

## **13-14** March, 2023 ONLINE EVENT

## 14<sup>TH</sup> EDITION OF GLOBAL CONFERENCE ON

## CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

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# 13-14

BOOK OF ABSTRACTS

14<sup>TH</sup> EDITION OF GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

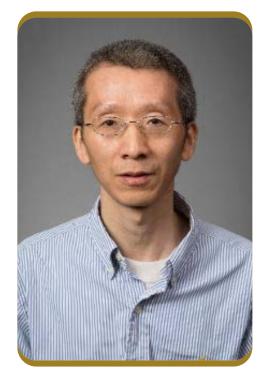
## INDEX

### Contents

| Keynote speakers            |  | 80 |
|-----------------------------|--|----|
| About the Host              |  | 09 |
| About CCET                  |  | 10 |
| About Publishing Partner    |  | 11 |
| Day 1 Keynote Presentations |  | 12 |
| Day 1 Oral Presentations    |  | 15 |
| Day 2 Keynote Presentations |  | 38 |
| Day 2 Oral Presentations    |  | 44 |
| Day 2 Poster Presentations  |  | 60 |
| Participants List           |  | 65 |

3

Dear congress visitors, it is my great pleasure and honor to welcome you on board. Organometallics, organocatalysis, and bioinorganic chemistry have witnessed great progress over the past few decades and have revolutionized the ways we think about the formation and cleavage of chemical bonds. Indeed, organometallics, organocatalysis, and bioinorganic chemistry already hold practical applications in pharmaceutical, agricultural, and material research and production. Future studies and developments in these fields will enrich our toolbox of methods and further improve the applicability of these synthetic strategies. Some exciting and recent progress in these fields will be communicated in this session in the hope of stimulating research interest among the wider scientific community.



Hailo De

**PROF. DR. HAIBO GE** Texas Tech University, USA

#### Dear Congress Visitors,

It is my honor and great pleasure to write a few notes to you. Through centuries people were fascinated with the possibilities of synthesis of new materials with extraordinary properties. New materials are practically needed in all domains of life. Design and synthesis of new materials is one of the most important and interesting part of materials sciences. Particularly a synthesis of new active and selective catalysis is a very important challenge. Our main aim concentrates on the new methods of the synthesis of singlesite hierarchical porous zeolite catalysts with acid-base and redox properties. Such zeolite catalysts with active sites formed by incorporation of hetero-elements in their framework are perspective as catalysts of protection of environment and bio-feedstock conversion into valuable chemicals.



Dangoy

PROFESSOR DR STANISLAW DZWIGAJ Sorbonne University - CNRS, France

#### Dear Distinguished Scholars, Engineers and Colleagues,

It is my great honour and pleasure as an Organizing Committee Member and Speaker to invite you to join with a contribution the 14th Edition of Global Conference on Catalysis, Chemical Engineering and Technology (CCET 2023), March 13-14, 2023, Online Event. The Conference will include Keynote speeches and Invited speeches which will be given by Distinguished Scholars, Colleagues and Experts from academic institutions and industry, and oral presentation by delegates and poster presentations by young junior participants. Devoted to the rapid development of Catalysis and Chemical Engineering, the conference will bring together distinguished experts, researchers, scientist, scholars, and young students from different cultures and different countries, providing them



with the opportunity to report, share, and discuss scientific questions, achievements, in these fields. This conference will provide excellent opportunity to meet distinguished scholars and experts and to exchange new ideas and application experiences, to establish research relations and collaborations for future research and projects.

As an Organizing Committee Member, I believe that **CCET 2023** will be a platform to discuss a broad range of topics related to Catalysis and Chemical Engineering for the academicians, scholars, investigators. Also, this conference will provide a facility for delegates to interact with each other, to conduct collaborations and to establish the research or business relations.

I am pleased to invite prospective authors to submit their original contributions to this important conference, where you are sure to have a meaningful experience with scholars and experts from different cultures and different countries.

DR. OSMAN ADIGUZEL Retired Professor of Physics, Firat University, Turkey

#### Dear congress visitors,

It is an honor and pleasure to write a few welcome notes. Bioelectrochemistry today covers a broad range of bioelectrocatalytic topics ranging from fundamental studies devoted to a deeper understanding of biomolecular systems on electrodes to electrochemical biosensor and energy conversion applications. Furthermore, the combinaKon of light with bioelectrochemistry will be also an attractive application to develop (biophotovoltaics). The environmental issue will be a particularly important part of this conferecen both for energy and for the development of new biodegradable systems.



#### PROF SERGE COSNIER

Director of Research exceptional rank at the CNRS, France

### **Keynote Speakers**



Thomas J Webster Interstellar Therapeutics, United States



Haibo Ge Texas Tech University, United States



Anne M Gaffney University of South Carolina, United States



Stanislaw Dzwigaj Sorbonne University, France



Serge Cosnier Universie Grenoble Alpes, France



Osman Adiguzel Firat University, Turkey

Thank You All.

### ABOUT MAGNUS GROUP

Magnus Group (MG) is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and researchers of same field or interdisciplinary research. Magnus Group is proficient in organizing conferences, meetings, seminars and workshops with the ingenious and peerless speakers throughout the world providing you and your organization with broad range of networking opportunities to globalize your research and create your own identity. Our conferences and workshops can be well titled as 'ocean of knowledge' where you can sail your boat and pick the pearls, leading the way for innovative research and strategies empowering the strength by overwhelming the complications associated with in the respective fields.

Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees' managing different conferences throughout the world, without compromising service and quality.

#### ABOUT CCET 2023

Magnus Group looks forward to welcoming you to its distinguished event 14<sup>th</sup> Edition of Global Conference on Catalysis, Chemical Engineering and Technology (CCET 2023) which is scheduled as a Virtual Event from March 13-15, 2023

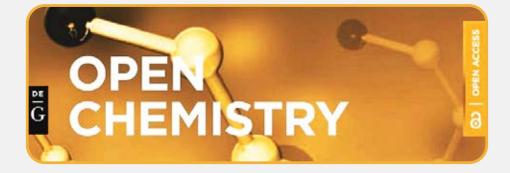
The congress is themed at Capturing and Exploring Panoramic Perspectives on Catalysis, Chemical Engineering and Technology.

We bring together all fields of chemistry, a varied audience of chemists, engineers, researchers and scientists at the conference. Parallel sessions comprising oral presentations, poster sessions, workshops, symposiums, panel discussions by junior and senior academics will be held in addition to keynote speeches.

This important colloquium has aimed to gather scientists from all corners of the world to share their interests in catalysis, chemical engineering and chemistry in general since its first edition. The programme of CCET 2023 will be tailored to attract chemists with ample chances for exchange and debate for PhD students, postdocs, and young researchers.

CCET 2023 will be a global scientific gathering bringing together scientists and clinicians from academia, industry, and government to debate the most recent advancements in the area in an informal virtual setting. This symposium will provide a stimulating and dynamic environment for scientists at all stages of their careers in this rapidly expanding subject to engage and inspire one another. We actively encourage students, the next generation of scientists and researchers, to participate.

We welcome you to join us at CCET 2023 virtually so that we may work together to improve the generation of catalysis, chemicals, chemical engineering while also improving the quality of life on the planet.



#### ABOUT Publishing Partner

Open Chemistry is a peer-reviewed, open access journal that publishes original research, reviews, and communications in the fields of chemistry in an ongoing way. Our central goal is to provide a hub for researchers working across all subjects to present their discoveries, and to be a forum for the discussion of the important issues in the field.

There are no submission charges. In order to sustain the production of our fully-refereed open access journal, each article accepted for publication in Open Chemistry is subject to Article Processing Charges (APC).

Note: We offer 30% discount on APC for the CCET 2023 conference participants.

For more details about the journal, please visit: https://www.degruyter.com/journal/key/chem/html magnus Group

# 13-14

DAY 01 KEYNOTE FORUM

14<sup>TH</sup> EDITION OF GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

## Application of metal single-site zeolite catalysts in heterogeneous catalysis

The metal ions well dispersed at zeolite framework are considered to L be active sites of catalytic processes. Therefore, the incorporation of these metals into zeolites as isolated tetrahedral sites appears to be the important task. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions results in the reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite. During my keynote talk the design of single-site zeolite catalysts with transition metal will be described and characterized by different physical techniques both at the macroscopic (XRD, BET, TPR, TEM) and molecular level (FT-IR, NMR, DR UV-Vis, XPS, EPR, XAFS). The application of metal single-site zeolite catalysts in environmental catalysis will be discussed. This twostep postsynthesis method applied in this work allowed obtaining metal single-site zeolite catalysts active in different catalytic processes such as oxidative dehydrogenation of propane into propene, selective catalytic reduction of NOx to N2, production of 1,3-butadiene or hydrogen from renewable sources, including ethanol obtained from biomass. Their catalytic activity strongly depended on the speciation and amount of metal incorporated into zeolite structure as well as their acidity.

#### Audience Take Away Notes

- The audience will be able to understand as control of preparation of catalyst systems
- They will see that catalytic activity depend on dispersion of metal in the framework of zeolite
- The researchers will be able, after my talk, do their own catalyst preparation using similar method



#### Stanislaw Dzwigaj

Sorbonne Universite, UMR 7197, Laboratoire de Reactivitede Surface, France

#### Biography

Professor Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris) he obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements he received the title of professor. His published work includes more than 170 papers published in reputable international journals.

## Bioelectrocatalytic materials based on buck papers and bio sourced glyconanoparticles

 ${f F}$  four decades, the functionalization of electrodes by biomaterials based on electrogenerated polymers, carbon nanotubes and / or nano-objects, was widely used in the field of analytical chemistry and energy conversion for the design of biosensors and biofuel cells. Some new approaches for developing nanostructured biomaterials based on functionalized carbon or tungsten nanotubes, glyconanoparticles and compressions of carbon nanotubes will be illustrated with enzymes or antibodies as catalytic or biosensing element.

In particular, the anchoring of biological macromolecules to the surface of electrodes has been carried out by chemically functionalizable electrogenated polymers. In addition, the self-assembly of carbon nanotubes via crosslinking polymers in the form of buckypapers was used. Composite bioelectrodes by compression of enzymes and carbon nanotube mixtures will be also reported. The concept of the hollow bioelectrode is based on the bonding of two conductive sheets composed of carbon nanotubes (buckypaper) whose assembly generates a microcavity defined by the thickness of the glue linking the two sheets. These buckypapers are permeable only to water and enzyme substrates but not allow the permeation of enzymes. Therefore, the enzyme trapped in powder form is then solubilized inside the microcavity leading to a high density of biocatalyst in solution with an electrical connection with the buckypapers. The electrocatalytic performance of the bilirubin oxidase hollow electrode was described as a function of pH, temperature and the amount of entrapped enzyme. The operational and storage stability of the bioelectrode in The development of glyconanoparticles resulting from the self-assembly of block copolymers composed of polystyrene and cyclodextrin as an inclusion site will be also reported. These glyconanoparticles, which are stable in water, constitute a multivalent platform for enzyme binding and hydrophobic electroactive molecules. These nanoparticles were applied to the elaboration of solubilized enzymatic fuel cell in solution or were grafted on surfaces for the development of amperometric enzyme electrodes.)

#### Audience Take Away Notes

- This presentation, in particular, presents an innovative and unpublished work on the design of a very thin, large surface area flat hollow bioelectrode configuration with an enzyme trapped inside a microcavity and its application to the electroenzymatic reduction of O<sub>2</sub>. The audience can learn how to fabricate hollow electrodes and exploit these electrodes for bioelectrocatalysis
- Moreover, this simple elaboration of hollow electrode can be easily extended to trapping other organic or inorganic catalysts offering thus promising applications, in particular in energy conversion
- An original approach of mixing and compressing CNT and protein powders to obtain easily mm-sized solid pellets will be described and the audience can used this method to develop original disks



Serge Cosnier<sup>1\*</sup>, Paulo Henrique M. Buzzetti<sup>1</sup>, Yannig Nedellec<sup>1</sup>, Monica Brachi<sup>1</sup>, Anastasiia Berezoska<sup>1</sup>, Dan Shan<sup>2</sup>

<sup>1</sup>Univ. Grenoble Alpes, DCM UMR 5250, F-38000 Grenoble, France CNRS, DCM UMR 5250, F-38000 Grenoble, France

<sup>2</sup>School of Environmental and Biological Engineering, Nanjing University of Science and Technology, Nanjing, 210094 Jiangsu, China

#### Biography

Dr Serge Cosnier is Research Director exceptional class at CNRS at the Grenoble university (France). He is member of the Academia Europaea, member of the European Academy of Sciences and Fellow of the American Institute for Medical and Biological Engineering. His activity is focused on molecular electrochemistry and bioelectrochemistry with the development of biosensors, biofuel cells and bio-nanomaterials based on carbon nanotubes. Dr Cosnier has authored over 390 publications (h-index Web of Science 69, Google Scholar 82), 3 books and 20 book chapters and holds 20 patents'.

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# 13-14

DAY 01 SPEAKERS

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## Chenchen Zhang<sup>1,2</sup>, Letian Wang<sup>1,2</sup>, Ubong Jerome Etim<sup>1</sup>, Yibing Song<sup>3</sup>, Oz M. Gazit<sup>2</sup>, Ziyi Zhong<sup>1</sup>\*

<sup>1</sup>Department of Chemical Engineering, Guangdong Technion-Israel Institute of Technology (GTIIT),Guangdong, 515063, China

<sup>2</sup>Department of Chemical Engineering, Institute of Technology (IIT), Haifa, Israel 32000

<sup>4</sup>Department of Chemistry, Shantou University, Guangdong 515063, China

## $\rm Co_2$ hydrogenation to methanol over $\rm Cu/TiO_2$ catalysts: The role of oxygen vacancies in $\rm co_2$ activation

Carbon dioxide ( $CO_2$ ) is a greenhouse gas in the atmosphere. In the last several decades, intensive efforts have been made to activate and convert  $CO_2$  through hydrogenation reactions to valueadded chemicals, particularly through thermal catalysis. Various catalysts are applied for these reactions, including supported noble metal and nonnoble transition oxide catalysts. The representative catalysts are Cu-based catalysts, such as the Cu-ZnO-Al<sub>2</sub>O<sub>3</sub> catalyst used in the industrial for CO hydrogenation. However, the Cu- based catalysts have several issues: the  $CO_2$  activation on them is quite difficult, and Cu is easily sintered. Also, it has been widely believed that the reducible metal oxides are not a good option for the supported Cu catalysts due to the strong Cu-support interaction, which often leads to the coverage of the Cu active particles by the oxide support in the catalysts. This work investigates the role of oxygen vacancy (Ov) in theCu/TiO<sub>2</sub> catalysts in the  $CO_2$  hydrogenation reaction to methanol. It is found that the Ov generated in TiO<sub>2</sub> could facilitate  $CO_2$  activation and promote methanol formation. We also observed a strong metal interaction (SMSI) between Cu and TiO<sub>2</sub>, which retarded the Cu sintering. These findings provide insights into catalytic  $CO_2$  conversion and new ways to design and develop highly efficient catalysts for  $CO_2$  conversion.

#### Audience Take Away Notes

- Yes the audience will learn why and how we convert CO<sub>2</sub> from the atmosphere into useful products through our experimental results
- Yes the knowledge and skills learned will help the audience to improve their research
- Yes CO<sub>2</sub> conversion is quite a popular research topic these years. Many people are workingin this area. The knowledge and findings to be reported will benefit many people's researchand widen their version

#### Biography

Prof. Ziyi Zhong mainly works on heterogeneous catalysis, sonochemistry and wastewater treatment; he received his Ph.D. in 1995 from Nanjing University. Later, he did his post-doctoral research at Bar-Ilan University in Israel, the University of Washington, and the National University of Singapore sequentially for5 years. From 2003 to 2018, he worked in the Institute of Chemical and Engineering Sciences under A\*STAR in Singapore; since 2018, he has been a full professor at Guangdong Technion Israel Institute of Technology (GTIIT).



**Ji Wang** Piezoelectric Device Laboratory, Ningbo University, Zhejiang, China

## An analysis of thermal effects on vibration frequency of a quartz crystal microbalance

A quartz crystal microbalance (QCM) is a high-precision gravimetric sensor for biological and chemical samples in research laboratories, hospitals, and industry. The accuracy of a QCM depends on the design of the quartz crystal resonator with the specially tailored electrode and affinity layer for the sensing function and the stability in operations. As a result, a careful and accurate analysis of the QCM structure with considerations of quartz crystal blank, electrodes, temperature, and sample characteristics is important in the evaluation of sample materials and configurations. Concerning these issues, there are some experimental studies on the material and structural parameters and frequency variations, and corresponding analyses are also made with simplified plate equations to ensure an analytical procedure to improve the design process. It is found that the approximate equation of plate vibrations is capable of accurate results in certain ranges of parameters, and the results are consistent with the finite element analysis. The refinement of the equation and techniques for the complication factors like electrodes, samples, and temperature will provide a more reliable procedure for the design and optimization of QCM with better precision. There will be detailed discussions on the analytical equations and comparisons of results from measurements with the consideration of temperature.

#### Audience Take Away Notes

- The thermal behavior of a quartz crystal microbalance is analyzed with plate equations
- Analytical results are consistent with measurement data
- Measurement of a QCM can be improved and calibrated systematically
- QCM design can be improved for better stability and accuracy
- Novel design of QCM is supported through the vibration analysis with thermal effects

#### Biography

Professor Ji Wang is the founding director of the Piezoelectric Device Laboratory, Ningbo University. Professor Ji Wang also held visiting positions at Chiba University, University of Nebraska-Lincoln, and Argonne National Laboratory. He received his PhD and Master degrees from Princeton University in 1996 and 1993 and a bachelor's degree from Gansu University of Technology in 1983. Professor Wang has been working on acoustic waves and high-frequency vibrations of elastic and piezoelectric solids for resonator design and analysis with several US and Chinese patents, over 200 journal papers, and frequently invited, keynote, and plenary presentations at major conferences around the world.





#### Md Nurul Islam Siddique<sup>1\*</sup>, Zaied bin Khalid<sup>2</sup>

<sup>1</sup>Faculty of Ocean Engineering technology & Informatics, University Malaysia Terengganu (UMT), 21030, Kuala Nerus, Terengganu, Malaysia

<sup>2</sup>Faculty of Engineering Technology University Malaysia Pahang 26300 Gambang Pahang Malaysia

#### Role of supplemented nutrients and intermediate temperature on biomethane generation from anaerobic digestion of agricultural waste: Feasibility & fertilizer recovery

The rise in demand for organisms pulled in by anaerobic digestion could be due to the simultaneous digestion of many substrates. The impact of supplements on the co-digestion of growth substrates was investigated in this study. In three phases, 37°C, 40°C, and 50°C, an extra improvement plan that anticipates a critical occupancy in anaerobic digestion was used. As a result of the changes, biogas output climbed to 1.38 times that of the control at 37°C. Furthermore, as a result of 40°C without additives, the excellent usage of this newly discovered mid-temperature considerably influenced an innovative philosophy (56 percent of VS end and 8.4 L-biogas). Biogas output surpassed 11.3 L with supplements during anaerobic co-digestion at 50°C, and mL-CH4/g-VS was 1.24 times that of the system without any extra improvement. The results reveal that at each temperature, the improved course of action promotes co-digestion. The most generally utilized temperature on the advanced scale was 37°C, which had the biggest influence on the utilization of improvements during the anaerobic process. Sludge was recovered at a rate of 0.09 m<sup>3</sup> sludge/m<sup>3</sup> substrate from the digester, while water was recovered at a rate of 0.86 m3 sludge/m<sup>3</sup> substrate from the digester. The processed sludge may be utilized as compost, and the water can be used to water plants. The time it took to recoup the investment was found to be 3.77 years. As a result, it may be inferred that the current research might soon be recognized as a potential green solution for trash management across the world.

#### Biography

Dr. Md Nurul Islam Siddique studied Civil Engineering at the Khulna University of Engineering & Technology, Bangladesh, and graduated as MS in 2012 from University Malaysia Pahang. He then joined the research group of Prof. Zularisam at the Institute of University Malaysia Pahang. He received her Ph.D. degree in 2015 at the same institution. After that, he obtained the position of Assistant Professor at the University Malaysia Pahang. He has published more than 40 research articles in ISI journals.



## Zibo Zhao<sup>1\*</sup>, Jiamei Quan<sup>1</sup>, RongRong Yin<sup>2</sup>, Ximei Yang<sup>1</sup>, G. Barratt Park<sup>3</sup>, Alec Wodtke<sup>1</sup>,Hua Guo<sup>2</sup>

<sup>1</sup>Max Planck Institute for Multidisciplinary Sciences <sup>2</sup>Department of Chemistry and Chemical Biology, University of New Mexico <sup>3</sup>Department of Chemistry and Biochemistry, Texas Tech University

#### Highly rotationally excited $N_2$ of $N_2O$ dissociation on Pd (110) surface

**T** o understand the energy transfer processes associated with chemical bond breaking and successive bond formation is essential to study the dynamics of surface reactions. Although the internal states measurements of desorption products deliver much dynamical information from the surface reactions, the mechanism underlying the energy partitioning in the reactions remains mostly unclear. In this study, we employ ion imaging methods to explore the quantum- state resolved dynamics of N<sub>2</sub>O decomposition on Pd (110). We find that N<sub>2</sub> directly desorbs with a narrow angular distribution from the decomposition of N<sub>2</sub>O adsorbed on bridge sites oriented along [001] azimuth of the surface. N<sub>2</sub> is highly rotationally excited up to J=50 (v=0) with a large mean translational energy of 0.62 eV. By combining with the density functional theory and ab initio molecular dynamics calculations, we estimated approximately 38%–76% of the energy released (1.5 eV) from the transition state is taken up by the internal and kinetic energies of the desorbing N<sub>2</sub>. The internal energy arises from a torque transition state and decoupled from translational energy. Applying the principle of detailed balance, we predict that rotational excitation and high incident kinetic energy of N<sub>2</sub> can effectively reduce the reaction barrier of N<sub>2</sub>O formation on palladium catalysis via Eley-Rideal mechanism.

#### Audience Take Away Notes

- Firstly, I will shortly introduce our experimental systems with ultra-high vacuum (UHV). We develop this system to allow a range of experiments of surface reactions and offer remarkable opportunities to advance our fundamental understanding of the dynamics and kinetics of heterogeneous catalysis. In the experiments, some reaction conditions, such as surface temperatures, the coverage of adatoms, and the energy of reactants can be well-controlled
- Secondly, we will show a sample study to reveal the energy transfer mechanism in the surfacereactions under the UHV conditions. In the practical catalytic reactions, due to the vast structural complexity of heterogeneous catalysts, it becomes possible if a well-definded modelcatalyst, such as a single crystal catalytic surface with atomic cleanness, is used. The experimental results of the surface reactions not only can set as a standard for the theoretical simulations, but also be useful for the understanding of the practical catalytic reactions
- Thirdly, the revealed dynamics of the surface reactions can be used to predict the reversed reaction on the basis of the principle detailed balance. Successful examples have been reported involving the activation of small molecule such as CO2. Inspired by this study, the mechanical activation of N2 would be great interest for the ammonia industry

#### Biography

Zibo Zhao studied Physical Chemistry at the University of Gottingen, Germany and graduated as Master in 2018. Now he is a PhD candidate in the Surface Dynamics Department led by Prof. Dr. Alec Wodtke at the Max Planck Institute for Multidisciplinary Sciences in Gottingen. His research focuses on the atomic scattering from surfaces and surface reactions.



#### Huiqin Li\*

College of Ecology and Environment, Inner Mogolia University, Hohhot, Inner Mongolia, China

## Preparation of catalyst with defective cerium-based structures and its application in vocs degradation

The effectively decontamination for atmosphere VOCs is getting more important whereas it is general facing the issues such as technical difficulties and high energy consumption. In this work, a Z-scheme Ag/Ag<sub>3</sub>PO<sub>4</sub>/CeO<sub>2</sub> heterojunction was prepared with a precipitation method and was applied to decompose gaseous benzene at very convenient ambient conditions. The prepared composite presents a 90.18% removal rate and 74.17% TOC efficiency within 3 h solar light irradiation at an initial 600 ppm benzene concentration. A photo-catalytic mechanism superimposed with solar light induced thermo-catalysis is proposed. Ag<sub>3</sub>PO<sub>4</sub> that has great solar light absorptive capacity is used as the photocatalytic component and CeO<sub>2</sub> is used as thermo-catalytic substrate due to its good thermo-conductivity in lower temperature. Ag0 produced from an in situ reduction of Ag<sub>3</sub>PO<sub>4</sub> is used as an electronic relay platform to form a Z-type heterojunction together with Ag<sub>3</sub>PO<sub>4</sub> and CeO<sub>2</sub>. Lots of vacancies of CeO<sub>2</sub> contribute to the enhanced pre-adsorption towards to VOCs. The assembled Z-scheme Ag/Ag<sub>3</sub>PO<sub>4</sub>/CeO<sub>2</sub> heterojunction is specially effectively for the separation of the photo-excited electrons and holes in space and maintains the highly redox potentials to decontaminate VOCs. Meanwhile, the composite is diverse, also having good oxidative power for HCHO, and thus could be a kind of promising material to purify VOCs in the convenient atmospheric environment.

#### Audience Take Away Notes

- A Z-scheme  $Ag/Ag_3PO_4/CeO_2$  heterojunction was prepared by a precipitation method
- Ag/Ag<sub>3</sub>PO<sub>4</sub>/CeO<sub>2</sub> presents high removal rate for gaseous benzene at ambient conditions
- A solar light-induced photo-thermal catalytic mechanism is proposed
- $Ag_3PO_4$  contribute to wide solar light harvesting and high oxidative ability
- CeO<sub>2</sub> is used as thermocatalytic substrate in low temperature driving by solar light

#### Biography

Dr. Huiqin Li studied Environmental Chemistry at the Inner Mongolia University, China and graduated as MS in 2013 at the North China Electric Power University. Before joined the Inner Mongolia University, she had worked in Environmental Science Academy of Inner Mongolia and Chinese Research Academy of Environmental Sciences, alternatively. She has published 14 research articles in SCI (E) journals.



Chi-Ping Li<sup>1\*</sup>, Bing Ze Li<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, National United University, Maioli, Taiwan

#### Tungsten trioxide cathode films for electro chromic devices

**T** emplate-assisted sol gel chemistry provides a versatile approach to introduce order and porosity into nanostructured materials. However conventional evaporation induced self-assembly techniques are not easily scaled to produce films with sufficient thickness over large areas at the throughput required by electrochromic windows. The principles of sol gel chemistry may be deployed using ultrasonic spray deposition (USD) for scalable syntheses of nanocrystalline WO<sub>3</sub> films with unrivalled electro chromic performance are demonstrated. Systematic manipulation of sol chemistry enabled the production of mesoporous films with high specific surface area (>100 m<sup>2</sup>/g), mean pore sizes of ~5 nm, and narrow pore size distributions. Film thickness is found to be proportional to the sol concentration and number of spray passes, and various combinations are shown to produce films capable of modulating >98% of incident solar radiation in the visible spectrum (450–900 nm). Elimination of haze enables full transmission in the bleached state, while the broadband coloration is attributed to the exceptionally high charge density (>120 mC/cm<sup>2</sup>). The materials have good switching speeds which improve with specific surface area, and the long term durability is promising.

#### Audience Take Away Notes

- The audience will be able to use what they learn to improve the performance of the materials
- This research will help the audience to design a material that exhibits higher charge density of opt electrochemical device
- This research can provide a practical solution to enhance the specific surface area of a material

#### Biography

Dr. Chi-Ping Li received his PhD of Materials Science from Colorado School of Mines (USA) in 2014 and followed by postdoctoral research in National Renewable Energy Laboratory (NREL, USA) in 2015. He joined Department of Chemical Engineering in National United University in Taiwan as an assistant professor in 2018. His research interests are mainly focused on synthesis of nanostructured films, nanocomposite films and nanoparticles. Those materials are used in electrochromic windows, lithium batteries, organic photovoltaics and LED encapsulants. His goal is to overcome the challenges and produce great but low cost materials in the fields of green and renewable energy.



**Vinod Agnihotr\*, Prof Dr A. Seetharaman, Dr S. Ranganathan** SP Jain School of Global Management, Australia

#### E-commerce adoption in B2B specialty chemical industry

E-commerce as a path breaking disruptive innovation of recent times, offers general businesses, a high level of customer satisfaction delivering noticeable cost benefits. Since the inception of E-commerce concept, we have been experiencing its exponential momentum in every corner of business. In fact, the significance of this concept is further recognized these days while experiencing the disruptions in global trade environment under the lock down scenarios in the ongoing Covid-19 pandemic.

The Specialty Chemical Industry deals with chemicals that have an impact on some industrial chemical processes and final products, including those for our most fundamental requirements such as food and pharmaceuticals; it would be practically impossible to survive and thrive without this industry's products and services. It has been observed that, despite many growth stories, this industry is trailing to follow latest technological suit versus peers. Challenges like fading innovation, evolving regulatory landscape, sustainability, rapid digitalisation under Industry 4.0 and dynamic geo-political developments instigating trade barriers disrupting feedstock supplies are affecting this industry significantly. Such challenging situations do instigate a need for conducting business research around connecting topics, one of them being looking at a business model of E-commerce, to address and possibly mitigate some of such challenges.

This exploratory study has been intended to run across South Asia and Southeast Asia cross-sectionally in the B2B Specialty Chemical Industry, and it is currently in the stage of quantitative assessment of the derived conceptual framework. This study was designed to run across South Asia and Southeast Asia. At this stage, I would like to share the background and significance of my research, as well as the literature review that was involved in arriving at my conceptual framework and leading to related research questions and hypotheses. In addition, I would like to provide some additional information regarding the research methodology that was adopted for the study. I will briefly describe the sampling strategy used for the pre-testing of the survey instrument and the pilot study, as well as the preliminary findings of the study. Finally, I'd like to outline the steps I intend to take to conduct my intended large-scale study, which includes gathering the necessary data and analysing it with a predetermined statistical tool to verify my research hypotheses derive outcomes, identify limitations, and define scope for further research.

#### Audience Take Away Notes

- Insight into the possible enablers/barriers to E-commerce adoption in the specialty chemical sector will be shared with the audience
- A portion of the audience may be influenced to become a catalyst for the spread of the idea within their own professional and business network (WOM)
- As such, this empirical research study is a formal attempt to explain the process driving E-com adoption in the B2B specialty chemical industry, and it is anticipated that this work may contribute to the body of knowledge in both, the academic and practical sectors
- The findings of this research in future may be useful in the education and training programs in relevant schools

#### Biography

Vinod Agnihotri graduated in Chemistry from Bombay University, India in 1993. Subsequently, he earned another graduation in Fiber Technology and Textile Chemistry from the Institute of Chemical Technology, Bombay University in 1996. In 1998, while working, he also earned a Master Diploma in Business Administration from Symbiosis, Pune (distance learning). After gaining valuable professional experience in operations, sales, marketing, business development, product management, and international business while working for several local and global specialty chemical companies, he has been actively serving the industry for the past 27 years. Currently, he serves as the Managing Director and Vice President of LANXESS Pte Ltd., Singapore (German MNC).



**Mamulaishvili** Associated Professor of Batumi Shota Rustaveli State University, Georgia

#### Thermolysis of petroleum oil and solubility of deposits

The article discusses the process of formation of deposits in the pipelines of the engine oil system and the factors affecting the conditions for their formation. The technological process of oxidation and the criteria for indicator parameters characterizing the thermolysis of used oil are shown. An extractive method is proposed that ensures the removal of deposits from the pipeline using special flushing process fluids based on regenerated petroleum oil.

To search for cheap and efficient hydrocarbon raw materials, regenerated petroleum oils were chosen from among the renewable resources of oil refining. The proposed process fluid was prepared on the basis of low-viscosity spent and then purified petroleum oil. The viscosity of the petroleum oil was adjusted with the addition of petroleum kerosene or diesel. Diluted surfactant solutions were used as additives. and detergent additive (alkali metal salts). It was revealed that in the oil system of an automobile engine at high temperatures (200-350 °C) oil thermolysis occurs, and the resulting deposits contain asphaltenes, carbons and carboids. The efficiency of dissolution of deposits in the mixture under study at low temperatures and the concentration of surfactants were revealed. The dependence of the interfacial tension on the concentration of various surfactants is shown. The limiting amounts of the content of the constituent components are found and the ratio of oily extract, from deposits of oxidized oil, is selected.

As a result of the tests, it was found that the washing liquid reduces the interfacial tension between the surface of the pipes and deposits and leads to an increase in the movement of the liquid. It has been established that the process of washing off deposits depends on the composition of the deposits, as well as on the composition of the oily extract. The optimal mode and prescription composition of the flushing liquid has been selected. The efficiency of washing off the studied liquid with other means is shown, while it should be noted that this liquid has a simple component composition and is much cheaper than other means.

**Keywords:** Oil Thermolysis; Deposits of Oxidized Oil; Regenerated Petroleum Oil; Interfacial Tension; Oily Extract; Surfactant

#### Biography

Nora Mamulaishvili is an Associated Professor in Batumi Shota Rustaveli State University, Georgia. She has developed several scientific projects and has supervised master's work. She has also participated in the creation of educational programs. She is the author of two monographs, a textbook (manual), three patents and 45 scientific works.



Zaur Berishvili\*, Marina Kipiani LEPL Institute Optica, Tbilisi, Georgia

#### Development and research of an innovative magnetron ion-plasma electrodispersion reactor for the fields of catalysis, chemical engineering and technology

T he work is dedicated to the development of an innovative construction of a magnetron ion-plasma electro dispersion reactor based on a planar-rotational magnetron sputtering device with improved capabilities in the direction of synthesizing catalysts, as well as general chemical engineering and technology, and its use in laboratory research.

For the synthesis of modern catalysts, the use of physical methods, in particular, the magnetron sputtering method, is very limited, since in the process of formation of nanoparticles on the coating, coagulation processes are observed and, as a result, a high probability of cluster formation, which prevents and makes it impossible to synthesize flat catalytic coatings on the entire surface of the samples. The magnetron sputtering method has certain advantages compared to chemical and other existing methods. The advantages of the innovative planar-rotational magnetron developed by us are as follows: it is compact; The flow of the cooling liquid not only provides effective cooling of the sputtering target and the cathode node as a whole but at the same time it is used for the rotation of the magnetic block; Has a high rate of use of target material; It is distinguished by a uniform erosion zone of the disk target; The stability of the plasma is ensured by the arrangement of permanent magnets along the involute circle in the rotating magnetic block and as a result, the creation of a closed magnetic field of a complex configuration; Are controllable technological parameters: the configuration of the magnetic field on the surface of the disk target, the frequency of rotation of the magnetic block and the distribution of the density of the discharge currents. We are introduced to the ion-plasma electro dispersion reactor created on the basis of the mentioned innovative, planar-rotational magnetron.

The method of forming nanomaterials in the process of sputtering the target material includes the formation of a flow of macro droplets in the active zone of erosion and their cascade division in the region of a toroidal shape magnetron plasma. The formation and electro dispersion of macro droplets occur under the action of intense ion bombardment between the inputs and outputs of the magnetic field lines in a closed circuit. The sputtered atoms and molecules of the target material freely pass through the toroidal shape plasma, and macro droplets from the target material in the plasma volume are recharged. Further, as a result of the development of the process of Rayleigh or capillary instability in plasma, they undergo cascade fission. The process of cooling and solidification of nanoparticles occurs outside the plasma region in the vacuum space between the target surface and the substrate holder. Due to the fact that the formed nanoparticles have the same charge, they are not attracted to each other and this eliminates the risk of increasing the size of nanoparticles due to maturation or agglomeration by Oswald. Rapid cooling of monodisperse nanoparticles formed in vacuum space and on the substrate, surface contributes to the save of their spherical shape, amorphous structure, and size of 2–4 nm. Obtaining a coating with an amorphous structure composed of individual spherical nanoparticles on the samples can be realized by maintaining the temperature of the

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nanoparticles formed as a result of cascade decomposition at such a level that ensures the conditions for the formation of Van Der Waals or metallic bonds.

#### Biography

Dr. Zaur Berishvili studied physics at Tbilisi State University Iv. Javakhishvili and received a diploma in radio physics and electronics in 1966. In the same year, he began working at the Research Institute of Semiconductor Devices, as an engineer, then as a leading engineer. He then joined the research group of Prof. Svechnikov at the Institute of Semiconductors of the Academy of Sciences of the Ukrainian SSR. In 1984, he received his Ph.D. He has published over 40 scientific articles in SCI (E) journals.



#### Yaddanapudi Varun<sup>1\*</sup>, I. Sreedhar<sup>2</sup>, Satyapaul A. Singh<sup>3</sup>

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Kapra Mandal, Hyderabad-500 078, India

## Role of ni, la impregnation and substitution in $\text{Co}_3\text{O}_4\text{-}\text{Zro}_2$ catalysts for catalytic hydrogen combustion

Ni and La were substituted and impregnated on  $\text{Co}_3\text{O}_4$ -Zr $\text{O}_2$  (CZ) nanocomposites by solution combustion and wetness impregnation methods for catalytic hydrogen combustion. In this study, our focus is to understand the role of active metals and their interactions with the support CZ in facilitating high oxidation rates. All the impregnated and substituted catalysts showed 100% conversion below 350°C. The hydrogen combustion is noticeable even at 200°C due to the activation of hydrogen and oxygen on the active sites. The Ni and La substituted with CZ catalysts showed better catalytic activity than the impregnated catalysts. To explore the mechanistic features and structure-property relations, X-ray photoelectron spectroscopy and TPR studies were carried out for substituted and impregnated catalysts. The regeneration ability was found with the Ni and La substituted catalysts and the redox coupling between Co and La/Ni indicated the possibility of a dual site redox mechanism. Overall, the lattice substitution is found to be desirable and offered high performance for catalytic H<sub>2</sub> combustion.

**Keywords:** H<sub>2</sub> Combustion; H<sub>2</sub>-TPR; Regeneration Ability; Reaction Pathway; Porous Network Structures; La Substitution.

#### Audience Take Away Notes

- This presentation helps in understanding the importance of  $\rm H_{2}$  safety majorly in nuclear power plants and fuel cells
- Mainly the people associated with designing and synthesis of new catalysts will help in understanding the importance of this work
- This presentation will give some idea about future development of H<sub>2</sub> safety applications.
- Catalyst regeneration ability and redox couple mechanism

#### Biography

On the surface, Yaddanapudi Varun is a successful chemical engineer who attended MVGR College of engineering in AP from 2009 to 2013 and graduated with a degree in 2013. In the academic year 2013–2015, he attended the JNTU Hyderabad department of chemical technology to get his master's degree in that field. He worked at the CSIR-IICT as a project assistant on a prominent project known as the Indo-US in developing second-generation fuel ethanol. Varun has been able to publish his works in journals that have a high degree of influence, such as the International Journal of Hydrogen Energy, Catalysis Science & Technology and Journal of Environmental Chemical Engineering.



**Shalini Arora\*, Sri Sivakumar** Department of Chemical Engineering, IIT Kanpur, Kanpur, U.P, India

#### One pot synthesis of ultra-small nimo catalysts supported on amorphous alumina with enhanced type 2 sites for hydrodesulfurization reaction: A combined experimental and theoretical study

he deep removal of high molecular weight sulphur compounds (e.g., 4, 6, dimethyl dibenzothiophene) L is challenging due to their steric hindrance. Hydrogenation desulfurization (HYD) pathway is the main pathway to remove these sulfur compounds and it is mainly governed by the number of type 2 sites. The formation of type 2 sites can be enhanced by modulating the pore structure and the interaction between the active metal and support. To this end, we report the enhanced HDS catalytic activity of ultrasmall NiMo supported on amorphous alumina  $(A-Al_2O_3)$  catalysts by one pot colloidal synthesis method followed by calcination and sulfidation. The amorphous alumina (A-Al<sub>2</sub>O<sub>2</sub>) was chosen as the support due to its lower surface energy, better physicochemical properties and enhanced acidic sites (due to the dominance of tetra and penta coordinated [Al] sites) than crystalline alumina phase. At 20% metal oxide composition, NiMo supported on A-Al<sub>2</sub>O<sub>3</sub> catalyst showed 1.4 and 1.2 times more reaction rate constant and turn over frequency (TOF) respectively than the conventional catalyst (wet impregnated NiMo catalysts) for HDS reaction of dibenzothiophene reactant molecule. A-Al<sub>2</sub>O<sub>3</sub> supported catalysts represented enhanced type 2 sites formation (because this catalyst possesses higher sulfidation degree (80%) and NiMoS sites (19.3 x 1017 sites/mg) with desired optimum stacking degree (2.5) than wet impregnated catalyst at same metal oxide composition 20%) along with higher active metal dispersion, Mo edge site fraction. The experimental observations were also supported by DFT simulations. Lower heat of adsorption (< 4.2 ev for MoS<sub>2</sub> interaction and < 3.15 ev for Ni doped MoS<sub>2</sub> interaction) values for A-Al<sub>2</sub>O<sub>3</sub> confirmed the presence of weaker metalsupport interaction in A-Al<sub>2</sub>O<sub>3</sub> in contrast to crystalline  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. The weak metal-support interaction for prepared catalysts clearly suggests the higher formation of type 2 sites which leads to higher catalytic activity for HDS reaction.

Keywords: Amorphous Alumina; Colloidal; Desulfurization; Metal-support Interaction

#### Audience Take Away Notes

- As described,  $A-Al_2O_3$  is a better catalytic support than  $\gamma-Al_2O_3$  so it can be used as a support for other heterogeneous catalysts
- The developed approach has drastically improved the sulfur removal from petroleum feedstocks
- The catalyst preparation method is just a one step process that make it easy to handle and increases the reproducibility

#### Biography

Shalini Arora studied at IIT BHU, Varanasi and graduated as M. Tech in 2016. She then joined her PhD in the nanotechnology and catalysis group of Prof. Sri Sivakumar at IIT Kanpur. She has filed an Indian patent based on her PhD thesis work and published articles in reputed journals.



#### Noorin Fatima<sup>\*</sup>, Sadam Ilaiah, Ginuga Prabhaker Reddy

Dept. of Chemical Eng., Univ. College of Technology., Osmania University, Hyderabad (TS), India

## Experimental studies on control of a two tank non-interacting liquid level system using internal model based PID controller

The flow and level control system play very important role in a Chemical Industry to achieve important objectives. The higher order processes tend to show unstable behavior and an advanced control system is required for such processes to meet set point tracking and disturbance rejection. In the present work, it is proposed to design an advanced control system such as internal model control based PID control for two tank non- interacting liquid level process. Real-time step test has been conducted for identification of the two tank non interacting liquid level process. The process has been identified as the first-order with dead time transfer function model. Based on above transfer function model, the IMC-PID controller has been designed. Experimental study shows that the IMC-based PID Controller results in superior performance with lesser overshoot and lesser settling time than conventional PID controller in case of set point tracking. Tuning factor (n) for IMC-PID is selected as 0.5 for best performance. Actual parameters of IMC-PID are selected as 40% of designed parameters by a trial and error method.

#### Biography

Noorin Fatima studied BTech. And M.Tech. In Chemical Engineering from University college of Technology, Osmania University, Hyderabad, India. Her research interests are in advanced control techniques such as Internal Model based control, Fuzzy logic control and Artificial Neural Network control. Her personal hobbies are reading and singing.





**Dr. Ashanendu Mandal** Energy Expertise and International Speaker University of Calcutta, India

## Removal of phenol from wastewater using biological and industrial wastes as adsorbents

This research aims for adsorptive removal of phenol from wastewater by solid materials generated L from biological wastes viz. guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and industrial wastes viz. rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina. The adsorbents are characterized by SEM, XRD, FTIR and BET analyzers. The experiments of phenol removal are carried out with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum removal obtained is 97.50%. The kinetics shows that the pseudo-second order model is best fitted for all adsorbents except red mud. The kinetic modeling's show that the adsorption mechanism is supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggests that Freundlich isotherm model is best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm are best supportive for rice husk ash and clarified sludge respectively. The thermodynamics shows the spontaneity, randomness and endothermic/exothermic nature of the adsorption processes. The ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient establishes that the experimental and predictive data are within allowable range. The scale-up designs are performed for their commercial applications. The regeneration and the safe disposal of used adsorbents are also studied for checking their wider industrial applicability.

#### Biography

Ashanendu Mandal has worked in ONGC for more than 34 years in offshore and onshore oilfields. He is graduated as B. SC (Chemistry) and B. Tech (Chemical Engineering) from University of Calcutta and post-graduated as M. Tech in Chemical Engineering from IIT, Kharagpur and MBA in Finance from IGNOU, New Delhi. He is the lifetime professional member of Indian Chemical Society and Indian Science Congress. He is now doing research in University of Calcutta. He has been recognized with the Best Researcher Award 2020 by VD Good International Professional Association. He has participated in many international conferences in more than 25 countries as invited speaker, panelist, roundtable moderator and session chairman.



**Dr P K Dash** Department of Aeronautical Engineering, NMIT, Bangalore, Karnataka, India

#### Roll of catalyst in space propulsion system

The space propulsion becomes more challengeable in current era of 21st Century. Lot of developments is happening to overcome the required speed and stability in this domain. But it is still going research for achieving the goal.

In 20th Century, the scientific community and engineers are able to achieve the target for exploring the space. For that, they used the chemical energy as the source from six different natural energies, and segregated the chemical energy in its physical form to rocket technology like Solid propulsion, Liquid propulsion, and hybrid propulsion. Their specific interests are concentrated to specific impulse, thrust etc. In this context they searched for faster burning rate and high-density exhaust gas using Newton's third law. To obtain that, they tried with several high energetic materials and various chemical compositions to be combust faster. Also, they tried with chemical catalysts and intermediate phases like Gel for higher volumetric loading.

Thus, catalyst played a major role in enhancement of the performance of propulsion system. Here they tried with different form of catalysts like homogeneous, heterogeneous (solid), heterogenized homogeneous catalyst and biocatalysts. In this presentation, the function of catalyst on achieving higher combustion and propulsion will be discussed with some examples. It will describe the selection process, roll and efficiency of using catalyst with combustion. Also the nano form of catalyst effect will be discussed for solid, liquid and hybrid propulsion systems. Also, emphasis will be given on role of catalyst in future propulsion system.

#### Audience Take Away Notes

- This present will give the past, present and future thoughts in space propulsion
- Especially the people associated with space technology and designing the future spacevehicles will look into the parametric benefit in using Catalysts
- This presentation will give some idea about future development of propulsion technologywhich is a major technology in current and future centuries
- It will give some new design concepts
- It will help in space related activities

#### Biography

Dr. P. K. Dash is the Professor and Head of the Department of Aeronautical Engineering, NMIT, and Bangalore, India. In addition to his administrative experience, he has held positions such as Dean, Principal, Director of Research, and Head of Department for over 30 years. He has several academic and research achievements to his credit. He has carried out number of funded research projects, guided more than 100 students both from UG, PG, and Ph. D. studies. In addition to winning best researcher awards, he has also been a recipient of numerous research paper awards. Additionally, he served as a panelist at international and national conferences. He is associated with number of National and International societies like AIAA, ERPS, and ASME etc. and served for national and international committees. As he relates to aerospace engineering, he is keen on innovating engineering disciplines in all dimensions with a view to developing a good pool of aerospace professionals for the future.



**Suman Dutta<sup>1</sup>\*, D.N.V.V. Konda Lutukurthi<sup>2</sup>** Department of Chemical Engineering, Indian Institute of Technology (ISM), Dhanbad, Jharkhand, India

## Synthesis of Zno via solution combustion method; Study the effect of ignition temperature and fuel quantity

Tinc oxide (ZnO) nanoparticle photocatalyst has been synthesized by solution combustion method Lusing zinc nitrate as the oxidizer and urea as the fuel. The effect of fuel-to-oxidizer ratio and ignition temperature on the properties of synthesized catalysts have been studied. The fuel-oxidant ratio is an important factor during the synthesis because powders with a variable degree of crystallinity and different morphologies were obtained at the fuel-lean and the fuel-rich combustion conditions. Pyramid shape morphology changed to sheet-like morphology with an increase in fuel content. Conversely, reducing the fuel content to the fuel-lean condition has resulted in powders with less surface area, improved crystallinity, and decreased bandgap energy. Properties such as crystallinity, morphology, surface area, and optical properties have been investigated by thermal analysis, X-ray diffraction (XRD), Scanning electron microscopy (SEM), Diffuse reflectance UV-Visible spectra, and Photoluminescence analyses. Ignition temperature is also crucial because it could fix the rate of heating of the precursor mixture. The Samples synthesized at an ignition temperature of 500°C have shown better photocatalytic activity for both the fuel-lean and fuel-rich conditions. Besides the ignition temperature, ignition time is also an important and optimizable variable as it influences the crystallinity and surface area of the synthesized powders. The degradation of an azo dye at ambient temperature (25±2°C) and solution pH was conducted to evaluate the photocatalytic activity of the synthesized materials. The photocatalysts prepared at fuel-rich conditions show higher photocatalytic dye degradation capability as they have a small crystallite size and more surface area. This study shows that the powder catalyst synthesized at the fuel-oxidant ratio of 1.8 and the ignition temperature of 400°C have the maximum percentage (99%) of dye degradation in 180 min. The photocatalytic (fuel-oxidant ratio of 1.8) dye degradation follows the pseudo-first order kinetic with a rate constant of 0.0253 min-1, which is 3.14 and 2.88 times higher than that of samples synthesized at fuel-oxidant ratios of 0.6 and 1. The outcomes of the present study help to design more pronounced experiments for the synthesis of photocatalysts by varying fuel amounts and ignition temperatures.

#### Audience Take Away Notes

- Knowledge of ZnO synthesis via solution combustion method
- Effect of various factors such as fuel-to-oxidizer ratio, ignition temperature, ignition time
- Details characterization of synthesized catalyst using SEM, XRD, etc
- Application of ZnO catalyst for dye degradation and other environmental pollution reduction

#### Biography

Dr. Suman Dutta is an Associate Professor in the Department of Chemical Engineering, Indian Institute of Technology (ISM) Dhanbad, India. He received his Ph.D. from Jadavpur University, Kolkata, India in 2011. Major research areas are production of renewable energy, photocatalysis, and membrane technology. He has authored one book Optimization in Chemical Engineering and edited two books Sustainable Fuel Technologies Handbook and Membranes with Functionalized Nanomaterials: Current & Emerging Research Trends in Membrane Technology. He also published almost 50 articles in reputed journals and 10 book chapters in various edited books.



#### H. Christian Schewe<sup>1\*,2</sup>, Bruno Credidio<sup>3</sup>, Aaron M. Ghrist<sup>1,4</sup>, Sebastian Malerz<sup>1</sup>, Christian Ozga<sup>5</sup>, Andre Knie<sup>5</sup>, Henrik Haak<sup>1</sup>, Gerard Meijer<sup>1</sup>, Bernd Winter<sup>1</sup>, Andreas Osterwalder<sup>3</sup>

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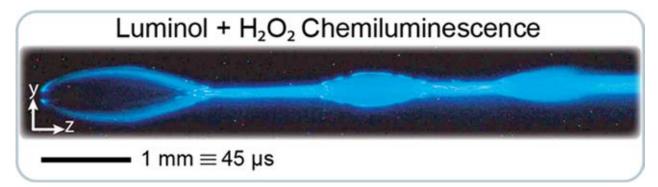
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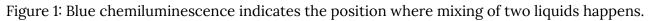
<sup>4</sup>Department of Chemistry, University of Southern California, Los Angeles, California 90089-0482, United States

<sup>5</sup>Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

#### Imaging of chemical kinetics at the water-water interface in a freeflowing liquid flat-jet

Two cylindrical liquid microjets are set up in a colliding geometry to generate a planar leaf-shaped flowing sheet. Using jets with two different aqueous solutions, each containing a reactant for a fast chemiluminescence reaction, we image the emitted photons to spatially visualize the mixing of the solutions at any position of the leaf – see Figure 1. We observe that under laminar flow conditions mixing in the first leaf happens differently compared to all consecutive leafs since the first leaf remains dark while all consecutive leafs show a homogeneous chemiluminescence glow. In the first leaf no turbulent mixing takes place in the planar region. Instead diffusion across the planar liquid-liquid interface leads to mixing of chemical species from the two solutions, also leading to chemical reactions and their chemiluminescence detection. We exploit this micrometer-thin flowing two solution structure for spectroscopic and kinetic studies at the liquid-liquid interface. We present a quantitative model that describes diffusion-limited reaction kinetics at the liquid-liquid interface, which can also be extended to account for interactions at the liquid-vapour interface. I will conclude with an overview of the current ongoing research.





#### Audience Take Away Notes

- Micrometer thin liquid sheets which they could adopt to their purposes. In fact flat-jets have started to be employed in numerous experiments such as collision studies, high-harmonic generation of light and to study chemical reactions. The audience will also learn how we made use of the unexpected flow dynamics and mixing properties of these flat-jets and how they allow the possibility to study diffusion limited kinetics given our special case of a very fast chemiluminescence reaction
- I will show the audience in the fluid dynamics session how we imaged the turbulent and diffusive mixing dynamics using a fast chemical reaction something that be used in many other hydrodynamic applications or setups. Furthermore, it should be helpful to see and to discuss how the model to describe diffusion controlled kinetics can also be adapted to other systems
- This research connects the fields of hydrodynamics, especially the mixing dynamics within laminar flow, chemical reactivity and chemiluminescence, and reaction kinetics
- Typical leaf surface dimensions are 1.5 mm  $\times$  0.5 mm with flow velocities of a few 10 m/s corresponding to a flow time through the first leaf of around 50–100 µs. This covers a time scale for chemical kinetics that is currently difficult to access by other methods. Indeed, conventional stopped-flow techniques are best suited for studies on time scales around a millisecond, while laser-induced techniques work best on faster time scales
- The flat-jets free flow through air or vacuum permits unobstructed optical access to the liquid and thus enables a wide range of spectroscopic detection i.e. photo- electrons that are incompatible with many solid container materials

#### Biography

Dr. Schewe studied Physics at the Free University Berlin, Germany and graduated as MS in 2009. He then joined the research group of Prof. dr. Gerard Meijer at the Fritz-Haber Institute of the Max-Planck society. He received his PhD in 2015. After a short period as risk-analyst at an insurance company he is currently a postdoctoral fellow at the Institute of Organic Chemistry and Biology (IOCB) and the J. Heyrovsky Institute of the Czech Academy of Science in Prague, Czech Republic.





#### Ieva Gaide<sup>1\*</sup>, Violeta Makareviciene<sup>2</sup>

<sup>1</sup>Department of Environment and Ecology, Faculty of Forest Science and Ecology, Vytautas Magnus University Agriculture Academy, Kaunas, Lithuania

<sup>2</sup>Department of Environment and Ecology, Faculty of Forest Science and Ecology, Vytautas Magnus University Agriculture Academy, Kaunas, Lithuania

#### Snail shells as a heterogeneous catalyst for biodiesel synthesis

The world is going through an energy crisis related to the transition to a wider use of renewable energy - resources. Due to climate changes, greenhouse gas emissions and fossil fuel depletion, the energy situation is not stable. There are also problems with obtaining oil due to the war in Ukraine. More and more legislations and concern about global warming and energy security encourage to pay huge attention to renewable energy sources. Renewable energy resources have influence energy security insurance and sustainable development. There are a lot of studies related with conventional biofuel production technologies by applying transesterification process of oil using alcohol and catalyst. Heterogeneous catalysis has the advantage of easy separation of catalyst from the final product. Snail shells are a waste which is composed mainly of calcium compounds. Using calcination process calcium compounds can be converted to calcium oxide (CaO) which is known as a good catalyst used in heterogeneous biodiesel synthesis. In the present work, we investigated optimum conditions for biodiesel synthesis from rapeseed oil and methanol using snail shells as a heterogeneous catalyst. Firstly optimum conditions for catalyst preparation was studied. Optimum catalyst fraction size was obtained 0.315-0.1 mm and calcination temperature 850°C was used to convert CaCO<sub>3</sub> to CaO, content of oxides in snail shells were investigated. It was obtained that calcinated snail shells which we used for rapeseed oil transesterification contained 91.69% of CaO. Transesterification tests were conducted in a conical flask, condenser, a thermometer with a temperature controller and a mixer (at a constant mixing speed of 350 min-1) were used. Response surface methodology central composite design (CCD) was employed to determine the optimal reaction conditions. The optimum conditions of transesterification process were obtained: the catalyst amount - 6.06 wt%, the molar ratio of methanol to oil – 7.51:1, the reaction duration – 7.99 hours and the reaction temperature – 64°C. The ester yield obtained was 98.15%. Our findings indicate the potential of snail shells as a heterogeneous catalyst for biodiesel production with methanol.

#### Audience Take Away Notes

- The research is related to the use of heterogeneous catalysts in biodiesel synthesis. After listening to the presentation, participants will know that materials rich in calcium can be used as catalysts in biodiesel synthesis
- They will be able to independently select such catalysts
- They will also learn the method of preparation of these catalysts for transesterificationreactions
- Conference participants will be introduced to biodiesel production and analysis methods, which could be useful in their work

#### Biography

Ieva Gaide is a third year PhD student (Environmental Engineering) in Vytautas Magnus University Agriculture Academy, Institute of Environment and Ecology, Faculty of Forest Science and Ecology. Her field of study is related to the heterogeneous synthesis of biodiesel using natural heterogeneous catalysts, for example, snail shells, dolomite, eggshells.





#### Hasan Saygili<sup>1\*</sup>, Gulbahar Akkaya Saygili<sup>2</sup>

<sup>1</sup>Vocational School of Technical Sciences, Department of Chemistry and Chemical Process Technology, Batman University, 72100 Batman, Turkey <sup>2</sup>Department of Science, Faculty of Education, Dicle University, 21280 Diyarbakır, Turkey

## An investigation on adsorption of heavy metal with hydro char developed from industrial waste: Kinetics, mechanisms, and desorption

As a result of the rapid development of the industry, heavy metal pollution of water environments is a very serious problem. Removal of heavy metal ions and derivatives from the environment has become a priority in order to preserve the quality of the ecosystem. Adsorption is an effective method that can be used to reduce the levels of heavy metals in wastewater. The motive of this work is to synthesis hydrochar from industrial processing waste (pomegranate bagasse (PB)) by a hydrothermal carbonization (HTC) process and the prepared hydrochar (PBHC) is been used as an effective functionalized sorbent for the removal of heavy metal ion (copper (Cu (II))) from simulated contaminated water in a batch mode. The adsorption kinetics was investigated at different initial concentrations (50 and 100 ppm) and times (3-300 min). Two different kinetic models were used to analyze the experimental copper adsorption kinetic data. Among the tested various models, the pseudo-second-order kinetic model provided the best simulation to the kinetic data of hydrochar with R2 of being 0.98. The results show surface complexation of -OH and -COOH groups with Cu (II) ions played an important role on the adsorption mechanism of Cu (II) on the above-mentioned sorbent. Desorption of Cu(II) from Cu(II) loaded sorbent was investigated with 0.1 M HCl at 298 K for 2 h. Overall, the results demonstrated that industrial processing waste are promising feedstock to be made into hydrochar for treatment of wastewater contaminated by Cu (II) and heavy metal.

#### Audience Take Away Notes

- Utilization of pomegranate bagasse (PB) via HTC was explored
- Prepared hydro char (PBHC) was examined as Cu(II) sorbent
- The adsorption kinetics performance of the hydrochar for Cu(II) was investigated
- Surface complication is played a major role in Cu(II) binding using PBHC
- Pomegranate bagasse hydrochar (PBHC) could be considered as a promising sorbent to remove heavy metals from the aqueous medium

#### Biography

Dr. Hasan SAYGILI is currently working as an Assoc.Prof. In the Chemistry and Chemical Process Technology Department, Vocational School of Technical Sciences, Batman University, Turkey. He has an experience in the field of carbon-based materials for environmental applications. He holds a PhD in activated carbon production from bio wastes from Dicle University, Turkey. His primary research interests include carbon nanomaterials, waste minimization, environmental pollution, hydrothermal carbonization, and cleaner production technology and wastewater treatment. He has published 27 SCI papers.



Ashiff Khan<sup>1\*</sup>, A.Seetharaman<sup>2</sup>, Abhijit Dasgupta<sup>3</sup> <sup>1</sup>SP Jain School of Global Management, Saudi Arabia <sup>2</sup>SP Jain School of Global Management, Singapore <sup>3</sup>SP Jain School of Global Management, India

### Antecedents of the adoption of big data by the global chemical industry

The new era of big data is influencing the chemical industry tremendously, providing several opportunities to reshape its operations. However, given the development of big data, the availability of free software, and the large amount of real- time data generated and stored, the chemical industry is still not fully adopting big data. Moreover, the industry is just starting to realise the importance of the large amount of data it owns to assist in making the right decisions and support its strategies. Therefore, this article explores the significance and influence of identified gap variables, namely professional competencies, business intelligence, data scalability, process monitoring, and investment in tools, for the adoption of big data in the chemical industry. This study follows a survey-based quantitative method using structural equation modelling. The data collected was studied to draw scientific conclusions about the myriad of hypothesised relationships. This was accomplished by employing a positivist paradigm in the research process. This study recognises the strong relationship between data scalability, process monitoring, and the investment in tools for big data adoption as a contribution towards industry application and practice. Mediation effects between the constructs and final measures were studied as part of this research, and the significance of their relationships was established. This study contributes to the application of the Unified Theory of Acceptance and Use of Technology. Based on the literature survey and research outcomes, this study also positions the chemical industry in Davenport and Harris's paradigm of analytical maturity. This article's conclusions and contributions towards practical application are expected to support a shift from conventional methods towards a data-driven approach to decision-making in the chemical industry. To further achieve the objectives, conclusions, and future research directions presented in this article, suggest government, academia, and industry must work together to overcome all present and potential challenges.

#### Audience Take Away Notes

- Factors influencing big data adoption in industries
- Use of quantitative study in research outcomes
- Application and contribution to theory and practice
- Future research directions

#### Biography

Ashiff Khan is a Lead Engineer for Saudi Aramco, handling process engineering, projects and master plans. He has more than 20 yr of experience in the chemical industry, and has multiple patents in the U.S. In addition to multiple advanced degrees, post-graduate diplomas, international certifications, and doctorates, including an MS degree in data science from Liverpool John Moores University in the UK, Dr. Khan also conducts research in business management as part of his doctoral studies at the SP Jain School of Global Management in Australia.

DAY

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# 13-14

DAY 02 KEYNOTE FORUM

14<sup>TH</sup> EDITION OF GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

## Basic lattice reactions in memory behavior of shape memory alloys

**C** ome materials take place in class of smart materials with adaptive **O**properties and stimulus response to the external changes. Shape memory alloys take place in this group, by exhibiting shape reversibility and capacity of responding to changes in the environment. These alloys exhibit a peculiar property called shape memory effect. This phenomenon is initiated by thermomechanical treatments with cooling and deformation and performed thermally on heating and cooling. With this deformation, strain energy is stored in the materials, due to the plastic deformation and released on heating by recovering the original shape. Shape of the materials cycles between deformed and original shapes on cooling and heating after the first processes in reversible way in bulk lecel, and this behaviour can be called thermoelasticity. These alloys exhibit another property called superelasticity, which is performed mechanically with stressing and releasing at a constant temperature in parent phase region, and shape recovery occurs instantly upon releasing, by exhibiting elastic material behaviour. Stress-strain profile exhibits nonlinear behaviour and hysteresis loop refers to energy dissipation. Thermoelasticity is result of two crystallographic transformations, thermal and stress induced martensitic transformations. These transformations are governed by the basic lattice reactions, twinning and detwinning. Thermal induced martensitic transformation occurs on cooling with the cooperative movement of atoms in <110>-type directions on {110}-type planes of austenite matrix, by means of shearlike mechanism, along with lattice twinning, and ordered parent phase structures turn into twinned martensite structures. Twinned martensite structures turn into detwinned martensite structures by means of stress induced transformation by stressing material plastically in martensitic condition. Superelasticity is also result of stress induced martensitic transformation and ordered parent phase structures turn into the detwinned martensite structure with stressing in parent phase region. Copper based alloys exhibit this property in metastable phase region, which has bcc-based structures. Lattice invariant shears and lattice twinning are not uniform in these alloys, and cause to formation of the layered structures with martensitic transformation. The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the parent phase.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging time



#### **Osman Adiguzel**

Department of Physics, Firat University, Elazig, Turkey

#### Biography

Dr. Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and studied were focused on shape memory effect in shape memory alloys. His academic life started following graduation by attending an assistant to Dicle University in January 1975. He became professor in 1996 at Firat University in Turkey, and retired on November 28, 2019, due to the age limit of 67, following academic life of 45 years. He supervised 5 PhD- theses and 3 M. Sc- theses and published over 80 papers in international and national journals; He joined over 120 conferences and symposia in international level with contribution. He served the program chair or conference chair/co-chair in some of these activities. Also, he joined in last six years (2014 - 2019) over 60 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. Additionally, he joined over 70 online conferences in the same way in pandemic period of 2020-2021. Dr. Adiguzel served his directorate of Graduate School of Natural and



at room temperature, and this result refers to a new transformation in diffusive manner.

**Keywords:** Shape Memory Effect; Martensitic Transformation; Superelasticity; Thermoelasticity; Lattice Twinning and Detwinning

#### Audience Take Away Notes

- Shape memory phenomenon is a multidisciplinary subject and used in many fields from biomedical to building industry
- I will introduce the basic terms and definitions, by addressing to all at the conference from different disciplines, and listeners will gain knowledge in elementary level

Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data).

## Human nanomedicine: Catalysts for improving health in the clinic

Tanomaterials have been widely tested in vitro and in small order animal studies for decades. Results have shown greater tissue growth, decreased bacteria growth, and inhibited inflammation. However, few studies exist examining human tissue response to nanomaterials. This presentation presents a cohort study of nano implants inserted into humans. In particular, one study includes the implantation of nanotextured spinal implants into over 14,000 patients over the past 5 years. Results demonstrated no cases of infections or other implant failures which is significantly better than statistics on conventional spinal implants which have up to 20% failure rates. This study will further explain that nano implants mimic the natural nano texture of bone itself and possess surface energy that can competitively increase the adsorption of proteins known to promote osteoblast (bone forming cells) functions, decrease bacteria functions, and limit inflammatory cell functions. Further, this invited presentation will highlight the role that environmentally friendly catalysts are playing in fabricating improved nanoparticles for medical applications. As such, this presentation will cover the few human clinical studies on nano implants showing improved human health.

#### Audience Take Away Notes

- How nanomaterials are serving as catalysts to improve human health
- How nanomaterials are being synthesized with biofriendly catalysts
- The past, present, and future of nanomaterials in medicine



#### Thomas J. Webster

Interstellar Therapeutics, Boston, MA, USA

#### Biography

Thomas J. Webster's (H index: 114; Google Scholar) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). He has served as a professor at Purdue (2000-2005), Brown (2005-2012), and Northeastern (2012-2021; serving as Chemical Engineering Department Chair from 2012 -2019) Universities and has formed over a dozen companies who have numerous FDA approved medical products currently improving human health. He is currently helping those companies and serves as a professor at Hebei University of Technology, Saveetha University, Vellore Institute of Technology, UFPI, and others. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology); 2022, Best Materials Science Scientist by Citations (Research.com); and is a fellow of over 8 societies. Prof. Webster has over 1,350 publications to his credit with over 53,000 citations. He is a current nominee for the Nobel Prize in Chemistry (2023).

#### Distal functionalization via transition metal catalysis

Celective carbon-carbon and carbon-heteroatom bond formation **U**reactions are among the most important processes in organic chemistry since it enables the construction of common organic molecules from simple precursors. Among various methodologies, the transition metal-catalyzed transient directing group-enabled C-H functionalization process represents one of the most efficient and straightforward approaches due to the avoidance of pre-functionalization of the reaction precursors. In comparison with the well-established sp2 C-H functionalization process, much less progress has been made to the unactivated sp3 carbons with the transient directing group strategy. In view of the prevalent presence of sp3 C-H bonds in organic molecules, advances in this area will allow for broad applicability by providing a powerful and valuable synthetic approach to access common organic frameworks, such as (hetero)cycles, privileged structures in medicines. This area will be advanced further by the development of site- and enantio-selective functionalization of unactivated sp3 C-H bonds. Furthermore, demonstration of these transformations through different reaction pathways will provide a new opportunity for the design of novel transition metal-catalyzed coupling reactions on sp3 carbons. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C-H functionalization reaction.

#### Audience Take Away Notes

- This study could potentially be used for others to build small molecules in an efficient way
- This study could potentially be used for others to carry out latestage functionalization of natural products or drug molecules
- This research could also be used by others to expand their research



#### Haibo Ge

Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX, USA

#### Biography

Haibo Ge received his PhD degree in Medicinal Chemistry from The University of Kansas in 2006, and then moved to The Scripps Research Institute for postdoctoral study. In 2009, he began his independent academic career at the Indiana University - Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by his group is mainly focused on the development of novel methods for carbon-carbon and carbonheteroatom bond formation through transition metal catalyzed C-H functionalization.

#### Plastic Trash to Monomers and Intermediates - PTMI

**T**o address the issue of waste plastics in landfills, a hybrid approach L is proposed. This would use low temperature plasma pretreatment followed by catalytic cracking to augment the conversion of waste polyolefins into monomers, intermediates, new polymers and valueadded chemicals. Lightweight packaging (LWP) comprises about 50% of total plastics consumption and consists mainly of single and multilayer films and containers. LWP is heterogenous, contaminated and is difficult to recycle. Mechanical recycling is currently the only commercial approach to recycling but is inadequate to address the growing volume of packaging plastics and degrades or downcycles both polyethylene (PE) and polypropylene (PP). In contrast, feedstock recycling converts polymers to monomer feedstock that can be used to make new products that have virgin-like performance in high volume single use packaging applications, thereby creating new value chains for what is currently a waste stream. Current high TRL feedstock recycling technologies like pyrolysis and gasification are highly energy intensive, require multiple steps (plastics-syngas-methanol-olefins) and have low selectivity to polyolefin building blocks (ethylene, propylene). Alternatively, plastics upcycling aims at selectively deconstructing polymer in a one-step process directly into monomers and high value chemicals (HVC). Consequently, it is proposed to use a hybrid approach of preconditioning with a low temperature plasma followed by catalytic cracking for conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. This offers improvement in carbon utilization, cumulative energy demand and selectivity to recycled high value products over current benchmark feedstock recycling processes like gasification and pyrolysis. It is suggested to use LTP treatment as a tunable polyolefin functionalization step to increase selectivity of subsequent catalytic deconstruction and reconstruction. The target waste stream is post-industrial and post-consumer packaging waste, mainly LDPE, LLDPE, and PP films. The primary target products from this novel process are C2-C4 olefins (ethylene, propylene, and butylene) which are the raw materials for bulk of the volume of single use plastic production (PE and PP). Aromatic and other HVC precursors like benzene, toluene, xylene (BTX), ethyl benzene and polyols are also expected as by-products from the process. All theproducts and by-products (C2-C4 olefins, BTX, polyols, HVC) can be upcycled to resins, bulk (polyethylene, polypropylene) and specialty polymers (polyurethanes, epoxy, polyester, Nylon-6) at different market entry points.



#### **Dr. Anne M. Gaffney** University of South Carolina, Columbia, South Carolina, USA

#### Biography

Dr. Anne M. Gaffney is the Chief Science Officer of Idaho National and Distinguished Laboratory National Lab Fellow (2014 present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 257 patents. Dr. Gaffney is also a distinguished Joint Appointment Fellow at the University of South Carolina (2018 - present) where she is the Technical Director of the National Science Foundation Center for Rational Catalyst Synthesis. Some of her recent awards include: the 2019 American Chemical Society, Energy & Fuels, Distinguished Researcher Award in Petroleum Chemistry; the 2015 Eugene J. Houdry Award of the North American Catalysis Society; the Chemical Heritage Foundation, Women in Science Inductee, 2014; and the American Chemical Society, Industrial Chemistry Award, 2013. Dr. Gaffney received her BA in chemistry and mathematics from Mount Holyoke College and her Ph.D. in physical organic chemistry from University of Delaware.

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# 13-14

DAY 02 SPEAKERS

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#### Delia Teresa Sponza

Department of Environmental Engineering, Engineering Faculty, Dokuz Eylul University, İzmir Turkey

# Removal of oxytetracycline antibiotic via photocatalytic process by $Sn_2/Bi_2Sn_2O_7$ nanocatalyst

 $SnO_2/Bi_2Sn_2O_7$  heterojunction photocatalyst was fabricated to determine the photocatalytic removal of oxytetracycline antibiotic. Experimental results indicated that the existence of the built-in electric field between  $SnO_2$  and  $Bi_2Sn_2O_7$  led to a direct Z-scheme charge transfer. The efficient separation and fast transfer of photogenerated charge carriers contributed to boosting the photocatalytic performance of  $SnO_2/Bi_2Sn_2O_7$ . The optimal photocatalytic tetracycline degradation efficiency of  $SnO_2/Bi_2Sn_2O_7$  was 98 % at a  $SnO_2$  to  $Bi_2Sn_2O_7$  ratio of 0.45, at a 1.80 mg/l  $SnO_2/Bi_2Sn_2O_7$  concentration at a power of 40 W after 20 min irrdiation. Radical trapping experiments and electron paramagnetic results indicated that the photocatalytic degradation process in  $SnO_2/Bi_2Sn_2O_7$  system was modulated by photogenerated electrons, holes and  $O_2^-$  active species. The synthesized composites were characterized by the XRD, TEM, DRS and FTIR spectroscopy. The surface area of  $C_2$  composite (42.8 m<sup>2</sup>/g) was measure from the nitrogen adsorption/desorption data using Brunauer-Emmett-Teller (BET). The performance enhancement of the photocactivity is because of improved electron-hole separation effciency due to active electron transfer between  $Bi_2Sn_2O_7$  and  $SnO_2$  from  $SnO_2/Bi_2Sn_2O_7$  composite.

#### Audience Take Away Notes

- It is very exiting issue
- The people learn more about my studies
- This research exhibited advanced data to share with my students and colleques

#### Biography

Prof. Dr. Delia Teresa Sponza is currently working as a professor at Dokuz Eylul University, Department of Environmental Engineering. Scientific study topics are; Environmental engineering microbiology, Environmental engineering ecology, Treatment of fluidized bed and activated sludge systems, Nutrient removal, Activated sludge microbiology, Environmental health, Industrial toxicity and toxicity studies, The effect of heavy metals on microorganisms, Treatment of toxic compounds by anaerobic/aerobic sequential processes, Anaerobic treatment of organic chemicals that cause industrial toxicity and wastewater containing them, Anaerobic treatability of wastewater containing dyes, Treatment of antibiotics with anaerobic and aerobic sequential systems, Anaerobic and aerobic treatment of domestic organic wastes with different industrial treatment sludges, Treatment of polyaromatic compounds with bio-surfactants in anaerobic and aerobic environments, Treatment of petrochemical, Textile and olive processing industry wastewater by sonication, Treatment of olive processing industry wastewater with nanoparticles and the toxicity of nanoparticles. She has many international publications.





**Jun Gou\*, Lixin Liu, Jin Chen, Zijian Zhang** School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu, Sichuan, China

## High-speed high-efficiency silicon-based photo detectors with photontrapping holes

Monolithic infrared detectors with high speed and high efficiency have important applications in optical communication, signal measurement and other fields. Si is the best candidate material for monolithic integrated photodetectors, but the absorption coefficient of Si in near-infrared band is significantly reduced. Aiming at the contradiction between high absorption (high efficiency) and high speed (large bandwidth) of Si-based photodetectors in the near-infrared band, a Si film based photodetector integrated with periodic photon-trapping holes is proposed, which can ensure ultra-fast response speed and significantly enhance the absorption of near-infrared light. The spectral response range is also improved by combining Si with other semiconductor materials such as lead selenite (PbSe) film and quantum dot. The author introduces the research progress in photon-trapping mechanism, material synthesis, structure design, manufacturing process, and test verification of Si film based infrared detector. High speed (FWHM < 30 PS) and high efficiency (EQE > 60%) Si based infrared detectors are realized. It lays the theoretical and technical foundation for the development and application of monolithic integrated photo detectors with high performance.

#### Audience Take Away Notes

- This study could potentially be used for others to enhance the infrared response of photodetectors in an efficient way
- This study could potentially be used for others to design surface microstructures and explain the photon-trapping mechanism
- This research could also be used by others to expand their research

#### Biography

Dr. Gou studied Optical Engineering at University of Electronic Science and Technology of China (UESTC) and graduated as MS in 2010. He then joined the State key laboratory of Electronic Thin Films and integrated devices of UESTC. He received his PhD degree in 2014 at the same institution. Now he works at School of Optoelectronic Information, UESTC. He is dedicated to the research of uncooled infrared and terahertz detectors. In recent years, he has presided over and completed 1 national key project and 2 NSFC projects, published more than 30 research articles in SCI (E) journals, co-authored 1 English monograph, and won the second prize of Technological Invention Award of Ministry of Education, the first prize of Science and Technology Progress of Sichuan Province, and more than 20 national invention patents.





#### Delia Teresa Sponza

Department of Environmental Engineering, Engineering Faculty, Dokuz Eylul University, İzmir Turkey

# Effects of NOM concentrations on the photocatalytic removal of 4-chloro-2-methylphenoxyacetic acid (MCPA) micropollutant from the surface water using CNT-TiO, nano catalytic systems

Previous studies have reported that NOM interferes with photocatalytic degradation via inner filter effect, radical scavenging, and competition between NOM and target OMPs over the active sorption sites. Such inhibitory effect of NOMs can be attributed to three main facts. Firstly, the NOMs present in water matrices act as the inner UV filter. NOMs have strong absorption in UV and near UV range; the presence of NOMs in water would decrease the availability of UV light for TiO<sub>2</sub> to produce ROS, thus decreasing the ROS and h+ production. This inner UV filters effect is dependent on the wavelength of photons, in general stronger inner UV filter effect is expected in shorter wavelength UV range. Secondly, NOM can also act as scavenger of ∙OH and h+ which are known as the primary oxidants in TiO<sub>2</sub> photocatalytic systems. Thirdly, NOMs can inhibit the target pollutant degradation via competitive adsorption on the TiO<sub>2</sub> surface. Therefore this study investigates the effect of dissolved natural organic matter (NOMs) on 4-chloro-2-methylphenoxyacetic acid (MCPA, a typical micropollutant found in many water bodies) photooxidation via CNT-TiO<sub>2</sub> nano catalytic system.The removal of MCPA decreased from 99% to 60% and 58%, in the presence of only 5 mg/L SWR-NOM and UMR-NOM respectively. At a pH 4.00 in the presence of 3 mg/l CNT-TiO<sub>2</sub> with a TiO<sub>2</sub> ratio of 23%

#### Audience Take Away Notes

- It is very exiting issue
- The people learn more about my studies
- This research exhibited advanced data to share with my students and colleques
- Advanced studies were shared with this way

#### Biography

Prof. Dr. Delia Teresa Sponza is currently working as a professor at Dokuz Eylul University, Department of Environmental Engineering. Scientific study topics are; Environmental engineering microbiology, Environmental engineering ecology, Treatment of fluidized bed and activated sludge systems, Nutrient removal, Activated sludge microbiology, Environmental health, Industrial toxicity and toxicity studies, The effect of heavy metals on microorganisms, Treatment of toxic compounds by anaerobic/aerobic sequential processes, Anaerobic treatment of organic chemicals that cause industrial toxicity and wastewater containing them, Anaerobic treatability of wastewater containing dyes, Treatment of antibiotics with anaerobic and aerobic sequential systems, Anaerobic and aerobic treatment of domestic organic wastes with different industrial treatment sludges, Treatment of polyaromatic compounds with bio-surfactants in anaerobic and aerobic environments, Treatment of petrochemical, Textile and olive processing industry wastewater by sonication, Treatment of olive processing industry wastewater with nanoparticles and the toxicity of nanoparticles. She has many international publications.



**Tulshi Shiyani**<sup>1</sup> <sup>1</sup>Saurashtra Research Institute, SRI, Rajkot, Gujarat, India

## Bio hybrid nanostructures for solar fuel generation

**S** olar energy is the greatest source of energy on earth. Sunlight can be converted into solar power and solar fuel (hydrogen and oxygen) using photoactive materials and devices. Inorganic materials absorb ultraviolet light whereas organic materials absorb major visible light. Therefore, hybrid materials can absorb multiple spectrum of light. This enhances the overall absorption of device. Biohybrid photoelectrodes were used to generate photocurrents, and photo voltages under illumination of light. Hybrid photoelectrodes were used for solar photoelectrochemical conversion to generate solar fuel such as hydrogen using water splitting process. This may lead the future generation of solar cells in clean energy sector.

#### Audience Take Away Notes

- The audience will learn about solar energy conversion using hybrid electrodes
- The presentation will help to the audience to explore this area at commercial scale and it may help to develop technology
- Yes, this research may be expanded to use in teaching and research
- Yes, it provides a practical solution to a global problem, i.e. alternative to fossil fuels
- The presented work will be the solution of current global problem, i.e. global warming
- Cheap fabrication, higher absorption of light, eco-friendly materials, solar energy conversion

#### Biography

Tulshi Shiyani studied Ph.D. in Nanosciences at Central University of Gujarat, India and MS in physics at Saurashtra University, India. He then joined Saurashtra Research Institute, Rajkot, India to work in the diverse areas of interdisciplinary areas in 2022. He also has worked at Indira Gandhi Centre for Atomic Research, Indian Institute of Technology Kanpur, Pandit Deendayal Petroleum University and Gujarat Technological University in the area of nanotechnology and physics. He has published many articles, books and reviews in reputed publications. He is a chief editor in Science & Engineering Letters.



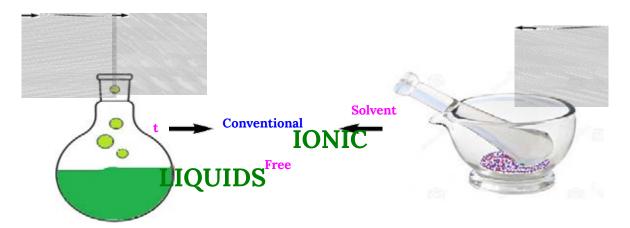


#### Dr. Kilivelu Ganesan

Assistant Professor, PG & Research Department of Chemistry, Presidency College, Tamilnadu, India

## Ionic liquids from simple synthetic approach and its catalytic response

I onic liquids have much attentions from chemist since last few decades because of their unique properties including chemical stability, very low flammability, less volatility and high thermal stability. Ionic liquids (IL) consist of hydrophobic moieties of organic cation with hydrophilic moiety of an inorganic anion; so, it can act as potential catalysts for most of the organic transformations. Organic segment of ionic liquid containing electro positive nitrogen are acted as second-generation Lewis acid. Pharmaceutically active organic molecules are prepared via carbon-carbon bond formations under Suzuki coupling reaction between some nitrile-functionalized pyridinium ionic liquids showed good catalytic activity.



#### Audience Take Away Notes

- Target molecules are obtained from shortest synthetic approach
- Researchers could minimize the toxic solvent during their synthesis
- Purification techniques are completely avoided during our current research
- Efficiency of recycled catalyst found to be very interesting
- Our approach has more merits than the conventional method so future researchers will follow

#### Biography

Prof. K. Ganesan received his Ph.D., degree in dendrimer chemistry from University of Madras, India. He has joined postdoctoral research associate at National Chaio-Tung University, Taiwan in combinatorial medicinal research group, then moved to University of Malaya, Malaysia as postdoctoral research associate in ionic liquids research group. Currently he is working as an assistant professor chemistry in the Presidency college, India which has been fifth place national level and first place in state level college ranked by NIRF 2020. Current research area of ionic liquids, catalysis and bio-organic chemistry. He has received Best Teacher award 2019 from PARE FOUNDATION; Outstanding Faculty in Science 2019 received from Venus International Foundation and Prestigious innovative research development and publishers (IRDP) award 2018 for teaching and research excellence national award.



#### Sidhartha Sondh, Darshit S Upadhyay\*, Sanjay Patel, Rajesh N Patel

Institute of Technology, Nirma University, Ahmedabad, Gujarat, India

## Sustainable municipal solid waste management system – a systematic review

The generation and accumulation of Municipal Solid Waste (MSW) is a major issue that most underdeveloped and developing countries around the globe are facing. The inefficiency of the waste management system is one of the major reasons for the current scenario of MSW mismanagement. A solid waste management system model that is effective for all sets of the country from high-income to low-income countries is required to preserve the environment and provide pollution-free air to breathe in. The study insights into the decision-making criteria to choose from various waste treatment methods. Different waste treatment methods such as gasification, incineration, pyrolysis, anaerobic digestion, and composting are critically reviewed to develop a better understanding of the characteristics of each method. The study highlights the practice of waste-to-value in the form of energy (heat and electricity) and material (bio-oil, soil quality amending material, construction materials, etc) to promote a multidimensional economy, known as circular economy. The solid waste management policies practiced by global leaders see the MSW management system gap strategically presented to sight the gap in the MSW management systems among different types of countries. The review will serve as an opportunity for underdeveloped countries to compare the present state of waste management systems and adopt better and more successful systems. This study attempts to develop a sustainable and healthy global economy to help in developing a sustainable and healthy economy across the globe.

#### Audience Take Away Notes

- To understand the severity of solid waste management
- To understand MSW management solutions and policies

#### Biography

Dr Darshit S Upadhyay is working as Assistant Professor in Mechanical Engineering Department since 2012. He has 13 SCI-indexed journal publications and presented more than 20 papers at international conferences. He has received different project grants from DST, and Nirma University. Dr Upadhyay has guided 15 postgraduate dissertations. Dr. Upadhyay is a recipient of Early Career Academic Grant from the Association of Commonwealth University, United Kingdom in 2016, and Indian Society for Technical Education (ISTE) awards. Dr Upadhyay is the reviewer of the international refereed journals in the fields of renewable energy, energy management, fuel, etc.



**Davood Fathi** Tarbiat Modares University, Iran

### Recent advances in perovskite-based nanostructure solar cell systems

**E** nergy and environment are two key issues in modern society which are necessities for the economic and social sustainable development of the world. In 2018, there is 79.5% energy economy that relies on conventional energy sources such as coal, petroleum oil, and natural gas, which are not renewable and environmentally benign. So far, fossil fuels account for about 87% of global energy. Since the beginning of the industrial revolution, economic growth has been driven by a continuous increase of power consumption, which has been possible thanks to the availability, high energy density and low price of fossil fuels. Currently, global demand for energy is growing faster than the capacity and utilization of fossil fuels, which leads to energy shortages. To deal with this problem, there has been a global drive seeking renewable and clean alternatives to fossil fuels.

Moreover, world energy demand due to population growth, Industrial development and Excessive use of modern electrical devices is constantly increasing. Therefore, finding reliable, cost-effective and renewable energy sources is needed for the future. Solar energy, as the cleanest and the largest exploitable resource of energy, can potentially meet the growing requirements for the whole world's energy needs beyond fossil fuels. Consequently, today, the development of renewable and clean energy sources has received global attention as an alternative.

Solar cells or photovoltaic cells are electrical devices that convert light energy directly into electricity by the photovoltaic effect. It is a physical and chemicalphenomenon. These types of cells have electrical properties such as current, voltage, or resistance that change when exposed to light.

Among various combinations of solar cells, Perovskite solar cells (PSCs) have emerged as one of the best in the photovoltaic industry in recent years. Power conversion efficiency (PCE) plays an important role in generating electricity from solar power. PSCs are one of the most important types of solar cells that can be used to produce cheaper solar energy.

#### Biography

Dr. Davood Fathi received the B.Sc. degree in the field of electronic engineering from Amirkabir University of Technology, Tehran, Iran, in 1990, and the M.Sc. degree in the field of biomedical engineering from Sharif University of Technology, Tehran, Iran, in 1994. After a couple of years working in industry, he worked toward the Ph.D. degree between 2006-2009 in the field of nanoelectronics with the Nanoelectronic Center of Excellence, Thin Film and Photonics Research Laboratory, School of Electrical and Computer Engineering, University of Tehran, Iran.

Dr. Fathi has joined from 2010 as a member of faculty to the Department of Electrical and Computer Engineering, Tarbiat Modares University (TMU), Tehran, Iran. He has been the reviewer for more than 15 international journals including IEEE, OSA, Elsevier, Springer, and so on. His current research interests include: Nanoelectronics; Nanophotonics and Optoelectronics; Solar cells and Water-splitting systems; Nanobiophotonics; Computational Optics-Photonics. He is also author or co-author of more than 85 scientific journal and conference papers in various fields of Nanoelectronics and Photonics, which most of the high impact publications during the past three years are in the field of solar energy. Dr. Fathi is currently an Associate Professor of Photonics and Optoelectronics at his department.

DAY



## Mohammadreza Yasoubi<sup>1</sup>, Zeinab Sanaee<sup>2</sup>\*

Energy Storage Laboratory, Department of Electrical and Computer Engineering, College of Engineering, University of Tehran, Tehran, Iran

# Formation of nanowires of silicon suitable for lithium ion battery application

C ilicon is regarded as an excellent candidate for anode of Lithium ion batteries, due to its extremely high Lithium storage capacity. The theoretical specific capacity of Silicon is around that of Lithium, showing its great potential as an electrode material for Lithium based batteries. However, this huge capacity for Lithium storage enforces a significant mechanical stress on the bulk Silicon material, which eventually can lead to its cracking and loosing the contact to the current collector. Using Silicon nanostructures, instead of its bulk format, can considerably alleviate this problem, providing sufficient space for expansion of Silicon during Lithium insertion through the intrinsic space between nanowires. In addition, nanostructures can better tolerate the expansion and resist against cracking, in comparison to the bulk material. The present paper reports the formation of Silicon nanowires using metal assisted etching (MAE) technique. This process is a fast and simple approach, that makes use of a thin nanometric layer of Gold as an effective catalyst to enhance the etching of Silicon. To accomplish this process, Si wafer has been placed in a RFsputtering system to deposit a 1 nm Gold layer on its surface. Applying Hydrogen plasma with a 250 W power, 200 sccm flow rate, and 5 min duration, using a RIE system, helps to form nano-islands of Gold on the Silicon wafer. Next, the sample has been immersed in the HF: H<sub>2</sub>O<sub>2</sub>: Ethanol (1:1:6) solution for 20 min. This solution would etch the Silicon much faster from the places that Gold nano-islands are on the surface, due to the catalytic effect of Gold layer, which yields the synthesis of Silicon nanowires on the surface of the sample. The nanowires can be released from the substrate through a tip sonication in an Ethanol environment. The obtained Silicon nanowires can be used as a high potential anode material in Lithium ion battery application.

#### Audience Take Away Notes

- Introduction to Lithium ion batteries will be explained
- Silicon based anode material is introduced as the pioneer anode in the modern Lithium ion batteries
- MAE synthesis of Silicon nanowires is explained
- These topics are part of the emerging technologies in the Lithium ion battery field, that can help the audience to be familiar with these topics and expand their research or teaching
- This research subject can lead to having higher performance Lithium ion batteries

#### Biography

Zeinab Sanaee received her BSc, MSc and PhD in 2005, 2009, and 2011, all in Electrical Engineering from University of Tehran. Then she started working at University of Tehran as an assistant professor in 2012. Her research interest is focused on fabrication of Lithium ion batteries and supercapacitors, and synthesis and implementation of nanostructured materials for their performance improvement. She is also director of Energy Storage Laboratory, where Fabrication of Silicon based Lithium ion batteries is followed as one of the main research subjects of the lab.



#### Florina Ștefania Rus\*, Madalina Ivanovici, Anamaria Dabici, Adrian Ionuț Cadis, Joao Nuno Goncalves

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# Conventional precipitation synthesis of $\rm Ca_2Bi_2O_5$ pure crystalline phase and its catalytic properties

The Ca-Bi-O materials have gained increasing interest within the scientific community due to their semiconductor and photocatalytic properties which were exploited for the degradation of different classes of substances such as antibiotics and organic dyes. The synthesis of these materials has been approached through the impregnation-calcination method, soft chemical method, flame spray method, sol-gel method, and others resulting in good photocatalytic properties in the visible range and high efficiencies for substances degradation. This work focuses on obtaining the Ca<sub>2</sub>Bi<sub>2</sub>O<sub>5</sub> system by a simple, conventional method - precipitation with environmental application in dye degradation from water.

The material obtained was investigated by X-ray diffraction to identify the crystalline phase and complementary analysis with Raman spectroscopy. Fourier transforms infrared spectroscopy, UV-VIS spectroscopy, and thermogravimetry completed the characterization of the obtained material, based on which the specific bands of the molecular bonds, mass loss, and diffuse reflectance were determined. The hybrid HSE06 functional was used in a first-principles calculation for this material to determine the energy band gap. The results highlighted a bandgap of 3.5 eV, similar to the bandgap obtained by diffuse reflectance recorded via UV-VIS spectroscopy on  $\text{Ca}_2\text{Bi}_2\text{O}_5$ . To determine the catalyst efficiency for purification, the obtained material was tested for the degradation of the dye at different pH values of the solution and dye concentration. The influence of parameters was studied on the adsorption and photocatalytic stages. Based on the time-dependent absorbance for RhB solution, the RhB degradation efficiency was calculated to be greater than 50%.

#### Audience Take Away Notes

- Novel and easy synthesis coprecipitation to obtain Ca<sub>2</sub>Bi<sub>2</sub>O<sub>5</sub>
- Characterization and identification of pure crystalline phase by Raman and XRD diffraction
- Analysis of RhB degradation as a response of Ca<sub>2</sub>Bi<sub>2</sub>O<sub>5</sub> activation to light
- Different behavior of Ca<sub>2</sub>Bi<sub>2</sub>O<sub>5</sub> activity depending on the parameters

**Acknowledgement:** This work was carried out through the Nucleus Program within the National Research Development and Innovation Plan 2022–2027, carried out with the support of MCID, project no PN 23 27 02 01, contract no. 29N/2023.

#### Biography

Florina Rus studied Materials Engineering at the Politecnica University of Timisoara, Romania and graduated as PhD in 2014. During this time she did a short research stage of approximately 8 months at Leibniz Institute for Solid State and Materials Research in Dresden where she gained experience in growing films using the pulsed laser deposition technique. She then joined the Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara Romania. She has published more than 27 research articles in the Scopus database.





#### Orlando Elguera Ysnaga

D.Sc. with Major in Analytical and Inorganic Chemistry- Universidade de Sao Paulo (Brazil)/ B.Sc. with Major in Chemical Engineering- Universidad Nacional de Ingenieria (Peru)

# Review of research topics for scaling-up of sonochemical reactors (sono-reactors)

This study is aimed to review the topics of chemical engineering to take in consideration for the L scaling-up of reactors, in order to perform processes based on the application of the sonochemistry at industrial level. Sonochemistry is an emergent technology, defined as chemistry made with ultrasound. The characteristic ultrasound frequencies are in the range of 1-10MHz, and in particular for sonochemistry in the sub-range 16-100 KHz. Chemical effects of ultrasound exist when there are changes in the pathways of reactions, yields and/or selectivities of the products due to the ultrasonic activation. At laboratory level, the sonochemistry has shown fantastic results, because it is based on the phenomenon of acoustic cavitation in liquids, thus, producing very high temperatures (some thousands of Kelvin degrees) and high pressures (some hundreds of atmospheres) during very short times (from tenths to hundreds of microseconds). Cavitation is the phenomenon with the most important effect for intensification of physical and chemical processing. Under these conditions, the yields of sonochemical reactions increase drastically, and their selectivities are improved, thus generating new mechanisms of reaction involving inorganic and organic syntheses. It is not easy to reproduce experimental results of quantification of sonochemical intensity, which is significant for the efficient scaling-up of sonochemical reactors (sono-reactors) for the progress of industrial applications of sonochemistry. This technology has application at industrial level for the treatment of waste-water and black-water. Sonochemistry can be considered as Green Chemistry, presenting the following advantages: low waste, low consumption of materials and energy with optimized use of non- renewable resources and use of renewable energies. Few studies were aimed about optimum design and scaling-up of sonochemical reactors. The implementation of sonochemistry at the industrial level will be feasible when the use of cavitational energy can be adequately controlled.

#### Audience Take Away Notes

- It is expected that this review can collaborate in the diffusion and development of this emergent technology, due to the advantages that possess: 1) Enhancement of the yields of chemical reactions significantly, 2) Improvement of selectivities, 3) Generation of new reaction pathways
- This technology has applications at industrial level for the treatment of wastewater
- Sonochemistry can be considered as Green Chemistry

#### Biography

D.Sc./B.Sc. Orlando Elguera studied Chemical Engineering at the National University of Engineering (Lima-Peru) with Master's studies in Chemistry Sciences at the National University of Engineering (Lima-Peru), and with Doctorate of Science with Major in Analytical and Inorganic Chemistry at the University of São Paulo (São Paulo-Brazil). He performed as Analyst of the Laboratory of samples of Geochemical Exploration and Inorganic Compounds at SGS del Perú S.A.C (almost 5 years). He has experience in the following method of analysis: Atomic Absorption Spectrometry, Inductively Coupled Plasma Optical Emission- Mass Spectrometry and X-ray Fluorescence. He has published 9 research articles in journals.



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## Detritiation of large volume of water with low tritium concentration by physicochemical methods of hydrogen isotope separation

The radioactive isotope of hydrogen, tritium, cannot be extracted from water by any selective methods used to remove, for example, Cs137 or Sr90. However, the operation of various industrial and experimental nuclear facilities, as well as scientific research using tritium-containing reagents, lead to the formation of tritiated water waste. As usual, the volumes of waste generated or accumulated over time are large and reach hundreds or thousands of m<sup>3</sup>, while the tritium concentration is low and amounts to 105–108 Bq/kg. Thus, these wastes are not of interest in the context of pure tritium recovery, however, the discharge of such wastes is unacceptable due to environmental reasons and exceeding the legally approved standards for tritium. The demonstrative example of the problems with such waste is the 10-year-old discussion about the destiny of some 1.3 million tons of tritiated water accumulated after the Fukushima accident. According to the latest information, the discussion ended with the TEPCO company starting construction of a kilometer-long pipeline into the ocean, through which this water is supposed to be drained within 30 years.

In Russia, over the past few years, the problem of detritiation of unbalanced water of Russian nuclear power plants has been discussed, the volume of which at each plant exceeds  $2000 \text{ m}^3$ /year at a tritium concentration in the previously mentioned range. This report discusses the prospects for using various physicochemical methods for the separation of hydrogen isotopes with the participation of water as a working substance for its purification. It is shown that the method of catalytic isotope exchange of hydrogen with water has the greatest prospects for use.

#### Audience Take Away Notes

- The presentation will formulate the problem of handling low-level tritiated water, which consists in a contradiction between environmental and economic requirements
- Possible technologies for the separation of hydrogen isotopes that can be used to solve the problem of water waste detribiation will be considered
- The advantages of using the method of catalytic chemical isotope exchange of hydrogen with water for detritiation of water are shown
- A variant of eliminating the contradiction between environmental and economic requirements is considered when using this method in conditions of large-scale production of hydrogen within the framework of the concept of hydrogen energy

#### Biography

Dr. Moseeva studied methods of physical chemistry at the D. Mendeleev University of Chemical Technology of Russia and graduated as MS in 2017. She received her PhD degree in 2022 at the same institution at the research group of Prof. Rozenkevich. During postgraduate supervised by Dr. Bukin at the Department of Isotope Separation Technology and Hydrogen Energetic conducted research of chemical isotope separation in water-hydrogen system. She has published 8 research articles in SCI (E) journals and 2 patents.



**Samira Rostom\*, Robert Symonds, Robin W. Hughes** Natural Resources Canada, CanmetENERGY, Ottawa, ON, Canada

# Comparative study of zeolite-5a and cu-BTC for $co_2$ adsorption using thermo- gravimetric analyzer in the application of hydrogen purification

H ydrogen is considered as one of the most important clean and renewable energy carriers for a sustainable energy future. However, its efficient and cost-effective purification remains challenging. This paper presents the potential of using metal-organic frameworks (MOFs) in combination with pressure swing adsorption (PSA) technology for syngas based H<sub>2</sub> purification. PSA process analysis is done considering high pressure and elevated temperature process conditions, it reduces the demand for off-gas recycle to the fuel reactor and simultaneously permits higher desorption pressure, thereby reducing the parasitic load on the hydrogen compressor. The elevated pressure and temperature adsorption we present here is beneficial to minimizing overall process heating and cooling demand compared to existing processes.

Here, we report the comparative performance of zeolite-5A, Cu-BTC and the mix of zeolite-5A/Cu-BTC for H2 purification from syngas typical of those exiting water-gas-shift reactors. The MOFs were synthesized hydrothermally and then mixed systematically at different weight ratios to find the optimum composition based on the adsorption performance. Synthesized MOF's were characterized excessively by thermogravimetric analyzer (TGA) for understanding their thermal stability and regeneration performance. Also  $CO_2$  adsorption at different temperatures and cyclic performance are also analyzed using TGA. The findings of this study suggest that the zeolite-5A/Cu-BTC composites are promising candidates for industrial H<sub>2</sub> purification processes.

#### Audience take-away Notes

- In literature, most PSA units operate at atmospheric temperature for better adsorption of gases. This study will help to evaluate PSA at high pressure and temperature that will minimize the process cost when considering not only the PSA unit, but also the systems integrated with the PSA unit. Therefore, the researchers from this field will have justification for the study of various adsorbents that could be stable enough at these conditions
- MOF's stability at high pressure and temperature has not been broadly reported before. Therefore, the audience could learn more details about the synthesis and performance of different MOFs at operating conditions of importance to this study
- In this study, the adsorption and desorption were done at elevated pressures. The syngas leaves the shift reactor at elevated pressure and keeping this pressure high reduces demands for off-gas recycle to the fuel reactor. In addition, the higher desorption pressure reduces the parasitic loads on the hydrogen compressors. Therefore, it simplifies the downstream power requirement of different hydrogen purification processes

#### Biography

Dr. Samira Rostom received her PhD degree in Chemical Engineering from University of Western Ontario (UWO) in 2018. She has published 4 journal articles including a review paper in the field she worked on during her PhD. Later she joined as a Post-doctoral Fellow at UWO in the field of oil-sand research. Then she joined Enerkem Inc., Edmonton while she worked mostly in the field of olefins production from syngas. She was involved in catalyst patent work along with piloting the process she was researching. Recently, she has joined at CanmetENERGY as a Research Scientist.



**Folayan Adewale Johnson<sup>1</sup>\*, Adewale Dosunmu<sup>2</sup>, Boniface Oriji<sup>2</sup>** <sup>1</sup>Department of Petroleum and Gas Engineering, University of Port Harcourt, Nigeria

<sup>2</sup>Professor of Petroleum Engineering, University of Port Harcourt, Nigeria

# Novel synthetic-based drilling fluid through catalytic and non-catalytic Trans esterification of linseed oil from $co_2$ -enhanced super-critical fluid extraction process

**T** n this study, the optimum reaction parameters as well as the effect of catalyst concentration and type L on the percentage yield and physico-chemical characteristics of linseed oil ethyl esters obtained from non-catalyzed (free catalyst system), super critical ethanol (SCE), homogeneous, heterogeneous and biocatalytic (enzymatic) trans-esterification reactions were experimentally investigated. The catalysts under investigation are sodium hydroxide (NaOH), calcium Oxide (CaO) and lipase catalyst (Candida antarctica) from Novozymes biotechnology company. The crude linseed oil was extracted from its seeds by super critical fluid extraction (SFE) process using carbon IV oxide as the extraction solvent and an oil yield of 43.50% was obtained. The fatty acids compositional analyses of the extracted oil were determined by an Agilent 8890 gas chromatography system coupled with Agilent 5977B mass selective detector (GC-MSD) and thermal desorption auto sampler (TD sampler). A Fourier transform Infra-Red (FTIR) spectroscopic technique was used to detect and measure the complete conversion of the triglyceride to fatty acid ethyl ester (FAEE). The physico-chemical properties of the synthesized ethyl esters were evaluated by using the American petroleum institute (API), ASTM D 6751-07b and the European committee for standardization (EN 14214) recommended standard procedures and techniques. The GC-MS analysis shows that the linseed oil contains essentially of poly-unsaturated fatty acids (about 53.15% of alpha Linolenic acid with 16.00% of Linoleic acid) and 20.80% of mono-unsaturated oleic acid. The major saturated fatty acids that were found in the oil GC-MS profile are 6.20% of Palmitic acid and 3.45% of Stearic acid with some traces of arachidic acid (0.30%). The Super critical ethanol (SCE) and the enzymatic ester production routes have the lowest quantities of free glycerine, water content, sulphated ash, carbon residue and total acid number as evident in their FTIR spectra because there was no production of soap and hence no washing steps were required. Though, with the former being more efficient than the latter in terms of ester yield, quality and superior cold flow, density, kinematic viscosity and oxidative stability characteristics. Finally, in comparison to catalytic reactions, non-catalyzed super-critical-alcohol trans-esterification process is faster with high triglyceride conversion efficiency in a very short time. However, the process requires higher temperature, pressure and alcohol to oil molar ratio when compared with the catalyzed reaction and hence higher cost of ester synthesis.

**Key words:** Key words: Bio catalyst (Candida Antarctica), ester yield and quality, Fatty acid ethyl ester (FAEE), Linseed oil, FTIR, GC-MS, heterogeneous catalyst, homogeneous catalyst, non-catalyzed, super critical fluid extraction (SFE), transesterification reaction.

#### Audience Take Away Notes

- The research showed the technical viability and environmental friendliness potential of linseed oil as new discovery and promising candidate in the endless search for novel synthetic drilling fluid
- The research article experimentally examined the effect of catalyst concentration and various catalytic routes as well as non-catalyzed transesterification reaction on the yield and physico-chemical characteristics of linseed plant oil fatty acid methyl ester (FAME)



- The research describes the optimum conditions under which production of Fatty acid methyl ester from linseed oil can be termed efficient
- The article will serve as guide to researcher, scientist and various bio-energy operators on the consequence of increasing and reducing one parameter or the other on Fatty acid methyl ester 'scold flow properties (cloud point and pour point) and critical fluid parameters (density, viscosity, acid number)

#### Biography

Folayan, Adewale Johnson is a young and vibrant academic of international repute. He has a Master's degree in Petroleum Engineering from University of Ibadan, Nigeria with distinctions. He is presently a final doctoral researcher in petroleum and gas engineering at university of portharcourt Nigeria. He has over twenty-five (25) novel scientific publications in high impact and Elsevier's Scopus indexed Journals covering drilling fluids, biofuels, energy conversion and management, green energy, nano science and nano technology, synthesis and environmental engineering. He has attended numerous scientific conferences both locally and internationally. His industry and academic experience in the field of chemical and petroleum engineering spans over a decade. magnus

# 13-14

DAY 02 POSTERS

14<sup>TH</sup> EDITION OF GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY



#### Alexandra Bakratsa<sup>1</sup>, Vasileios Athanasiou<sup>1</sup>, Vasiliki Zacharopoulou<sup>1</sup>, Georgia Kastrinaki<sup>1</sup>, George Karagiannakis<sup>1</sup>\*, Vasileios Zaspalis<sup>1,2</sup>

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# Effect of catalyst acidity and reduction step on carbon dioxide valorization

ver the last decades, carbon dioxide (CO<sub>2</sub>) is incessantly accumulated in the atmosphere due to human activities, especially in countries with developed economies. CO<sub>2</sub> constitutes one of the main greenhouse gases and CO<sub>2</sub> emissions are linked with global warming and several environmental concerns, thus strategies and technologies for immediate mitigation of CO<sub>2</sub> emissions should be adapted. CO<sub>2</sub> valorization techniques have been developed, using CO<sub>2</sub> as feedstock for the production of high added value products (chemicals and/or fuels) by heterogeneous catalysts with multifunctional structures. Within this context, mixed metal-based oxides were synthesized in order to catalyze the Reverse Water-Shift (RWGS) reaction (CO<sub>2</sub> is converted into CO), as well as Fischer – Tropsch (FTS) like reactions (CO hydrogenation). Alkali promoters were added to enhance selectivity into olefins, while the synthesized oxides were dispersed on acidic supports that promote deoxygenation reactions. Preliminary experiments were conducted to elucidate the effect of the reduction of the metal oxides and the zeolitic acidity/SAR on materials' catalytic performance. Samples were reduced for four hours prior to RWGS resulting in the production of C1-C3 deoxygenated species, such as methane, ethane, propene and propane. Further reduction did not improve CO<sub>2</sub> conversion and selective product distribution. Overall, reduced alkali promoted magnetite nanoparticles dispersed on H-ZSM5 (140-160 SAR) showed the most promising results with 9.3% CO<sub>2</sub> conversion, as well as 16.4 and 81.1% selectivity to CO and methane, accordingly.

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#### Audience Take Away Notes

- Catalytic carbon dioxide valorization aspects
- Effect of specific catalytic properties on the reaction product distribution

#### Biography

George Karagiannakis (MEng ChE, MSc, PhD) is principal researcher and head of the newly established ARTEMIS Laboratory (ARTEMIS stands for Laboratory of novel materials & Technologies for sustainable Energy & environmental Integrated applications) of the Chemical Process and Energy Resources Institute (CPERI) of CERTH, Greece. His main research focuses on materials and subsystems for production of energy carriers from solar-thermal/thermochemical processes, as well as on technologies using alternative fuels in gasification and fuel cell systems.



**Minjae Baek**<sup>1</sup> <sup>1</sup>Korea International School Jeju, Jeju, South Korea

# Quantitative analysis on collective interlaboratory adsorption data on ZIF-8

G as adsorption, a surface phenomenon leading to densification of gas molecules on a solid surface, is important in many energy and environmental applications, such as efficient separation processes, carbon capture, and geological carbon storage. Experimental measurements of adsorbed amounts of gases, generally expressed as adsorption isotherms, on various adsorbents are crucial in estimating the adsorption capacity and gas selectivity of the adsorbents and evaluating their performance in the applications stated above. However, there has been a lack of reproducibility in the experimentally measured adsorption isotherms reported in the literature, which potentially leads to incorrect estimation of the adsorption properties of adsorbent materials. In this study, experimental adsorption isotherms of  $CO_2$  on ZIF-8, a commonly studied adsorption system for future separation processes, that are available on the Database of Novel and Emerging Adsorbent Materials established by the National Institute of Standards and Technology have been collected and fitted using an empirical adsorption equation. The spread of the isotherms has been then quantified using the box-and-whisker plot analysis and its impact on the determination of the adsorption properties, specifically the limiting heat of adsorption, is reported. The results demonstrate a significant spread of the collected isotherms with clearly identified outliers, showing the importance of increasing the reproducibility of adsorption isotherm measurement.

#### Audience Take Away Notes

- The importance of repeatability of experimental measurements
- Possible sources of differences in experimental measurements
- The need to report experimental details in reporting data

#### Biography

Minjae Baek is a student at Korea International School who is passionate about the environmental challenges that the world faces and potential solutions that make the world more sustainable.





Maria Syrigou, George Karagiannakis\* Chemical Process & Energy Resources Institute, CERTH, Greece

### Mathematical model of a solar irradiated monolithic reactor

**S** olar-aided hydrogen production seems an interesting solution in the transition towards a carbon-free energy future. In this context, redox materials are employed to directly dissociate water in extremely high temperature processes (T>1000°C), where the required energy is provided via concentrated solar energy. Depending on the redox material and out of the variety of the possible routes, solar thermochemical hydrogen production using non-stoichiometric, non-volatile redox materials in a two-step process is of paramount interest. The material undergoes consecutive cycling between its reduced and oxidized state, thus hydrogen and oxygen are separately produced.

The current computational work investigates the performance of a solar irradiated monolithic reactor. The model considers nickel ferrite as the active material but is capable of describing any non-stoichiometric, non-volatile redox material. Due to the symmetry of the geometry, the simulation of single channel of the monolith is representative of the entire reactor. Furthermore, taking advantage of the characteristics of the honeycomb monolithic structures, low-dimensional modelling suffices to assess the flow regime inside the reactor. The developed model incorporates the energy conservation equations for the gas and the solid phase, the surface coverage evolution and the species conservation equations. The system of the coupled differential equations is solved using finite difference numerical methods, under steady state and dynamic conditions. Furthermore, the algorithm takes into account an in-house kinetic model that has already been developed [1] and is capable of accurately describing the evolution curves of the products under various operational conditions. The parametric study investigates the impact of the critical parameters on the performance of the process, while different scenarios (both thermal and chemical) are simulated in order to increase the productivity of the product yield.

**Acknowledgements:** We acknowledge support of this work by the project PROMETHEUS: A Research Infrastructure for the Integrated Energy Chain (MIS 5002704) which is implemented under the Action Reinforcement of the Research and Innovation Infrastructure, funded by the Operational Programme Competitiveness, Entrepreneurship and Innovation (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

#### Biography

George Karagiannakis (MEng ChE, MSc, PhD) is principal researcher and head of the newly established ARTEMIS Laboratory (ARTEMIS stands for Laboratory of novel materials & Technologies for sustainable Energy & environmental Integrated applications) of the Chemical Process and Energy Resources Institute (CPERI) of CERTH, Greece. His main research focuses on materials and subsystems for production of energy carriers from solar-thermal/thermochemical processes, as well as on technologies using alternative fuels in gasification and fuel cell systems.



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## Thermodynamic properties of aqueous l-threonine-[BMIm][Cl] solutions

mino acids as fundamental structural units of peptides and proteins have an important role in biological Asystems by affecting solubility, denaturation and activity of biomolecules [1-3]. Study of these effects on thermo physical properties of model compounds in the presence of electrolytes solutions provide information about solute-solvent and solute-solute interactions on biomolecules [4-5]. Ionic liquids (ILs) as organic electrolytes and green solvents are composed of an organic action and an inorganic anion which are liquid at ambient conditions. In the past decade, extensive investigations showed that the use of ILs as reaction media for processes involving biologically relevant compounds is promising in view of their successful application in kinetic resolution, biocatalysts, and biosynthesis, separation and purification processes [6]. The scope of this information is valuable to explore the interactions of amino acids in ILs. To reach this purpose, densities,  $\square$  of L-threonine in water and in aqueous 1-butyl-3-methylimidazolium chloride, [BMIm][Cl] solutions of different molarities over the temperature range T = (288.15-318.15) K have been determined using vibrating-tube digital density meter (DMA 4500M, Anton Par, Austria). The density data have been used to calculate the apparent molar volume, V\_I partial molar volume, V\_2^o and partial molar volumes of transfer,  $\Delta_{tr} V_2^{o}$ . The V\_2<sup>o</sup> values of L-threonine in aqueous [BMIm] [Cl] solutions are higher than those in water and thus exhibit positive  $\Delta_{tr} V_2^{o}$ , which are indicative of strong interactions between L-threenine and [BMIm][Cl]. The volumetric interaction parameters, V\_AB and V\_ABB and hydration numbers, n\_H have also been calculated to discuss the solute-solvent interactions occurring in these systems.

**Keywords:** L-threonine; 1-butyl-3-methylimidazolium Chloride; Partial Molar Volume; Partial Molar Expansibilities; Hydration Numbers

## **Participants List**

| Anne M Gaffney                                                  | 43      |
|-----------------------------------------------------------------|---------|
| University of South Carolina, United States                     | 40      |
| Ashanendu Mandal                                                | 30      |
| University of Calcutta, India                                   | 00      |
| Ashiff Khan                                                     |         |
| Saudi Aramco, Saudi Arabia                                      | 37      |
| SP Jain School of Global Management, Australia                  |         |
| Chi Ping Li Bing Ze Li                                          | 20      |
| National United University, Taiwan                              |         |
| Darshit S Upadhyay                                              | 50      |
| Nirmal University, India                                        |         |
| Davood Fathi                                                    | 51      |
| Tarbiat Modares University, Iran                                | 0.      |
| Delia Teresa Sponza                                             | 45 & 47 |
| Dokuz Eylul University, Turkey                                  |         |
| Folayan Adewale Johnson                                         | 58      |
| University of Port Harcourt, Nigeria                            | 00      |
| George Karagiannakis                                            | 61 & 63 |
| Chemical Process & Energy Resources Institute, CERTH, Greece    | 01000   |
| Haibo Ge                                                        | 42      |
| Texas Tech University, United States                            | 72      |
| Hanns Christian Schewe                                          | 33      |
| Czech Academy of Sciences, Czech Republic                       |         |
| Hasan Saygili                                                   | 36      |
| Batman University, Turkey                                       | 50      |
| Huiqin Li                                                       | 20      |
| Inner Mongolia University, China                                | 20      |
| leva Gaide                                                      | 35      |
| Vytautas Magnus University Agriculture Academy, Lithuania       |         |
| Ji Wang                                                         | 17      |
| Ningbo University, China                                        | 17      |
| Jun Gou                                                         | 46      |
| University of Electronic Science and Technology of China, China | 40      |
| Kilivelu Ganesan                                                | 49      |
| Presidency College, India                                       | 49      |

## Participants List

| <b>Md Nurul Islam Siddique</b><br>University Malaysia Terengganu, Malaysia                                                          | 18 |
|-------------------------------------------------------------------------------------------------------------------------------------|----|
| <b>Minjae Baek</b><br>Korea International School Jeju, Korea, Republic of                                                           | 62 |
| <b>N Mamulaishvili</b><br>Rustaveli State University, Georgia                                                                       | 24 |
| Noorin Fatima<br>Osmania University, India                                                                                          | 29 |
| <b>Orlando Elguera</b><br>Institute of Chemistry of Sao Carlos, Peru                                                                | 54 |
| Osman Adiguzel<br>Firat University, Turkey                                                                                          | 39 |
| <b>P K Dash</b><br>NMIT, India                                                                                                      | 31 |
| <b>Rus Florina Stefania</b><br>National Institute for Research and Development in<br>Electrochemistry and Condensed Matter, Romania | 53 |
| Samira Rostom<br>University of Western Ontario, Canada                                                                              | 56 |
| Serge Cosnier<br>Universie Grenoble Alpes, France                                                                                   | 14 |
| Shalini Arora<br>IIT Kanpur, India                                                                                                  | 28 |
| <b>Stanislaw Dzwigaj</b><br>Sorbonne University, France                                                                             | 13 |
| Suman Dutta<br>Indian Institute of Technology (ISM) Dhanbad, India                                                                  | 32 |
| <b>Tarnveer Kaur</b><br>Punjabi University, India                                                                                   | 64 |
| Thomas J Webster<br>Interstellar Therapeutics, United States                                                                        | 41 |
| <b>Tulshi Shiyan</b><br>Saurashtra Research Institute, India                                                                        | 48 |
| <b>Valeriia Moseeva</b><br>D Mendeleev University of Chemical Technology, Russian<br>Federation                                     | 55 |

66

## Participants List

| Vinod Agnihotri<br>SP Jain School of Global Management, Singapore                   | 22 |
|-------------------------------------------------------------------------------------|----|
| Yaddanapudi Varun<br>Birla Institute of Technology and Science (BITS) Pilani, India | 27 |
| Zaur Berishvili<br>LEPL Institute Optica, Georgia                                   | 25 |
| Zeinab Sanaeem<br>University of Tehran, Iran                                        | 52 |
| <b>Zibo Zhao</b><br>Max Planck Institute for Multidisciplinary Sciences, China      | 19 |
| <b>Ziyi Zhong</b><br>Guangdong Technion-Israel Institute of Technology, China       | 16 |

67



We wish to meet you again at our upcoming events next year...

## **Questions?** Contact

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