **"Thermal Degradation of Li-Ion Batteries in Hybrid Evs"**
11.25-11.30 h	Buffer time
Session II: Sustainable Development **Chair: Sh. Sudip K. Ganguly**	
11.30-11.50 h	**K-2: Dr. S. Venkatamohan**, Senior Principal Scientist, CSIR-IICT Hyderabad (K-2) **"Urban Biocycles: Circulating Metabolic Loops for Regenerative and Sustainable Ecosystem"**
11.50-12.05 h	**G-3: Dr. Sanat Kumar**, CSIR-IIP Dehradun **"Utilization of Waste Plastic for Sustainable Development"**
12.05-12.20 h	**G-4: Dr. Chinmmoy K. Hazra**, Assistant Professor, IIT Delhi **"Borane Catalyzed Ring Opening and Closing Cascades of Furans and Reductive Carbocyclization of Homoallylic Alcohols (Post-doc work) and Main-group Catalysis: Activation of Small Molecules (Current/Future Work)"**

12.20-12.35 h	**G-5: Dr. Rabah Boukherroub**, University of Lille, France **"CO2 Utilization in the Context of Climate Change Mitigation"**
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12.45-12.53 h +0.02 h	**O-4: Ms. Ruchi Shrivastava**, ITS Engineering College, Greater Noida **"Eco – friendly Corrosion Inhibitors"**
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Session III: Innovation and Change Management **Chair: Dr. Pranab Das**	
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14.20-14.28 h + 0.02 h	**O-5: Mr. Shubham Saxena**, MNIT, Jaipur **"Performance Modelling of Bituminous Mixtures with High Rap Content"**
14.30-14.38 h + 0.02 h	**O-6: Mr. Sreeja P.**, NIT, Calicut **"Paper on Development of Anti-Virus Filter Mask"**
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Session IV: Digital Application in Energy **Chair: Smt. Poonam Gupta**	
14.45-15.05 h	**K-4: Dr. Anoop Singh**, Associate Professor, IIT Kanpur **"Digital Applications in Energy (Power Sector)"**
13.05-15.20 h	**G-6: Dr. Devaraj S.**, Senior Assistant Professor, SASTRA Deemed University, Thanjavur **"Mesoporous Graphitic Carbon Nitride: A New Promising Electrode for High Energy Supercapacitors"**
15.20-15.35 h	**G-7: Dr. Saptarshi Debroy**, Assistant Professor, City University of New York, USA **"Energy Efficiency in the World of '5G' and Beyond"**
15.35-15.50 h	**G-8: Mr. Santosh Srinivas**, HYDAC India **"Condition Monitoring as Enabler for Industry 4.0"**
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16.15-16.30 h	**G-9: Dr. Venkata Krishnan**, Associate Professor, IIT Mandi **"Rational Design and Development of Nanostructured Heterogeneous Catalysts for Energy and Environmental Applications"**
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16.40-16.48 h + 0.02 h	**O-8: Mr. Viney Ghai**, IIT, Ropar **"Broadband Flexible Absorber for Energy Harvesting"**
16.50-17.00 h 17.00-17.10 h 17.10-17.15 h 17.15-17.20 h	**Guest and Honor: Dr. Rajendra Singh,** Waterman of India: Valedictory Address **Dr. Pranab Das,** Coordinator SEFCO-2020: Summarize the Event **Dr. Bipul Sarkar,** Coordinator SEFCO-2020: Announcement of Oral/Poster Awards **Mr. Amar Kumar Jain,** Chief Scientist, CSIR-IIP: Closing Note

***K- Keynote Speakers, *G- Guest Speakers, *O- Oral**

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Keynote
&
Invited
Abstracts

K-1

Energy Efficiency: The Shape of Things to Come

Dr. Ajay Mathur
Director-General
The Energy and Resources Institute
E-mail: dg@teri.res.in

The Bureau of Energy Efficiency reported last month that verified energy savings in 2018-19 amounted to nearly 10% of the electricity consumption, and 2.7% of the total primary energy supply in that year, which contributed nearly 152 million tons of CO_2 savings, which is estimated to be in excess of 6% of India's CO_2 emissions in 2018-19. The vast amount of the savings are due to the standards and labeling program (and especially due to enhanced efficiency of air conditioners and refrigerators), the perform, achieve and trade (PAT) program (due to enhanced efficiency in large industry), and the Ujjwala program (due to the replacement of incandescent and compact fluorescent bulbs by LED bulbs). These programs will continue to expand, and enhanced stringency in the energy efficiency norms for air conditioners, industries, and lighting will continue to bring increasing energy efficiency savings.

Where do we go from here?

Two sectors in which energy efficiency will probably in the near and medium-term are affordable housing and SME. Both these sectors have come centre stage because of the COVID-19 crisis, and there is a public policy urgency to greatly expand the affordable housing stock (to replace slums such as Dharavi) and strengthen the size, productivity, and profitability of SME industries, which are the backbone of job creations in the country. In both these sectors, the prime driver of energy efficiency will be the finance sector, largely because both these sectors will grow because of increased financial sector credit – often without collateral – and so energy efficiency norms could become one of the bases for credit availability in these sectors – especially since energy-efficient homes and industries are more likely to be able to repay the loans.

In the longer term, carbon emissions reductions will drive the energy efficiency agenda. We note that batteries (for grid stability in the presence of high levels of variable renewables, and for electric mobility largely to minimize urban pollution), cold storages (for food preservation which would also reduce emissions from food wastage), and zero-carbon steel will be essential for the move towards a zero-carbon future. The enhanced energy efficiency of these products (batteries, cold storages, and zero-carbon steel) is essential for them to become economically competitive (in both performances and price) with existing options. A related application is that of biofuels. While biofuels have many applications, there is no other zero-carbon substitute for aviation fuel applications; however, its utilization in this sector is crucially dependent on the energy efficiency of the conversion of biowastes into aviation fuel.

Energy efficiency opportunities in these sectors represent both an increasing demand for energy-efficient technologies, but equally, the need for the development and supply of these technologies, by universities and research institutions, together with manufacturing and sales companies, as well as with testing organizations, and with standards or specifications setting bodies. I am convinced that energy-use optimization has to be as much a part of industrial design as are the concepts of ease in manufacturing and use. After all, what is wanted – is what is developed and delivered.

K-2

Urban Biocycles: Circulating Metabolic Loops for Regenerative and Sustainable Ecosystem

Dr. S. Venkata Mohan
Senior Principal Scientist and DBT-Tata Innovation Fellow, Bioengineering and Environmental Sciences Lab, Department of Energy and Environmental Engineering, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad-500 007, India
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Urban concentrates are confronting challenges posed by increasing population growth, climate change, and faltering livability, which are prompting to chart the novel path towards adopting sustainable production/consumption strategies. The concept of circular economy (CE) that focuses on reuse and recycling of materials in technical and biological cycles to reduce waste generation is a critical intervention. Present communication establishes the immense potential of biogenic materials to be transformed into a source of value in an urban ecosystem and sets the scope for implementing 'urban biocycles' that strategically directs the flow of resources, extracting the value in the form of nutrients, energy, and materials for post-consumption within the urban metabolic regime. The emerging technologies that may support the functioning of urban bicycles will also be discussed.

K-3

Efficient System for Transporting Future Fuel "Hydrogen"

Dr. Rajesh B. Biniwale

CSIR-National Environmental Engineering Research Institute, Nehru Marg, Nagpur

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Future energy scenario will be moving away from fossil fuels for obvious reasons of resource constraints and environmental aspects. In fact, currently, many ways of renewable energy such as solar (PV), wind, etc. are available commercially and being adopted in a large extent. One of the clean and possibly renewable fuel is hydrogen. Application of hydrogen as a fuel has several challenges, such as generation from renewable sources, storage, transportation, delivery, efficient utilization, and safety. These are being addressed by researchers and technologists worldwide. One of the very important aspects is the delivery of hydrogen from the hydrogen production facility to the point of utilization.

This paper gives details of an efficient method for storage and delivery of hydrogen using liquid organic hydrides. The complete account of the method covering concept, catalytic reactions, reactor design, the effect of feed structure, life cycle analysis, etc. will be presented. The developed method can transport hydrogen at a gravimetric capacity of 6 wt% and a volumetric capacity of more than 60 kg/m^3. A prototype developed at this stage can deliver 1 Nm^3/h of hydrogen with a purity of 99.999%. The prototype of hydrogen delivery is integrated with a fuel cell stack of 1 kW. LCA study indicates that the method of supply of hydrogen using LOH is more sustainable, with a distance between two points goes beyond 250 km.

K-4

Digital Application in Energy (Power Sector)

Prof. Anoop Singh
Department of Industrial and Management Engineering (IME),
Indian Institute of Technology, Kanpur
Founder & Coordinator, CER & EAL
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K-5

"Hybrid Perovskite Solar Cells: Promise and Challenges"

Dr. D. Venkataraman
Advanced Laboratory for Iontronic, Electronic, and Nanomaterials (ALIEN)
Department of Chemistry, University of Massachusetts Amherst
E-mail: dv@chem.umass.edu

My talk will focus on a new class of materials, hybrid perovskites, that are being considered as active materials for solar cells. These solar cells have shown record power conversion efficiencies but are unstable to solar light. I will discuss our current understanding of the origins of this instability and ways to make them stable.

G-1

Managing Future Automotive Emissions with Technology and Infrastructure

Dr. David Checkel
University of Alberta, Canada
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Increasing population density and transportation demand lead to higher automotive exhaust emissions. These make a significant contribution to urban and regional air quality problems. To combat this issue, governments have a range of regulatory and economic tools at their disposal. Direct regulatory changes can affect emission control levels, fuel economy standards, fuel choices, and specific vehicle technologies such as electrification. Some economic tools include fuel-specific taxes or subsidies, transit subsidies, and capital investments in mass transit or road transportation infrastructure. Upgraded infrastructure may significantly improve transportation efficiency and mode splitting, though possibly at the expense of higher traffic volumes.

Given the scale of automotive emissions and the range of control tools available, it is important to get a measure of current emission levels and to evaluate the effect of various government actions on future emission levels. This presentation describes how physics-based microsimulation techniques are used to produce a transportation emissions inventory and to accurately forecast the changes due to government actions that affect future traffic demand, transportation mode split, vehicle technology, fuel choices, and other factors.

G-2

Mono/Bimetallic Heterogeneous Catalysts for the Conversion of Fructose to Various Value-Added Products

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Mono/Bimetallic heterogeneous catalysts showed promise in catalytic conversion of biomass-derived platform molecules to value-added products as they offer the potential of increased activity and selectivity combined with enhanced stability as compared to their monometallic counterparts [1]. In this work, we have prepared various bimetallic catalysts like Co-Al, Ru-Mg-Al-Si, Ru-ZrO_2MCM-41, and Ru@GOIL were synthesized. These catalysts were tested for synthesis 2,5-diformylfuran, 2,5-dimethylfuran, pyrrolidone from biomass-derived substrates.

In the first case study, we have studied the one-pot conversion of fructose to diformylfuran using Co-Al hydrotalcites. The catalytic properties of the prepared Co−Al hydrotalcites in the different molar ratios were investigated for the dehydration of fructose to 5-hydroxymethylfurfural (HMF), and then selective oxidation of the HMF into 2,5-diformylfuran (DFF) was studied [2]. Next, the synthesis of Ru metal supported on Mg-Al-Si was prepared and characterized by different characterization techniques. The catalytic effect of the prepared Ru-MMT in varied wt% of Ru metal was discovered for dehydration reaction of fructose to HMF, and for efficient oxidation of the HMF into DFF. The practical applicability of the developed catalyst was successfully demonstrated for the direct transformation of various carbohydrates (glucose, inulin, sucrose, starch, raffinose, and maltose) to DFF in moderate to good yield (35-64% yield).

In another work, we have developed an effective catalytic route for the selective hydrogenolysis of HMF to high-quality bio-fuel 2,5-dimethylfuran (DMF) by using Ru supported on ZrO_2-MCM-41 [3]. With the use of 2 wt % Ru-ZrO_2-MCM-41 catalyst, 90% yield of DMF was obtained from HMF with a very short reaction time of 1 h. The catalyst was recycled up to six-time with a marginal decrease in the yield after the 4th cycle. Moreover, the synthesis of ruthenium ion supported on ionic liquid immobilized into graphene oxide (Ru@GOIL) catalyst and characterized using
different analytical techniques. The catalyst is highly active for the synthesis of N-aryl/alkyl pyrrolidones derivatives by reductive amination reaction and afforded products in a 78-93% yield [4]. The catalyst was recycled for six reaction runs with slight drop-in activity after the 4th cycle. The practical applicability of the developed catalyst was successfully demonstrated by direct transformation of biomass waste (rice husk and wheat straw) derived LA to N-substituted pyrrolidones.

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G-3

Utilization of Waste Plastic for Sustainable Development

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Plastics are cheap, light weight, versatile and durable polymeric materials, derived mainly from petroleum, which provide many direct economic benefits, contribute to resource efficiency and boost development. They help in preserving natural species by replacing wood, cotton etc, help farmers and consumers by increasing shelf life of food, boost food processing and health care, facilitate growth of electrical and electronics industry , support building and construction etc. Moreover, these require less energy than metal or glass during processing as well as being relatively light weight consume lesser fuel during transportation. This has led to an enormous increase in the consumption of plastics and the world wide consumption is expected to increase from 0.3 billion in 2012 to more than 30 billion MT by 2050 (Nature, 2013). However, since plastics are non-biodegradable, there is a continued accumulation of waste plastics in land and marine environment, which is threatening the ecosystem and the biodiversity. Hence sustainable development warrants a proper techno-economic solution for mitigating the menace of waste plastics.

The present methods of disposal like landfilling, incineration and mechanical recycling are fast proving to be inadequate and hence new environment benign technologies are required that can utilize these waste plastics as a resource . CSIR-Indian Institute of Petroleum alongwith GAIL has developed a process for converting waste polyolefinic (polyethylenes and polypropylenes) into automotive grade diesel and gasoline (BS VI) as well as petrochemicals. 1 kg of clean plastics can give either 750-800 ml of diesel or 600-ml of gasoline. These meet the specifications of BS IV/VI and their performance on engines to are comparable refinery fuel. Plants based on this technology can be set up at capacities of 10 TPD or higher, which are likely to be economical and can provide multiple environmental benefits like proper disposal of waste plastics, reduction in green-house gases, cleaner land and oceans as well socio-economic benefits like reduced consumption of crude oil, employment generation etc.

G-4

Borane Catalyzed Ring Opening and Closing Cascades of Furans and Reductive Carbocyclization of Homoallylic Alcohols (Post-doc work) and Main-group Catalysis: Activation of Small Molecules (Current/Future Work)

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First part of my talk will be on *''Borane Catalyzed Ring Opening and Closing Cascades of Furans''*. Here we present the development of tris(pentafluorophenyl)borane–catalyzed conversion of furans via ring-opening and closing cascade processes to afford silicon-functionalized synthetic chemicals under transition metal-free conditions. The furan ring-opening with hydrosilanes is highly efficient and atom-economical without forming any byproduct to give rise to *α*-silyloxy-(*Z*)-alkenyl silanes. Additional equivalents of silane smoothly induce a subsequent $B(C_6F_5)_3$-catalysed cyclization of initially formed olefinic silane compounds to produce *anti*-(2-alkyl)cyclopropyl silanes, another versatile synthon being potentially applicable in the synthesis of natural products and pharmacophores. After that, I will focus on *''Borane Catalyzed Reductive Carbocyclization of Homoallylic Alcohols''*. The organoborane-catalyzed reductive carbocyclization of homoallylic alcohols has been developed by using hydrosilanes as reducing reagents to provide a range of 1,2-disubstituted arylcyclobutanes high yields and with excellent selectivity. The reaction proceeds in a cis-selective manner with high efficiency under mild conditions. Mechanistic studies indicate that stepwise dual ring-closing pathways are operative, whereas the condensative intramolecular cyclization is turnover limiting. Tuning the electronic nature of the C_4-aryl groups of homoallyl substrates can alter the reaction pathway to lead to cyclopropanes. Mechanistic studies, including deuterium scrambling and Hammett studies, and DFT calculations, suggest a dual ring-closing pathway.

Second part of my talk will be on the main group catalysis of activation of small molecules. Mostly, I am working with catalysis field where I can use organocatalyst to activate small molecules such as carbon dioxide (CO2). After searching many literature, I have found that Brookhart acid and Lambert salt would be the very good choices for the conversion of the volatile molecule, such as alkenes to the value-added products. In the near future, I will also be working with feedstock molecules such as CO2, CO, toluene, alkenes, and alkynes to get value-added products under metal-free conditions.

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G-5

CO_2 Utilization in the Context of Climate Change Mitigation

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The anthropogenic activities such as the burning of fossil fuel, deforestation, and energy generation have led to intensive greenhouse gases emission. The unceasing rise of greenhouse gas emission has, in turn, caused global warming and climate change. Carbon dioxide (CO_2) represents a major greenhouse gas, and its atmospheric concentration continues to rise over the last decades. The increase is still ongoing, l and it is likely that the level of CO_2 will reach 500 ppm by 2045, as compared to 280 to 390 ppm from the pre-industrial revolution to 2013. As a consequence, this may cause the Greenland and Antarctic ice sheets to melt, resulting in sea levels rising and extinction of about 24% of plant and animal species.[1-3]

In this context, conversion of CO_2 into feedstock chemicals, fuels, and electrical energy, represent an appealing approach to meet these threats, namely, energy security issues, global warming, and climate change.

In this presentation, I will discuss several key technologies and approaches that are able to environmentally and economically address these challenges.

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G-6

Mesoporous Graphitic Carbon Nitride: A New Promising Electrode for High Energy Supercapacitors

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Among various energy storage devices, supercapacitors have received significant attention due to their fast charging-discharging capability, extended cycle-life, wide operational temperature, etc. Supercapacitors can be used either as a standalone device or coupled with rechargeable batteries to power many appliances. However, their energy density is low, which seriously limits their applications in high energy demand appliances. Therefore, to fully harness the potential of supercapacitors, researchers continue to develop unique materials capable of delivering high energy without compromising power at relatively low cost.

Mesoporous graphitic carbon nitride (meso g-C_3N_4) is a layered semiconducting material which possesses outstanding chemical and thermal stability, mechanical rigidity, high surface area, adjustable pore size, good electronic structure and environmentally benign. Despite these unique properties, the potential of meso g-C_3N_4 as an electrode material for supercapacitors remains unexplored. Herein, we report for the first time capacitance properties of meso g-C_3N_4 synthesized by facile, cost-effective carbonization of the polymer-surfactant composite under static air. The electrochemical studies revealed that that the meso g-C_3N_4 is a potentially promising electrode material for high-performance supercapacitors.

G-7

Energy Efficiency in the World of '5G' and Beyond

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'5G' in and of itself is one of the most disruptive technologies the world has seen in decades. What makes the design and implementation of '5G' (and beyond) technologies truly challenging and transformative is the growing need of real-time 'Big Data' processing using 'Machine Learning' (ML) and 'Artificial Intelligence' (AI) algorithms. In this world of the omnipresence of 'Internet of Things' (IoT), mission-critical use cases (e.g., Smart Manufacturing, Edge/Fog assisted Disaster Response and Smart Health) that are built around low-power 'IoT' devices are in fact motivating such technology designs to be more energy-efficient. This talk will introduce the building blocks of energy-efficient future technology roadmaps, such as 'Big Data' processing, '5G' to '6G' vision, and 'Edge/Fog Computing.' The talk will also introduce the future use cases around which such energy-efficient technologies are being built upon.

G-8

"Condition Monitoring as Enabler for Industry 4.0"

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Intelligent sensor system, IoT gateways, edge computing, cloud services, big data analysis, machine learning, digital twin, administration shells, greenfield, brownfield, data hub, energy management…is that everything? These topics are spoken and written and implemented constantly.

The so-called fourth industrial revolution aims to link together people, production plants, and products, digitize them and thus incorporate them into the value creation process. But this digitization process is only possible with specific tools, or "enablers."

The predictions for the life expectance of components and system, pending consumable changes, and process-related errors are all communicated in real-time. Data from ERP systems are linked with machine and process data to improve co-ordination between production jobs and machine availability and to optimize productivity and production.

G-9

Rational Design and Development of Nanostructured Heterogeneous Catalysts for Energy and Environmental Applications

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Energy crisis and environmental deterioration have emerged as a major problem around the world in recent times, mainly due to the combustion of fossil fuels and their depletion. The utilization of solar energy for the production of chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. The design and development of highly efficient, eco-benign, and cost-effective photocatalysts, which can utilize the naturally abundant solar light, is highly desired for energy generation through water splitting and environmental remediation through the degradation of pollutants. Our research group has recently developed several two-dimensional carbons (reduced graphene oxide and graphitic carbon nitride) supported nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles, which can utilize the full solar spectrum from ultraviolet to infrared regions for energy generation and environmental remediation applications. In addition, our group has also developed efficient Green catalysts for organic transformation reactions to synthesize medicinally relevant indole alkaloids in water. Furthermore, our group has also worked on the development of bioinspired scaffolds for heterogeneous catalysis and also on the development of carbon-based catalysts for biomass conversion. The highlights of the ongoing research works of our group will be presented.

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Oral
&
Poster
Abstracts

Theme: 1

Energy Efficiency

&

Management

O-1

Energy Efficient Buildings: Quantification of Parameters

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The National Building Code of India, 2016 classifies buildings as naturally ventilated, mixed-mode, and air-conditioned buildings. Quantifying energy conservation measures in buildings refers to estimating the impact of each parameter vis-a-vis passive and active strategies that can be deployed by architects and engineers to make all the typology of buildings energy efficient. There are energy simulation tools and algorithms that can be used by professionals and are helpful to architects and engineers during the concept stage of the design of their projects or retrofitting existing buildings. However, quantification always remains a challenge for the majority of designers & architects. The Bureau of Energy Efficiency (BEE) has developed Energy Conservation Building Codes for Residential (2018) and Commercial Buildings (2017). Similarly, there are green rating systems like GRIHA, LEED - IGBC, etc. covering a wide spectrum of parameters, including energy efficiency. However, these Codes and rating systems do not quantify the energy savings and the payback period, which is left to designers. It has been observed from the opinion surveys of about 350 architects, and about 100 engineers across the country that majority (more than 96%) find hard to quantify the impacts. The reasons are manifold, and one of the reasons is the validation of theoretical and real-time data. The author has done extensive research on quantifying different parameters and carried out full – scale experimental studies for 18 months to monitor the performance by constructing two full-scale buildings one baseline and the other energy-efficient and compared the theoretical and experimental results. In this talk, the Scientist/author will put forth some basic questions and try to answer them with a view to make buildings energy efficient varying from 10% to 70% by appropriate deployment of passive systems and active technologies, with a payback period of 2-5 years, which can further be made Net Zero energy buildings (nZEB) by adopting renewable technologies with a payback of 5-7 years.

O-2

Thermal Degradation of Li-ion Batteries in Hybrid Evs

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Li-ion batteries are widely used in Hybrid Electrical vehicles at present. One of the major problems faced by these batteries is the capacity loss due to varying conditions like operating temperature. In this work, Li-Ion Batteries are simulated to study their dynamics and performance under different Indian weather conditions.
An Equivalent Circuit Model of a Battery (BECM) that can replicate the exact behavior of Li-ion batteries is first built. Then, a Battery Thermal Model (BTM) is made to determine the temperature change inside the battery pack with respect to the ambient temperature conditions that change Battery's usable capacity and, in turn, affects its State of Charge (SOC), Open Circuit Voltage (OCV), etc. Further, a Battery Degradation Model (BDM) is built-in which cycling losses and calendar losses are incorporated. Combination of these two losses gives the sum of total losses, used to determine the final decreased Capacity of the Li-ion Battery over a definite time and working conditions.

The simulated battery is benchmarked with the results of a 40 kWh Lithium Nickel Manganese Cobalt (NMC) Oxide battery used in the Nissan LEAF 2018. After validation of the model, it is tested for other input variables and can be used for different surrounding conditions. The developed model will be useful for predicting the life of Li-Ion batteries used in EVs on Indian roads.

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Theme: 2

Sustainable Development

O-3

Self-assembled graphene oxide for hydrogen storage applications

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There is a demand for renewable, eco-friendly and non-polluting zero-emission alternative sources of energy that could sort-out the energy dependency on fossil fuels due to the rapid globalization and increasing population. Among all the potential candidates for renewable energy including nuclear, solar, wind, tidal, biofuels, hydro, geothermal and hydrogen; hydrogen is emerged as a competent alternative source of energy because of zero carbon emission with high calorific value, lightweight and high gravimetric energy density (~33 kW h Kg^{-1}). Hydrogen can be stored in the fluid and solid-state medium. Significant progress has been achieved in hydrogen storage technologies development and demonstrated throughout the world. Graphene and its composites have considerable interest in the development of hydrogen storage technologies. Here, we will discuss the hydrogen storage properties of self-aligned graphene oxide (GO) at room temperature [1]. We will show how hydrogen storage capacity changes with interlayer spacing in aligned graphene oxide structure, as shown in Figure 1.

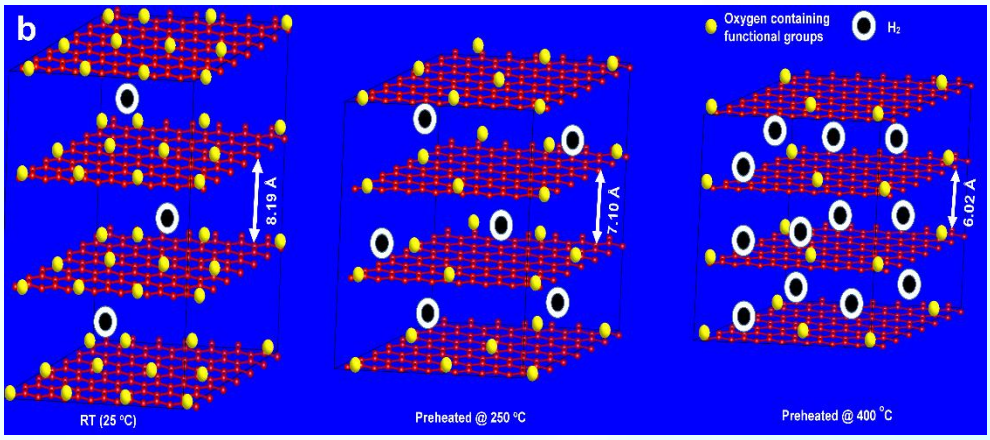

Figure 1: Schematic illustration for a temperature-dependent interlayer distance along with hydrogen adsorption.

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O-4

Eco–Friendly Corrosion Inhibitors

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The protection of materials from corrosion enhances the lifetime of equipments, saves industries from substantial economic loss, and also reduces the disintegration of toxic chemical from the components into our ecosystem. The use of natural products as green corrosion inhibitors is one of the most important methods to protect metallic materials against corrosion in acidic medium, containing hydrochloric acid (HCl) in particular. Acid solutions are widely used in various industrial processes such as cleaning, pickling, descaling, acid oil-well acidification, etc. and mild steel is frequently used in industry, and machinery could corrode in acid media. So, the corrosion prevention of steel in acidic media is one of the challenging problems in current research. The corrosion inhibition effect of methanolic extract of Elsholtzia communis inflorescence (ECI) has been studied by means of weight loss, potentiodynamic polarization, and electrochemical impedance spectroscopy (EIS) techniques. The temperature effect on the inhibition effect of plant extracts has also been discussed. The adsorption of inhibitor on the MS surface was found to obey the Langmuir adsorption isotherm. The GC-MS and FT-IR studies indicate that the adsorption centre in green inhibitor probably due to the presence of beta retinoid and its derivatives in ECI. Thus ECI extract shows effective inhibitive capacity towards the mild steel corrosion in acidic environment. Quantum mechanical study using Density Function Theory calculations provides strong support of the electron-donating tendency of inhibitor molecules and the mechanism of the inhibiting process.

P-1

Alternative Production of Light Olefins from CO_2 Hydrogenation

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Light olefins (ethylene, propylene, butene, etc.) are the basic building blocks for petrochemical and are very important intermediates in the chemical industries. Currently, more than 50% of these are being produced from the steam cracking of naphtha, which is one of the 10th most energy-intensive operations in the industry. The single-step hydrogenation of CO_2 to olefins is very novel, and there is no commercial intervention existing till date. Research is still underway for fine-tuning of catalysts and processes for developing a one-step route strategy.[1] The direct route to olefins involves a feed having hydrogen in deficient composition instead of that as required for the methanol route (H_2/CO_2, >2). Hence, there is a requirement of a catalyst and a process to address both in a single platform. We have synthesized Fe-Mo_2C catalyst for the continuous production of olefins rich hydrocarbon stream through selective activation of CO_2 in the presence of hydrogenation. The catalyst morphology obtained using TEM, and TGA also shows good catalytic stability of fresh as well as the spent catalyst. Our synthesized catalyst and their study provide an important contribution for CO_2 conversion to value-added chemicals.

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P-2

Sustainable Development and Sustainability

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The development that meets the needs of the present without compromising the ability of future generations to meet their own needs is known as Sustainable development. Sustainability is often thought of as a long-term goal (i.e., a more sustainable world). There are four dimensions to sustainable development – society, environment, culture, and economy – which are intertwined, not separate. Sustainability is a paradigm for thinking about the future in which environmental, societal, and economic considerations are balanced in the pursuit of improved quality of life. For example, a prosperous society relies on a healthy environment to provide food and resources, safe drinking water, and clean air for its citizens.

The principles of sustainable development are as follows:

- Conservation of ecosystem.
- Development of sustainable society.
- Conservation of biodiversity.
- Control of population growth.
- Development of human resources.
- Promotion of public participation.

The main challenges to sustainable development which are global in character include poverty and exclusion, unemployment, climate change, conflict, and humanitarian aid, building peaceful and inclusive societies, building strong institutions of governance, and supporting the rule of law.

P-3

Visible Light-Induced α-Amino Acid Synthesis from Carbon Dioxide using Nanostructured ZnO/CuO Heterojunction Photocatalyst

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Utilization of carbon dioxide for chemical synthesis has become an integral part of carbon management for sustainable development, mainly due to the growing environmental concerns.[1, 2] Despite the highly energy-intensive thermal processes, photocatalytic activation of CO_2 is a green and sustainable approach, which occurs at room temperature using solar energy. α-Amino acids are referred as essential constituents of proteins, peptides, and various bioactive compounds that play a vital role in our life.[3] Light assisted activation of carbon dioxide for the carboxylation reactions has come out to be a sustainable approach for the synthesis of carboxylic acids under mild conditions.

In the present work, we describe an efficient and green approach from the coupling of CO_2 and amines to α-amino acids using a nanostructured ZnO-CuO heterojunction semiconductor photocatalyst under visible light irradiation. The developed protocol provided the selective α-carboxylation of different amine substrates bearing various functional groups and afforded moderate yields of corresponding carboxylated products. The photocatalyst could easily be recovered from the reaction mixture and reused for at least five runs without any vital loss in activity.

Keywords: benzylamines, photocatalysis, carbon dioxide, heterojunction, carboxylation, α-amino acid

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P-4

Synthesis and Application of Waste Peels Derived Photoactive Carbon Dots

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Photoactive carbon dots (CD) were fabricated from waste peels of traditionally valuable/known Bitter Apple (BA) fruit. The sustainable approach involves carbonization of dried peels in a muffle furnace at ~ 300 ˚C. The photocatalytic activity of CD was tested under the presence of sunlight for photodegradation [1] of organic pollutant dye named crystal violet (CV). These Photoactive CD showed remarkable results concerning the photodegradation of CV (20 ppm in ~ 90 minutes) shown in figure 1. The NMR analysis supports the break down of complex organic aromatic framework of CV breaks into smaller aliphatic versions. A plausible mechanism governing dye degradation was investigated by trap experiment, where electrons and holes were identified as an active species responsible for photodegradation. Being water-insoluble CD has been easily separated from the photodegraded CV water and hence been used for multiple cycles. Generally, BA peels were discarded as waste, so, fabricating them into photoactive CD makes the whole process extremely economical.

Figure 1: Photographic image of sunlight-induced photocatalytic degradation of crystal violet dye.

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Theme: 3

Innovation & Change Management

O-5

Performance Modelling of Bituminous Mixtures with High Rap Content

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RAP is Reclaimed Asphalt Pavements. These materials are generated when asphalt pavements are removed for reconstruction or resurfacing. It is a useful alternative to virgin materials because it reduces the need to use virgin aggregates, which is in a scarce commodity in some areas. Also, it reduces the amount of costly new asphalt binder. Indian specifications allow the usage of 30% RAP in the construction of the pavement. However, various studies have been carried out on the usage of a high percentage of RAP in the mixes. Also, trial sections were laid down in order to evaluate its performance after a particular period of its service life. With increase in the percentage of RAP, some properties improve and become far better than that of the virgin mix, whereas few properties get affected by the increase in RAP percentage. The present focus of research is to increase the percentage usage of RAP in the Hot Mix Asphalt mixes. In the present study, an attempt shall be made to concise all the researches that were carried on the usage of 100% RAP in the Hot Mix Asphalt mixes and to conclude its performance as compared to that of the virgin mix.

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O-6

Paper on Development of Anti-Virus Filter Mask

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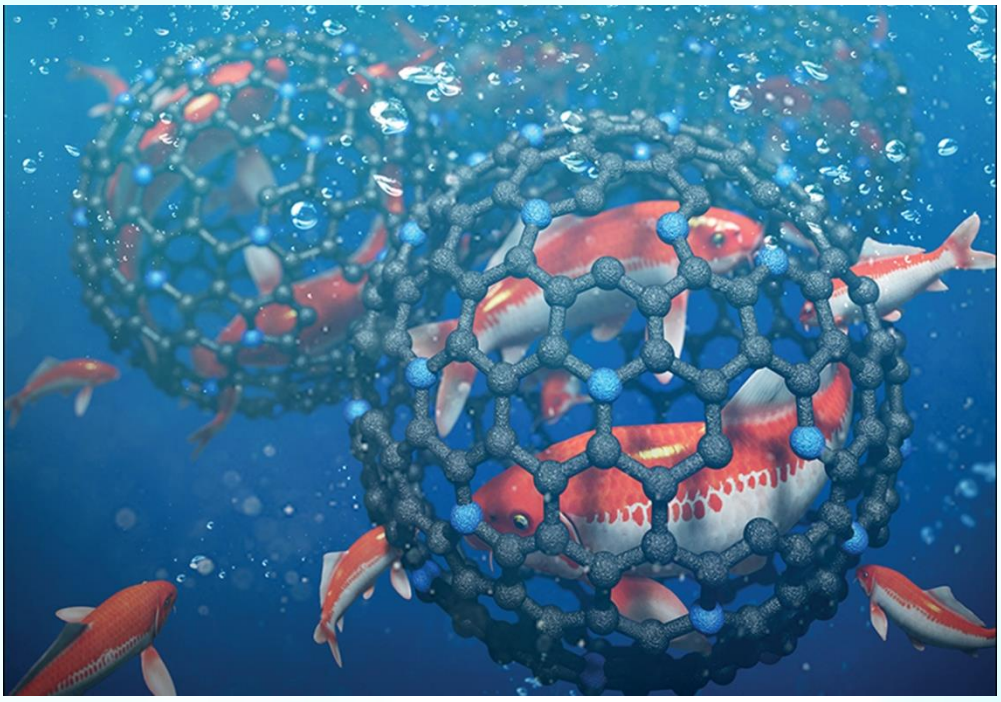
We know that due to the outbreak of a virus known as coronavirus, the whole world is facing difficulty in controlling the spread of Covid-19. These are spread through the droplets of patients while sneezing or coughing or through close contact, also known as primary contact. In this paper, it describes about the development of cough and sneezes containment mask using polymer composite, which makes people to travel outside confidently. Since these virus particles persist in the atmosphere, the cloth used by the person, which becomes a source of transmission again**.** In order to prevent this, the cough and containment device can be used, this kind of mask can be useful for the health workers, all other medical professionals in hospitals. We hereby aim to describe about reusable mask in this paper at a low cost, which is affordable for all the people. An infection containment mask that consists of a cavity which covers mouth and nose that holds a filter in the filter chamber. There are pressure vents on the unit that releases the air pressure when coughing or sneezing into the unit. The filter, in preferred embodiments, consists of a sub-micron and/or standard filter and/or anti-microbial filter. Another embodiment of the infection containment mask with an interchangeable filter for capturing and containing the infectious aerosolized droplets (viral, bacterial, and/or mycobacterial micro-organisms) from a sick person's cough and/or sneeze. It gives high safety for the health workers, medical professionals who are handling virus-infected patients.

Figure 1: Face shield

Theme: 4



Advanced Materials for

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4th National Symposium on Shaping the Energy Future: Challenges & Opportunities (SEFCO 2020)

O-7

Pd decorated Functionalized Carbon Nitride as an Efficient Heterogeneous Catalyst for Hydrogenation Reactions using $KHCO_2$ as a Hydrogen Source

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Functionalization of the widely known graphitic carbon nitride (GCN) material has been performed, and a novel heterogeneous catalyst is reported by incorporating palladium over the surface of functionalized GCN. GCN was functionalized using an optimized ratio of sulfuric acid, nitric acid, and hydrogen peroxide. The developed catalyst was characterized by various microscopic and analytical techniques. The developed material containing ≤1% Pd exhibits superior catalytic activity in comparison to other carbon support materials (such as 5% Pd/C) for various hydrogenation reactions under mild conditions. Potassium formate has been chosen as the best hydrogen source among other alkali metal formates. The developed catalyst was also able to catalyze a one-pot three-step reaction for the synthesis of N-benzylaniline, which is a precursor of various antihistamine and anticholargenic drugs. Moreover, the catalyst could be recycled multiple times, and consistent activity was reported.

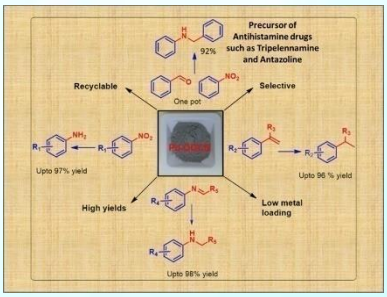

Figure 1: Use of Pd-OGCN for various hydrogenation reactions

Recently, we developed metal functionalized GCN for the transfer hydrogenation of aldehydes and ketones.[1] In pursuit of our efforts toward sustainable heterogeneous catalysis, we oxidized GCN to OGCN and decorated it with Pd. The synthesized Pd-OGCN nanocomposite has been found to be a reason efficient heterogeneous catalyst for in situ hydrogenation of nitro, imine, and alkene functionalities.[2] The Pd-OGCN nanocomposite exhibited better catalytic activity than its counterpart Pd-GCN material. The for good catalytic performance can be contemplated because of oxidative surface modification of GCN to OGCN. The extensive functionalization of the GCN surface has been supported by solid-state CP-NMR data also. We assume that the functionalized surface holds the Pd metal strongly and also helps the reactants to interact with the catalytic surface more efficiently. Alkali metal formates are noncorrosive sources of hydrogen gas. Hence, potassium formate has been used as a mild and noncorrosive source of hydrogen in this study.

O-8

Broadband Flexible Absorber for Energy Harvesting

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Most of the existing absorber find limited applications due to the fact that they are rigid and work efficiently only in the visible region of the solar spectrum. Consequently, there is a need to develop flexible absorber that can efficiently utilize the available solar energy. The present study focuses on the design and fabrication of novel multifunctional flexible absorber (flexorb) to harness the solar energy in a broader wavelength region of UV-Vis-NIR. To this end, untextured nanocomposite (UNC) is first synthesized by reinforcing 1 wt. % of nanofillers [carbon nanotubes (CNTs), zinc oxide nanorods (ZnO), and iron nanoparticles (Fe)] in polydimethylsiloxane (PDMS) matrix. Homogeneous mixture of these nanoparticles led to an ultra-high absorption of more than 96 % in the broadband range (300-2000 nm). Subsequent texturing of UNC enhances the absorption capacity to more than 99 % in the entire UV-Vis-NIR wavelength range. This increase in absorption is attributed to the multiple scattering of incident beam induced by textured surface (conical pillars) along with different nano-fillers present in PDMS. In addition, incorporation of CNTs in flexorb provides better impedance matching, which results in lower reflection losses at flexorb/air interface. Peel-off tests performed with flexorb show better bonding with different types of substrates. Due to the flexible nature, the fabricated flexorb can be deformed in a variety of shapes without any damage or creasing failure and, therefore, can be easily mounted on curved as well as other non-planar surfaces in real-life applications.

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P-5

Intense-Blue Bipolar Pyrene-Based Emitters Based on Hybridized Local and Charge Transfer (HLCT): A Promising Candidate for Future Lighting

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Deep blue emitters are attractive due to their use in full-color displays as well as their use as a host material for low energy dopant emitters. Two blue emitters **PypNPC** 9,9'-((7-(tert-butyl)pyrene-1,3-diyl)bis(4,1-phenylene))bis(9H-carbazole) and **PymNPC** 9,9'-((7-(tert-butyl)pyrene-1,3-diyl)bis(3,1-phenylene))bis(9H-carbazole) are synthesized by selecting *t*-butyl-pyrene as the core group and electron-donating *N*-phenylcarbazole (NPC) as side groups and characterized by photophysical, electrochemical, thermal, theoretical and electroluminescence studies. Among all three possible cases for a donor-acceptor (D–A) molecule, 1) a π–π* state (a localized excited state), 2) a charge-transfer (CT) state (a delocalized electronic state) and a mixed or hybridized state of π–π* and CT (named as the hybridized local and charge transfer (HLCT) state, HLCT is believed to be present in these molecules as confirmed by photophysical studies. The solvent-independent absorption spectra of the compounds indicate the absence of donor-acceptor interactions in the ground state due to twisted *N*-phenylcarbazole moiety with respect to pyrene. But despite the significantly twisted non-planar structure, these molecules still displayed efficient intramolecular charge-transfer emissions with clear solvatochromic shifts on increasing solvent polarity attributable to the reorganization of the *N*-phenylcarbazole orientation in the excited state. Emission wavelength under pure deep blue color of CIE coordinate (0.15, 0.08), low FMHW (~40 nm), high thermal stability (490 ^{o}C), and high quantum yield (FQY= 84%, EQE= 2%) make them as promising candidates for OLED applications.

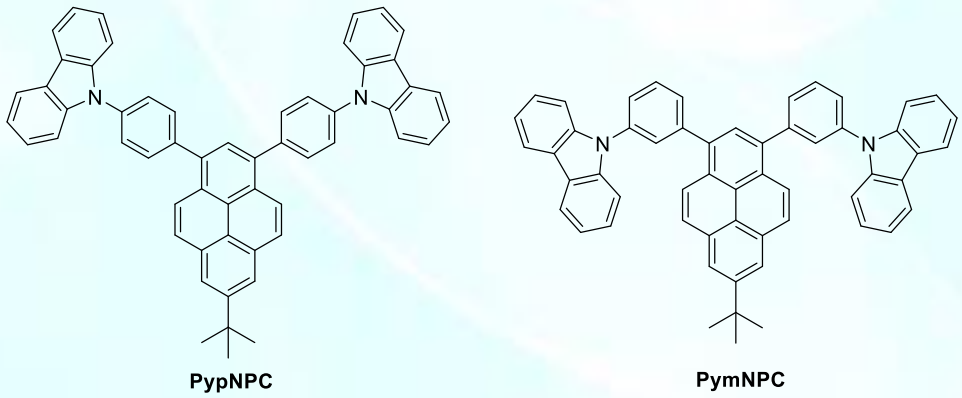

Figure 1: Structure of synthesized Dyes

P-6

Resorcin[4]arene-based Porous Organic Polymers for CO_2 Fixation and Micropollutant Removal from Water

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Resorcin[n]arenes are an important class of macrocycles possessing tractable cavity, heteroatom rich functionality, and excellent host-guest complexing ability.[1] They have been extensively used for catalysis,[1] molecular separation to drug delivery. Knitting the '*preporous*' cavitands using aromatic linkers may lead to a new generation porous organic polymers (POPs), where the inherent properties of the cavitands are augmented many folds. Herein, we demonstrated a '*cavitand-to-framework*' design strategy by connecting *C*-phenylresorcin[4]arene core (specific BET surface area: 156 $m^2 g^{-1}$) through different functional linkers to obtain a series of POPs.[2] The surface areas of the POPs were increased up to 8 fold than that of the cavitand monomer (156 $m^2 g^{-1}$ to 1230 $m^2 g^{-1}$). *C*-phenylresorcin[4]arene-based POPs exhibiting excellent performance towards metal-free CO_2 fixation and size-selective, charge-specific separation of organic micropollutants from water. Thus, cavitand-based POPs opens up an interesting field of research where we can address many unresolved problems related to sustainable development and environmental remediation.

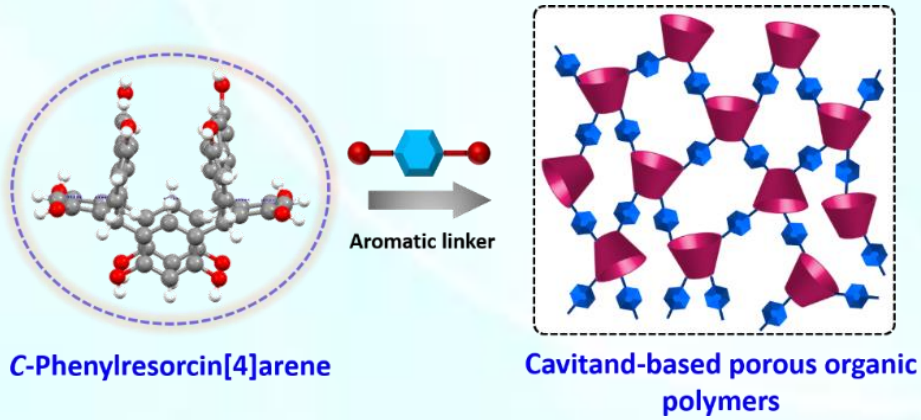

Figure: Connecting phenylresorcin[4]arene core with aromatic linkers leads to cavitand-based porous organic frameworks (POPs).

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P-7

An Efficient Supported Molecular Co-N Complex for Photoelectrochemical (PEC) Reduction of CO_2 to C1 Products

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The study aims to develop an efficient and robust hybrid via covalent immobilization of cobalt phthalocyanine tetrasulfonamide (CoPcS) to carboxylated graphene oxide (GO-COOH) that has been used as an active photo-electrode material for carbon dioxide reduction reaction (CO_2RR). The formation mechanism of a hybrid (CoPcS/GO-COOH) and their intermolecular covalent bonding is persuaded to create a proficient interface for photoelectrochemical (PEC) CO_2RR. Here, we achieved high current density (-1.7 mA cm^{-2}) at an applied voltage of -1.0 V vs. Ag/AgCl under visible light irradiation, and the PEC study recognizes the C1 (formate) as a key product. The difference in photocurrent density of CoPcS/GO-COOH is reasonably higher than pristine CoPcS & GO-COOH. AC impedance indicated significantly increased numbers of charge carriers and decreased e-/h+ pair

recombination in the case of hybrid CoPcS/GO-COOH. The developed hybrid molecular system showed improved efficiency for PEC CO_2RR as compared to the reported ones.

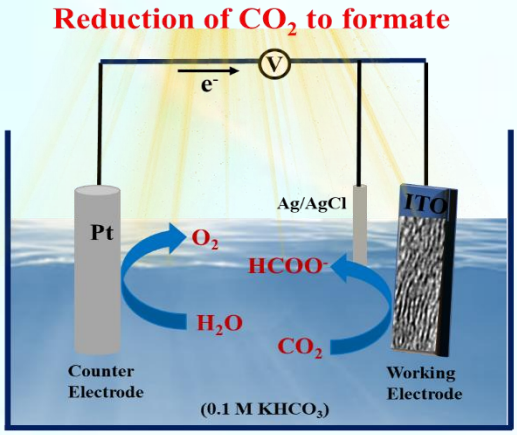

Figure 1: PEC reduction of CO_2 to formate by CoPcS/GO-COOH

P-8

Morphology-Controlled Mesoporous Perforated NiO Nanostructures for High Energy Density Supercapacitor Electrodes

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We report the morphology-controlled approach to improve the specific capacitance (C_s) and energy/power density of the supercapacitor. The randomly oriented irregular morphologies of NiO are converted into the perforated mesoporous nanobelts and further transferred into the nanoflakes under controlled reactions. The nanobelts and nanoflakes of NiO with an average width of ~74 nm and ~215 nm forms the thin film of thickness ~5.8 and 2.7 µm, respectively. The mesoporous NiO nanobelts deliver the high C_s of 794 F/g compare to the nanoflakes (146 F/g) and a thin film of irregular morphologies (742 F/g). Moreover, nanobelts show 88.6 % retention after continuous 2500 charging-discharging cycles. The NiO nanobelts exhibit the power density of 2963 W/kg, and energy density of 57 Wh/kg is significantly higher than the pristine NiO nanoflakes, nanorods, 2D thin films, porosity tunned nanowalls, nanofibers, and its heterostructures with $NiCo_2O_4$ and Ni_3S_2 nanosheets. The perforated mesoporous NiO nanobelts with clearly visible textural boundaries provide relatively larger surface area and excellent interconnecting network than that of irregular morphologies and nanoflakes, which provide easy access to the OH^- ions for diffusion. This suggests that the perforated mesoporous NiO nanobelts hold the potential as electrode materials for the supercapacitor with ultra-high rate capabilities.

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P-9

Bimetallic Ru-Pt and Ru-Ge High Nuclearity Complexes for Hydrogen Storage

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The reaction of $Ru_3(CO)_{12}$ with $Pt(IMes)_2$ in benzene solvent at room temperature afforded the monoplatinum–triruthenium cluster complex $Ru_3Pt(IMes)_2(CO)_{11}$, **1** and the trigonal bipyramidal cluster complex $Ru_3Pt_2(IMes)_2(CO)_{12}$, **2**. The reaction of **2** with hydrogen at 80 °C afforded the tetrahydrido–tetraruthenium complex $Ru_4(IMes)(CO)_{11}(\mu\text{-}H)_4$, **3** (Figure 1) and the dihydride–diruthenium–diplatinum complex $Ru_2Pt_2(IMes)_2(CO)_8(\mu\text{-}H)_2$, **4** [1]. In heptane solvent, $Ru_3(CO)_{12}$ reacts with tertiary butyl germane at reflux, to afford three new bimetallic ruthenium- germanium carbonyl cluster complexes $Ru_4(CO)_8(\mu_4\text{-}GeBu^t)_2(\mu\text{-}GeBu^tH)_2(\mu_3\text{-}GeBu^t)(H)$, **5**, $Ru_5(CO)_{12}(\mu_3\text{-}GeBu^t)_2(\mu_4\text{-}GeBu^t)(H)$, **6**, $Ru_6(CO)_{12}(\mu_3\text{-}GeBu^t)_4(H)_2$, **7** [2]. All six compounds were structurally characterized by single-crystal X-ray diffraction analyses, and compounds **3-7** contain hydride ligands. Supported bimetallic clusters have been shown to exhibit high activity for catalytic hydrogenation reactions when immobilized on mesoporous silica. These high nuclearity hydride clusters will be used for the storage and conversion of hydrides into hydrogen.

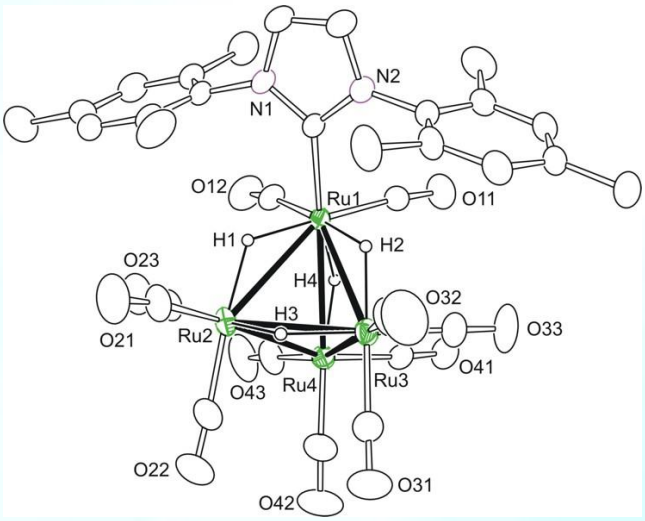

Figure 1: An ORTEP showing the molecular structure of $Ru_4(IMes)(CO)_{11}(\mu\text{-}H)_4$, **3** at 30% thermal ellipsoid probability.

P-10

Interchangeability Potential of Selected Seed Feedstocks from Wildly Growing Tree Species for Biogas Production

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Anaerobic digestion (AD) is a potent option for treating biodegradable matter in rural areas as it yields two valuable products, biogas and bio-fertilizer [1]. Biogas can cater to a whole spectrum of energy demands, including heating, cooking, electricity, and transport [2]. In this study, seeds of wild tree species, namely *Acacia nilotica*, *Prosopis juliflora*, *Albizia lebbeck*, and *Leucaena leucocephala*, have been explored as new alternative feedstocks for AD [3]. The selected trees grow widely almost all across India, primarily in arid, semi-arid, tropical dry, and humid subtropical tracts [4]. To tackle the seasonal availability of these feedstocks, a study was conducted for the interchangeability of different seeds in a mixed-feeding mode. Investigations were carried out in 300L anaerobic digester under daily feeding mode for 120 days retention period. The average specific biogas yield and the specific methane yield was found to be 0.425 m^3/kg VS and 0.228 m^3/kg VS, respectively. The average methane content in biogas was observed as 54.7%, and the total volatile solids mass removal efficiency for the entire period of operation was 46%. The study reveals that the seeds have a higher biogas production potential than cattle manure. Successful outcome with interchangeability of seeds thus enable sustained operation of digester without depending on the seed species and the seasonal availability as different seeds are available at different times of the year, and all of them can be used together to run a digester. Further, their use can help in checking the ecological risk these seeds pose by growing into invasive trees.

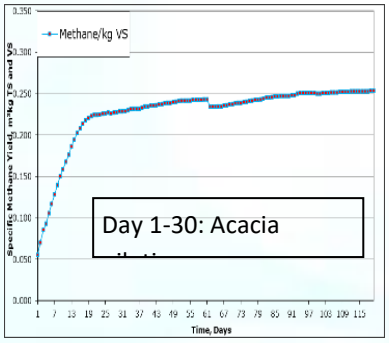

Figure 1: Specific methane yield from selected seeds fed in succession.