VIRTUAL EVENT

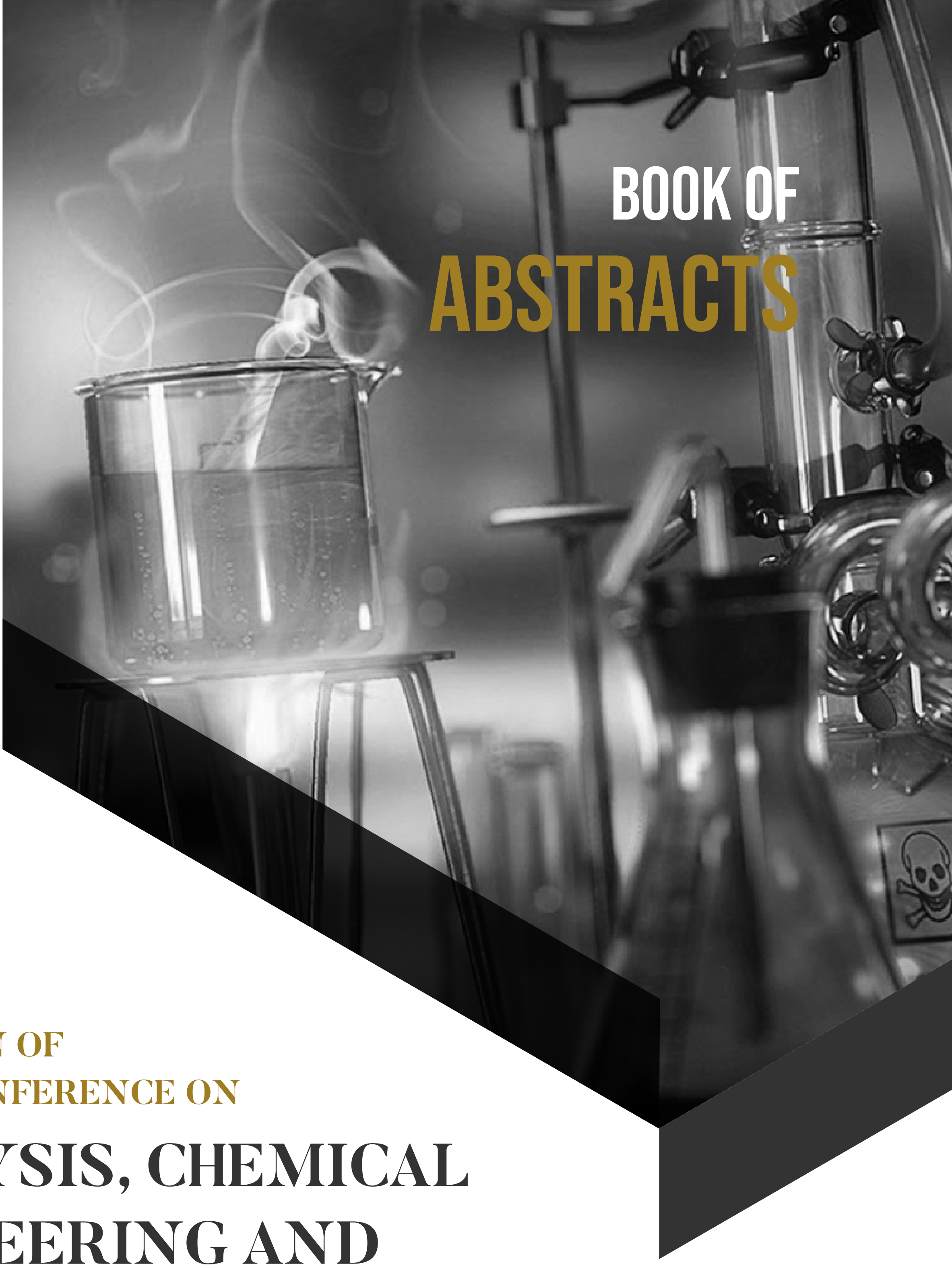
28-29

MARCH 2022

10TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

Contact us:
Ph: +1 (702) 988-2320
Email: catalysis-chem@magnusconference.com
Website: https://catalysis.magnusconferences.com/



BOOK OF ABSTRACTS

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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 conference 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 2022

CCET 2022 welcomes members from different parts of the world to join our Online Event - “10th Edition of Global Conference on Catalysis, Chemical Engineering and Technology” scheduled during March 28-29, 2022. It includes prompt Keynote presentations, Oral presentations, and Poster presentations, interactive and informal exchanges. This is going to be one of the most remarkable events of the year. Through the theme “Neoteric Advancements Fostering Chemical Engineering and Catalysis” conference will explore the advances in the field. CCET 2022 goal is to bring together bright minds to give talks that are ideas-focused, and on a wide range of scientific sessions, to faster learning inspiration. It will provide an international platform to share expertise, foster collaborations, discover new information, and stay current with trends and networking.

KEYNOTE FORUM

DAY 01

10TH EDITION OF
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CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

28-29 MAR

Stanislaw Dzwigaj

Sorbonne Université, France

Chemical engineering of metal single-site zeolites for application in heterogeneous catalysis

The incorporation of metal ions into zeolites as isolated tetrahedral sites appears to be the important task because such sites are considered to be active sites of several catalytic processes. 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 chemical 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 chemical engineering of single-site zeolites with transition metal will be described and characterized by different physical techniques both at the macroscopic and molecular levels. The application of metal single-site zeolites in heterogeneous catalysis will be discussed. The post-synthesis 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 NO_x to N_2, production of 1,3-butadiene 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:

- 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.

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.

Saim Ozkar

Middle East Technical University, Turkey

How to increase the catalytic efficacy of platinum-based nanocatalysts for hydrogen generation from the hydrolysis of ammonia borane

Hydrolysis is the best way of releasing H_2 from ammonia borane (AB) in the presence of catalysts. Significant achievements have been obtained in increasing the rate of releasing H_2 from AB by employing transition metal nanoparticles (NPs) as catalysts. Platinum is one of the most active transition metals providing high TOF for hydrogen generation from the hydrolysis of AB. However, high price of platinum hampers its large-scale applications in catalysis. Achieving high catalytic performance with the smallest amount of metal is critical for any catalytic applications of noble metals. While continuous efforts have been devoted to improve the catalytic activity of non-noble metals, an immense challenge is the enhancement of utilization efficiency and catalytic performance, and thus ultimately lowering the cost of noble metal catalysts. For example, reducing the particle size of platinum catalysts to nanoregime increases their surface area and thus, the number of active sites. However, colloidal NPs are unstable and tend to aggregate to larger particles, which greatly hampers their recyclability and catalytic performance. A proper way of overcoming this problem is the immobilization of platinum NPs on materials with large surface area. The catalytic activity and stability of supported platinum NPs depend on the particle size distribution, surface area of support, and strength of metal-support interaction. Selecting suitable supports is of paramount importance in obtaining NPs which are stable and still catalytically active. The strength of platinum-support interaction turns to be crucial for catalytic activity and stability of NPs on the support surface. Although no mathematical correlation between the catalytic activity and strength of metal-support interaction could be obtained yet, almost all the highly active platinum(0) catalysts have high Pt-4f binding energy as determined by XPS analysis. Increasing the lifetime and reusability of nanocatalysts can certainly help to improve the atom efficiency of Pt catalysts. Lifetime is used as a measure of stability which correlates well to the strength of metal-support interaction relative to metal-metal bond while reusability is mainly determined by the isolability of nanocatalysts for subsequent runs and measures the stability of catalysts. Low reusability is largely caused by material loss during the isolation of catalyst from solution and re-dispersing in a new reaction solution for the succeeding run of catalytic reaction. A recyclability test, which is performed by adding a new batch of AB to the reactor when the hydrolysis is complete for the subsequent cycle of hydrolysis without isolating the catalyst or removing the reaction solution from the reactor, measures the durability of catalysts. A short prelude on the mechanism of catalytic hydrolysis of AB will give insight to understand and appreciate the reported achievements in enhancing the catalytic performance of platinum-based catalysts in the hydrolysis of AB. The progresses in developing highly efficient platinum(0) nanocatalysts which have been reported to be active catalysts in H_2 generation from the hydrolysis of AB will be discussed along with the available parameters including temperature, particle size, surface area, the catalyst to substrate ratio, TOF, and the XPS determined Pt-4f binding energy.

Audience Take Away:

- The employment of colloidal platinum(0) NPs as nanocatalysts significantly enhances the catalytic activity. Supporting NPs on materials with large surface area provides a competent way of stabilizing them against agglomeration.
- The strength of platinum-support interaction turns to be crucial for catalytic activity and stability of NPs on the support surface. The high Pt-4f binding energy is caused by charge transfer from platinum(0) NPs to the support

through the platinum-support interaction. Such a charge transfer makes the platinum(0) NPs highly active and stable on the surface of support. In this context, reducible oxides appear to be promising candidate as supporting materials for platinum(0) NPs in the hydrolysis of AB.

- Using single-atom Pt catalyst seems to be an effective way of increasing atom efficiency of platinum nanocatalysts. However, an increase of the Pt loading of single-atom nanocatalyst is impossible without causing agglomeration, which is a key impediment in large scale application of single-atom catalysts.
- Platinum(0) NPs can be made readily separable when supported on magnetic powder materials. As reducible and magnetic support, $CoFe_2O_4$ and Co_3O_4 turn to be the most suitable supports providing high catalytic activity and reusability for the platinum(0) NPs, ultimately lowering the cost of precious metal catalysts.

Biography

Dr. Ozkar graduated from Faculty of Chemical Engineering, Technical University of Istanbul in 1972, worked for two years in industry, received Ph.D. in inorganic chemistry at Technical University of Munich in 1976 before joining Middle East Technical University. He spent one year at Max Planck Institute in Mülheim as Scholar of Alexander von Humboldt-Foundation in 1986, two years at University of Toronto as visiting professor in 1988-1990, and a total of 5 years at Colorado State University between 2000 and 2019. He was awarded Science Prize by the Scientific and Technological Research Council of Turkey in 1996 and has been a permanent member of Turkish Academy of Sciences since 1996. His research interests involve the synthesis and catalytic use of transition metal nanoparticles. He has published more than 300 research articles in SCI(E).

Osman Adiguzel
Firat University, Turkey

Crystallographic basis of thermal and mechanical memory in shape memory alloys

A series of alloy systems take place in class of advanced smart materials with adaptive properties and stimulus response to the external changes. Shape memory alloys take place in this group, with the thermal and mechanical memory characteristics. These alloys exhibit a peculiar property called shape memory effect, which is characterized by the recoverability of two certain shapes at different temperatures. This phenomenon is initiated by cooling and deformation processes and performed thermally on heating and cooling. Therefore, this behavior can be called thermal memory or thermoelasticity. These alloys have dual characteristics called thermoelasticity and superelasticity, from viewpoint of memory behavior. Two successive structural transformations, thermal and stress induced martensitic transformations govern thermal and mechanical memory in crystallographic basis. Thermal induced transformation occurs along with crystal twinning on cooling and ordered parent phase structures turn into twinned martensite structures, and twinned structures turn into the detwinned structures by stressing material in low temperature condition by means of stress induced transformation. Superelasticity is performed mechanically by stressing and releasing material at a constant temperature in parent phase region, and shape recovery is performed simultaneously upon releasing the applied stress. Therefore, this behavior can be called mechanical memory. Superelasticity is performed in non-linear way; stressing and releasing paths are different in the stress-strain diagram, and hysteresis loop refers to energy dissipation. The elementary processes involved in such martensitic transformations are lattice invariant shear, lattice twinning and detwinning. It is well known that crystal twinning and detwinning reactions play a considerable role in shape memory effect and superelasticity. Thermal induced martensitic transformation is lattice-distorting phase transformation occur with the cooperative movement of atoms by means of shear-like mechanism in <110>-type directions on {110} -type planes of austenite matrix.

Copper based alloys exhibit this property in metastable β-phase region. Lattice invariant shears are not uniform in these alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures. 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 ordered lattice. The unit cell and periodicity are completed through 18 layers in direction z, in case of 18R martensite, and unit cells are not periodic in short range in direction z.

In the present contribution, electron diffraction and x-ray diffraction studies performed on two copper based CuZnAl and CuAlMn alloys. Electron diffraction patterns and x-ray diffraction profiles exhibit super lattice reflection. Specimens of these alloys aged at room temperature, and a series of x-ray diffractions were taken duration aging. Reached results show that diffraction angles and peak intensities change with aging time. Especially, some of the successive peak pairs providing a special relation between Miller indices come close each other, and this result refers to the rearrangement of atoms in diffusive manner.

Keywords: Shape memory effect, martensitic transformation, thermal memory, mechanical memory, lattice twinning, detwinning.

Audience Take Away:

Shape memory effect is a multidisciplinary phenomenon. Shape memory alloys are multifunctional materials and used as shape memory devices from biomedical to the aeronautical and every field of the industry. This phenomenon is based on microstructural changes in the materials. Crystal structure of copper-based shape memory alloys is complicated; I will start my presentation with elementary knowledge and continue the importance and application on copper-based shape memory alloys. Audience will find the answer of many questions, and my presentation will be beneficial for every delegate and participant.

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 on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has been retired due to the age limit of 67, following academic life of 45 years. He published over 80 papers in international and national journals; He joined over 100 conferences and symposia in international and national level as participant, invited speaker or keynote speaker with contributions of oral or poster. He served the program chair or conference chair/co-chair in some of these activities. In particular, he joined in last seven years (2014 - 2020) over 80 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. He supervised 5 PhD- theses and 3 M.Sc- theses.

Dr. Adiguzel served his directorate of Graduate School of Natural and 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) also appreciates cooperation of his group and interest in Powder Diffraction File.

Alexander G. Ramm

Kansas State University, United States

Solution of the millennium problem concerning the navier-stokes equations

The Navier-Stokes problem in R3 consists of solving the equations:

$v_j + (v, \nabla)v = -\nabla p + \nu\Delta v + f, x \in R3, \ t \geq 0, \nabla \cdot v = 0, v(x, 0) = v0(x)$, where $v = v(x, t)$ is the velocity of the incompressible viscous fluid, $p = p(x, t)$ is the pressure, the density of the fluid is $\rho = 1$, $f = f(x, t)$ is the exterior force, $v0 = v0(x)$ is the initial velocity.

The aim of this talk is to analyse the Navier-Stokes problem (NSP) in R3 without boundaries. It is proved that the NSP is contradictory in the following sense:

If one assumes that the initial data $v(x, 0)$ ƒ≡ 0, $\nabla \cdot v(x, 0) = 0$ and the solution to the NSP exists for all $t \geq 0$, then one proves that the solution $v(x, t)$ to the NSP has the property $v(x, 0) = 0$.

This paradox (the NSP paradox) shows that the NSP is not a correct de- scription of the fluid mechanics problem for incompressible viscous fluid and the NSP does not have a solution defined for all $t > 0$. In the exceptional case, when the data are equal to zero, the solution $v(x, t)$ to the NSP does exist for all $t \geq 0$ and is equal to zero, $v(x, t) \equiv 0$.

These results are proved in [1]–[4].

These results solve one of the millennium problems.

Key words: The Navier-Stokes problem

Biography

Alexander G. Ramm was born in Russia, emigrated to USA in 1979 and is a US citizen. He is Professor of Mathematics with broad interests in analysis, scattering theory, inverse problems, theoretical physics, engineering, signal estimation, tomography, theoretical numerical analysis and applied mathematics. He is an author of 708 research papers, 20 research monographs and an editor of 3 books. He has lectured in many Universities throughout the world, gave more than 150 invited and plenary talks at various Conferences and had supervised 11 Ph.D students. He was Fulbright Research Professor in Israel and in Ukraine, distinguished visiting professor in Mexico and Egypt, Mercator professor, invited plenary speaker at the 7-th PACOM, he won Khwarizmi international award in 2004, and received many other honors. A.G.Ramm has solved inverse scattering problems with fixed-energy scattering data, with non-over-determined scattering data and studied scattering problems with under-determined scattering data. He solved many specific inverse problems and developed new methods in this area. He solved the many-body wave scattering problem when the bodies are small particles of arbitrary shapes and used this theory to give a recipe for creating materials with a desired refraction coefficient. These results attracted attention of the scientists working in nanotechnology. He gave formulas for the scattering amplitude for scalar and electro- magnetic waves by small bodies of arbitrary shapes and formulas for the polarizability tensors for such bodies. He gave a solution to the Pompeiu problem, proved the Schiffer's conjecture and gave first symmetry results in harmonic analysis. He has developed the Dynamical Systems Method (DSM) for solving linear and non-linear operator equations, especially ill-posed. He developed a random fields estimation theory and studied convolution equations with hyper-singular integrals. recently, he solved the millennium problem, the Navier-Stokes problem (NSP) and proved a paradox in the NSP which shows the contradictory nature of the NSP and the non-existence of its solution on the interval $t \in [0, \infty)$ for the initial data $v0(x)$ ƒ≡ 0 and $f(x, t) = 0$.

Dr. Anne M. Gaffney

University of South Carolina, USA

Plastic trash to monomers and intermediates – PTMI

To address the issue of waste plastics in landfills, a hybrid approach 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 value-added 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, 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 the products 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.

Biography

Dr. Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished 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.

SPEAKERS

DAY 01

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Md Nurul Islam Siddique*, Zaied bin Khalid
University Malaysia Terengganu (UMT), Malaysia

Application of additional nutrients on Bio-methane generation from anaerobic digestion of agricultural waste: Viability & Fertilizer recovery

The enhancement of demands for the organisms drew in with anaerobic digestion could be the result of different substrates digested simultaneously. The effect of supplements on the co-digestion of growing substrates was investigated in this study. At three phases, 37 °C, 40 °C, and 50 °C, an extra improvement plan that anticipates a crucial occupancy in anaerobic digestion was applied. The results showed that with improvements, biogas output increased to 1.38 times that of the control at 37 °C. Furthermore, the fantastic use of this mid-temperature that had been discovered hugely influenced an interesting philosophy as a result of 40 °C without additives (56 percent of VS end and 8.4 L-biogas). The anaerobic co-digestion at 50 °C revealed that biogas output exceeded 11.3 L with supplements, and mL-CH_4/g-VS was 1.24 times that of the system without any additional enhancement. The results show that the enhanced course of action improves co-digestion at each temperature. On the advanced scale, 37 °C was the most commonly used temperature and had the greatest impact on the use of improvements during the anaerobic process. From the digester, sludge was recovered at a rate of 0.09 m^3 sludge/m^3 substrate, and water was recovered at a rate of 0.86 m^3 sludge/m^3 substrate. The sludge that has been processed can be used as compost, and the water can be used for irrigation. The amount of time required to regain the investment was observed to be 3.77 y.

Audience Take Away:

- Anaerobic digestion (AD) collects methane and provides a source of renewable energy that is carbon neutral i.e. provides energy with no net increase in atmospheric CO_2. Fertilizer - compared to undigested slurry, the nitrogen in digestate is more readily available as a plant nutrient.
- Farming waste production around the globe is up to 6 million tons yearly. From these wastes, those that originate from regular trade are yet disposed of in landfills and used for the ignition method with no treatment. This methodology, along these lines, prompts higher GHG emanations and environmental pollution. Anaerobic co-fermentation has been demonstrated to be a successful methodology for improved bio-methane generation from wastes. The mix of different substrates improves nutrition in the digestion system. Thus, microbes have access to supplemented media with an appropriate nutrient equalization. The fundamental targets of co-digestion ought to support valuable associations, keeping away from hindrance and upgrading methane generation. Yes, this research that other faculty could use to expand their research or teaching. Yes, this provides a practical solution to a problem that could simplify or make a designer's job more efficient. Yes, it improves the accuracy of a design or provides new information to assist in a design problem. all other benefits are listed below:
- Improved hydrolysis, pathogen removal, and minimum odor are the key benefits of a thermophilic run.
- On the other hand, the mesophilic run saves energy and is not affected by shock loading than a thermophilic run.
- Besides, a vast microbial community is estimated under a mesophilic state that may help to digest numerous types of organic substances.
- The thermophilic state helps the elimination of pathogens and produces enhanced methane. Nevertheless, the use of intermediate temperatures has not been studied deeply which can influence the system.
- The related works found in the literature didn't study the gap between the feasibility study and fertilizer recovery. Therefore, our work is novel and has detailed data and explanations on the feasibility study and fertilizer recovery.

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. She has published more than 40 research articles in ISI journals.

Nur Zalin Khaleda Razali, Sheikh Ahmad Izaddin Sheikh Mohd Ghazali, Suhaila Sapari, Fazira Ilyana Abdul Razak, Nur Nadia Dzulkifli*
Universiti Kebangsaan, Malaysia

Synthesis, characterization and corrosion inhibition study on 2-chloroacetophenone 4-ethyl-3-thiosemicarbazone: Weight loss and DFT methods

Corrosion is a process of continual deterioration of metals caused by the action of the corrosive medium. Mild steel is often used as a construction material in the industry because of its relatively low price. However, it has low corrosion resistance, therefore some form of a protective film should be applied to prevent it from rusting in the corrosive environment. Therefore, a corrosion inhibitor is used to overcome the corrosion problem. Thiosemicarbazone derivative is one of the Schiff base ligands that can inhibit corrosion due to the presence of electronegative atoms such as N, S, and π electrons that can cause an efficient adsorption action on the mild steel surface. This research aims to synthesise a thiosemicarbazone ligand derived from 2-chloroacetophenone and 4-ethyl-3-thiosemicarbazide, namely as 2-chloroacetophenone 4-ethyl-3-thiosemicarbazone (2ClAcTSC). The structure of 2ClAcTSC was confirmed using an elemental analyser, UV-Vis, NMR and ATR-FTIR. The inhibitive effects of 2ClAcTSC were studied on mild steel in 1 M hydrochloric acid (HCl) and sulfuric acid (H_2SO_4) by using the weight loss method and Scanning Electron Microscopy (SEM). It was found that the 2ClAcTSC has better effectiveness in HCl rather than H_2SO_4 solution. Moreover, the inhibition efficiency increases as the inhibitor concentration increases. The SEM results verified that the inhibitor had been adsorbed on the mild steel surface to form a protective layer. DFT computations are performed to correlate inhibitor efficiency with intrinsic molecular parameters. The study revealed that the results obtained are consistent with the experimental data reported.

Audience Take Away:

- Introduction of thiosemicarbazone derivatives that have potential to be applied in various fields.
- The thiosemicarbazone derivatives potential to coordinate with metal ions to form complexes.
- The properties of thiosemicarbazone derivatives potential to be explored using computational method.

Biography

Dr. Nur Nadia Dzulkifli studied Chemistry by Research (Inorganic Chemistry) at Universiti Kebangsaan Malaysia as Ph.D. student in 2018. Her research group is called as MaterInOleo Research Group (Material Science, Oleochemistry, and Inorganic Chemistry). She is currently working as a Senior Lecturer at Universiti Teknologi MARA, Negeri Sembilan Branch. Her research field is mainly in corrosion study and inorganic chemistry. Besides that, she is planning to expand her research into DFT study and Material Science.

Ashanendu Mandal
University of Calcutta, India

Adsorptive removal of toxic phenol from industrial wastewater to reduce water pollution

Phenol being toxic in nature needs to be removed from industrial wastewater to protect the environment. Among various technologies for phenol removal, adsorption has been considered most popular due to simplicity and low-cost. In this research adsorptive removal of phenol has been investigated using eight adsorbents viz. guava tree bark, rice husk, neem leaves, activated carbon from coconut coir, rice husk ash, red mud, clarified sludge from basic oxygen furnace and activated alumina. The surface characterizations of the adsorbents have been carried out by SEM, XRD, FTIR and BET analyzers. The experimental investigations of phenol removal have been carried out by changing the 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 phenol removal percentage was obtained as high as 97.50%. The kinetic, isotherm and thermodynamic studies have been incorporated in details to analyze the actual adsorption mechanisms. The innovative ANN modeling have been studied to check the applicability of experimental results in the unknown process conditions in the industry. The scale-up designs have been worked out for using the pilot results for their commercial applications. The safe utilizations of used adsorbents for manufacturing bricks have also been studied for their effectiveness. The regenerations of adsorbents have been studied to meet the supply criticalities of fresh adsorbents. The research concludes that this simple and safe adsorptive removal process of phenol from wastewaters using these low-cost adsorbents is effective for practical applications in several industries and also for creating circular economy in third world countries.

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 17 countries as invited speaker, panelist, roundtable moderator and session chairman.

T. Shiyani
Asiatic Institute of Science & Technology, India

Solar photoelectrochemical energy conversion

Solar energy harvesting through photoelectrochemical conversion is the most promising technology for renewable energy production. Nanoscience and nanotechnology have enabled the development of hybrid and multifunctional materials for harnessing solar energy. Hybrid nanomaterials consist of more than two nanomaterials to improve the individual performance of the components. Natural photosynthetic biomaterials such as photosystem I, photosystem II, proteins and bacteria extracted from various leaves, plants or fruits can be used with inorganic nanomaterials to enhance the efficiencies of hybrid solar cells. Natural dyes can absorb the light in a wide range of wavelengths. Artificial photosynthetic systems such as photoelectrochemical cells may be built using biohybrid materials for solar energy conversion at a low cost and in an eco-friendly manner. The dye-sensitized PEC achieved energy conversion efficiency from 0.2 to 0.7% with zinc oxide. Solar energy conversion using these hybrid photoelectrodes may lead to an eco-friendly and cheap way of generating solar fuels in the future. The hybrid devices can also be useful for photoelectrochemical cell and water splitting applications. Hybrid solar cells can change the path of next-generation hybrid solar cell technology. Hybrid devices may be useful to generate solar fuels to meet the energy demand in the future.

Audience Take Away:

- Audience will learn about photoelectrochemical energy conversion for generating solar power and solar fuel.
- The talk will explore green energy production and upcoming students and faculties may involve in this area for research and may provide job in green energy.
- The proposed technology can be commercialized with collaboration of academia and industries.

Biography

T. Shiyani studied Physics at Saurashtra University, Rajkot, India and graduated as MS in Physics. He then joined the research group of Prof. R. C. Budhani at IIT Kanpur and PDPU. He pursued research at Central University of Gujarat, India. He has established a non-profit research organization, named Shiyani Research Institute to research. Recently, he joined Asiatic Institute of Science & Technology for education and research.

Bijoy Biswas

CSIR-Indian Institute of Petroleum (IIP), India

Catalytic hydrothermal liquefaction of macroalgae for the production of higher ester functional compounds

Liquefaction of biomass with proper solvents is a process that can prospectively be integrated with optimized conditions to produce fuel and valuable chemicals. Thus, the solvent might have an effect on the yield and composition of the crude bio-oil and other fractions produced from hydrothermal liquefaction (HTL). HTL of macroalgae using ethanol and methanol as the solvent produced ester compounds. However catalysts can be enhanced the ester compounds and several researches using the different catalysts for the production of ester compounds. While homogenous base catalytic HTL of macroalgae has been reported by several researchers, the use of solid base catalyst as a more economically viable choice has not been examined. The production of selective functional group compounds or quality bio-oil would call for further catalytic screening of algal biomass. In this study, higher selective ester compounds were produced by using various solid base catalysts (CaO supported on CeO_2, Al_2O_3, and ZrO_2) in HTL of macroalgae at different reaction temperatures, catalyst amounts and also involving the use of co-solvent. The possible reaction mechanism of ester functional compound formation was also explored.

Biography

Dr. Bijoy Biswas graduated (M.Sc) in Chemistry at the Indian Institute of Technology, Chennai, India, in 2013. He then joined the research group of Prof. Thallada Bhaskar at the CSIR-Indian Institute of Petroleum, India, at Material Resource Efficiency Division (MRED). He has contributed for the conversion of lignocellulosic biomass lignin, and aquatic biomass into high value products by applying thermochemical process such as pyrolysis and hydrothermal liquefaction (HTL). He optimized the reaction parameter for the production of selectively higher functional chemicals. The novelty also includes the role of temperature, solvents, catalysts, environment for enrichment of high value compounds using low value and abundantly available waste biomass. He has to his credit around 37 research publications in international peer-reviewed journals, 10 reputed conferences, and 8 book chapters and having more than 1212 citations with an h-index of 16.

Meera Yadav*, Takio Nene, Anindita Hazarika and Shilpa Saikia

North Eastern Regional Institute of Science and Technology, India

Oxidoreductase-metalloenzymes: Catalysis in green chemistry domain

Metalloenzymes namely lignin peroxidases, manganese peroxidases, versatile peroxidases, peroxidases and catalases are oxidoreductase group of enzymes that catalyses H_2O_2 dependent oxidation reactions. Discussion will deal on kinetics of enzyme catalyzed reaction with respect to aims of enzyme kinetic studies, steady state and transient state kinetics, enzyme activity measurements. These specific enzymes will be taken into account with respect to their isolation, different techniques used in purification of enzyme from crude extract, determination of enzyme characteristic parameters like Michelis-menten constant (Km), turnover number (Kcat), Kcat/km, Vmax, pH optima and temperature optima and nature of inhibition studies will be discussed. Mechanism of action, Immobilization studies on beads isolated from crustacean species and application of these enzymes in delignification of lignin containing cellulose materials, the degradation of recalcitrant organic pollutants such as phenol containing compounds, pesticides, azodyes, and polyaromatic hydrocarbons (PAHs), development of enzyme-based biosensors for monitoring of H_2O_2 and other hazardous wastes, and remediation of wastewater achieved by enzyme based immobilized micromotors, decolorization of pollutant dyes, soil treatment and conversion of high molecular weight coal fractions to low molecular weight coal fractions will be discussed. Consequently these enzymes provide very efficient tools for the removal and control of high H_2O_2 levels. Provide an understanding of role of an enzyme in metabolic pathways. Studies will be helpful to sort out complex kinetic mechanism, regulatory strategies of enzyme, identify new enzyme inhibitors and measure their potency for development of drugs.

Audience Take Away:

- Enzyme technology will provide efficient tools for removal of pollutants that persist in environment.
- Studies will be helpful to sort out complex kinetic mechanism and regulatory strategies of enzyme.
- Identify new enzyme inhibitors and measure their potency for development of drugs.

Biography

Dr. Meera Yadav completed her Master's and Ph.D in Chemistry from DDU Gorakhpur University, Gorakhpur, U.P. India. She was awarded CSIR-SRF, twice as DST- Woman scientist A and UGC- Dr. D. S Kothari Postdoctoral Fellow at Department of Chemistry, Gorakhpur University, Gorakhpur. Her research area includes, purification, characterization and applications of Metalloenzymes namely Lignin peroxidase, Mn-peroxidase, Laccase and Chloroperoxidase. Use of enzymes in synthetic inorganic and organic chemistry. Currently she is working as an Assistant professor in the Dept. of Chemistry, North Eastern Regional Institute of Science and Technology (NERIST), Nirjuli, Itanagar, A.P., India. She has participated in more than 30 national and international seminars and conferences. She has guided two Ph.D and five students are being involved in research activities and has published more than 30 research papers in reputed national and international peer reviewed journals, 3 books, 6 chapters in reputed standard books. She is life member of American Chemical Society, Indian Council of Chemists and Indian Society of Chemists and Biologists.

Prashanth S Adarakatti* and Mallappa M
SVM Arts, Science and Commerce College, India

Electrochemical sensing of mercury(II) using a nickel ferrite/graphitic carbon nitride nanocomposite modified screen-printed electrode as one-shot disposable sensor

A simple and novel strategy for electrocatalytic detection of mercury(II) ion was successfully achieved on nickel ferrite embedded graphitic carbon nitride modified screen-printed electrode (g-C_3N_4/$NiFe_2O_4$/SPE). g-C_3N_4/$NiFe_2O_4$ composite was prepared by co-precipitation method and was characterized by various analytical spectroscopic techniques. The detailed studies confirmed that the synthesized g-C_3N_4/$NiFe_2O_4$ were crystalline, grown well in high density and exhibited good electrocatalytic properties. The electrochemical detection of mercury(II) ion at g-C_3N_4/$NiFe_2O_4$/SPE has been studied by using cyclic voltammetry (CV) and differential pulse anodic stripping voltammetry (DPSV). The results illustrate that g-C_3N_4/$NiFe_2O_4$ composite modified SPE has showed better electrocatalytic activity towards mercury(II) detection than that of bare SPE, g-C_3N_4/SPE and $NiFe_2O_4$/SPE in acetate buffer solution of pH 5. The proposed sensor showed acceptable reproducibility and stability under optimal conditions with high accessible surface area and antifouling properties. Additionally, the sensor showed very good linear range from 10 - 900 nM and based on the calibration plot, limit of detection (LOD) was calculated and was found to be 2.35 nM. Further, the proposed electrochemical sensor has been successfully employed to determine mercury(II) content in real sample matrices.

Audience Take-Away:

- Here in this proposed research work, a simple and rapid detection of mercury ions have been determined as this element is toxic to mankind and environment.
- The fabrication of electrode opens a new avenue for the determination of various analytes.
- The audience will be able to understand some fundamental terminologies like linear range, detection limit, repeatability, reproducibility and stability of the modified electrode.
- Especially, in designing new electrodes, these kind of work really help them to understand this basic phenomenon.
- Researchers can be used these bespoke screen-printed electrodes for the analysis of various real sample matrices which in turn they do get a job in industries.
- The prepared low cost material can be prepared in bulk and can be used for various applications.
- It really opens a new avenue in analytical chemistry domain. As these electrodes are one-shot disposable sensors and can be analyzed the target analytes on spot and these electrodes required no polishing or smoothening. And it demands very low volume of the analyte which is being analyzed.

Biography

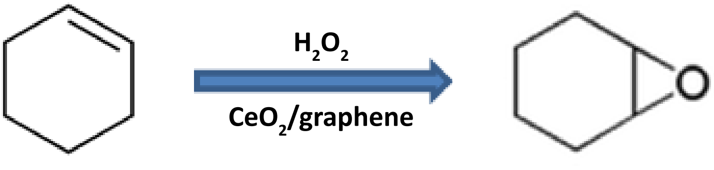
Dr Prashanth S. A., completed his Graduation in 2010 from JSS Degree College, Dharwad, India. He did his Post graduation in 2012 from P. C. Jabin Science College, Hubballi, India. He completed his Doctorate degree in 2017 from Central College, Bangalore University, India. Then he started his Postdoctoral studies in Indian Institute of Science (IISc), Bengaluru, India. Presently he is working as Assistant Professor of Chemistry in SVM Arts, Science and Commerce College, ILKAL, affiliated to Rani Channamma University, Belagavi, Karnataka, India. He published more than 50 international peer-reviewed articles in refereed journals which includes ten book chapters in RSC and Elsevier publications. He recently awarded International Young Scientist award and Member of Royal Society of Chemistry (MRSC), Cambridge, UK. Presently, he joined as a Visiting Scientist under the guidance of "Bharat Ratna Prof. CNR Rao" ICMS, JNCASR, Bengaluru, India. His research interests are electrochemical sensors, electroanalytical chemistry and materials chemistry for energy storage applications.

Salga E G and Binitha N Narayanan*

University of Calicut, India

Green synthesis of CeO_2/graphene nanocomposite for cyclohexene epoxidation

Liquid phase exfoliation of graphite has the advantage of producing high-quality graphene sheets. But the successful solvents chosen for graphene production via graphite exfoliation are toxic in nature and the yield is also limited. The commonly employed graphite oxide assisted route proceeds in a highly corrosive medium liberating enormous pollutant gases. Here a surfactant assisted exfoliation of graphite is preferred due to the improved yield of graphene and the eco-friendly nature of the process. Water is employed as the exfoliating agent in the presence of Pluronic triblock copolymer P123 surfactant. Incorporation of CeO_2 is performed via hydrothermal treatment of the cerium hydroxide – graphene dispersion. Material characterization studies revealed the presence of fluorite structure of ceria and exfoliated nature of graphite. The prepared nanocomposite is effectively used in the oxidation of cyclohexene using hydrogen peroxide with a very high selectivity to cyclohexene epoxide.



Audience Take Away:

- A green preparation method of graphene that can be used as an alternate to commonly investigated graphite oxide assisted routes.
- The whole preparation can be done in aqueous medium without employing any drastic oxidizing medium in graphene preparation.
- Audience can extend this green method of preparation of graphene for the preparation of different composites of graphene in aqueous medium. This preparation can be taken as a model of practicing green chemistry in graphene preparation. Can be executed as a prototypical for nanomaterial preparation even in UG laboratories.

Biography

Dr. Binitha N Narayanan studied Chemistry at the Cochin University of Science and Technology, India and graduated as MSc in Applied Chemistry in 2001. She then joined the research group of Prof. Sugunan S at the Department of Applied Chemistry, Cochin University of Science and Technology, Kochi, India. She received her PhD degree in 2007 at the same institution. She joined as Assistant Professor in Chemistry at Sree Neelakanta Govt. Sanskrit College Pattambi in 2006 and meanwhile had done one-year postdoctoral fellowship (2008-2009) supervised by Prof. Dr Zahira Yaakob at the Department of Chemical and Process Engineering, National University of Malaysia, Malaysia. She was an Associate professor at Sree Neelakanta Govt. Sanskrit College Pattambi from 2019-2022. She moved to University of Calicut as Professor in the Department of Chemistry in March 2022. She has published more than 60 research articles in SCI(E) journals.

Jie XU*, Brodu N, Youssef B, Taouk B

INSA Rouen Normandie, France

Biobased novolac resins cured with DGEBA using water-insoluble fraction of wood pyrolysis bio-oil: Synthesis and characterization

The water-insoluble fraction of bio-oil products obtained from intermediate pyrolysis and fractional condensation of beech wood biomass were used as a phenolic source to substitute phenol for the synthesis of Novolac Resin. The replacement of formaldehyde considered an atmospheric pollutant was also studied. The ratio of phenolic fraction from bio-oil were added to partially substitute for phenol and until completely replace from 25% to 100% to synthesize bio-oil phenol acetaldehyde (BPA) resins. Simultaneously, two concentrations of hydrochloric acid catalyst (1% and 10%) were examined to understand the effect of the catalyst on the reaction between bio-oil and aldehyde. The kinetic parameters of the curing reaction using Bisphenol A diglycidyl ether (DGEBA), as a formaldehyde-free cross-linker for bio-oil based novolac resins were evaluated with model-free methods using data obtained from differential scanning calorimetry (DSC). Physicochemical and thermal properties of BPA resins were determined before and after curing and compared in the function of different synthesis conditions.

The results showed that the higher the proportion of bio-oil is, the more the properties of Novolac resin deviated from standard phenol resins. The presence of bio-oil promoted the curing reactions. Indeed, the curing reaction of all the BPA resins started early than PA resin. The peak temperature at maximum rate and the activation energy (Ea) of BPA resins were lower than that of PA at a low bio-oil ratio (≤75 wt %). It was also observed that the char yield at 800°C of resins increased and reached the highest value at 100% BPA due to the occurrence of cross-linking reaction between novolac resins and DGEBA.

Under 10% of HCl catalyst, all cured and uncured Novolac BPA resins are more stable. The high catalyst content can shorten the defect of incorporating bio-oil and can produce excellent bio-oil based resins with less free phenols and aldehydes, higher yield, and higher molecular weight. High content of catalyst allows BPA to decrease the activation energy (Ea) when curing with DGEBA and its properties are also closer to PA resin.

Audience Take Away:

- The audience will be able to learn some skills of applying bio-oil to replace phenol to synthesize bio-oil novolac resin.
- At the same time, many analytical instruments have also been applied to characterize the physical and chemical properties of the prepared resin (FT-IR, H-NMR, GPC, HPLC, GC-FID, GC-MS, DSC, and TGA), which will also help readers in their future studies.
- The audience will know how to use differential scanning calorimetry (DSC) to study the curing reaction of bio-oil based novolac resin and DGEBA. The obtained data will further use model-free methods to calculate the kinetic parameters of curing (Ea, reaction order).

Biography

PhD student Jie XU studied Chemical engineering and technology at the Shaanxi Normal University, China, and graduated as MS in 2018. She then joined the research group of Prof. Taouk at INSA Rouen Normandie, France. She started her PhD in chemical process engineering and will receive her PhD degree in 2022. She has participated in two international conferences and published 2 research articles in SCI journals. And there are also some research articles in preparation.

Salima Bouteraa*, Sarah Hamoud, Nourredine Bettahar

University of Sciences and Technology of Oran - USTO, Algeria

Study on structure and photocatalytic activity of lanthanum-containing mixed metal oxide derived from ZnFe- layered double hydroxides: An outstanding strategy for promoting visible light in indigo carmine photodegradation

With attempts to tune the photocatalytic activity of hydrotalcites catalysts and improving the photocatalytic performance via efficient separation of photoexcited electron-photogenerated hole. $ZnFe_{(1-x)}La_x$-LDH with variable Lanthanum cation contents (x = 0 to 5%) were prepared by well-known co-precipitation method followed by heat treatment at 600 °C. The synthesized photocatalysts were characterized by X-ray diffraction (XRD) and UV-visible diffuse reflectance spectroscopy (UV-Vis DRS). The analytical results showed that the crystallinity of the layered materials decreases as the La contents increases, probably due to the distortions introduced by the large difference in the ionic radii of the cations. UV-Vis DRS analysis demonstrated a decrease in the band gap of Lanthanum-substituted LDH compared to ZnFe-LDH. $ZnFe_{0.97}La_{0.03}$-600 was used as a photocatalyst to improve the degradation of IC under visible light in the presence of H_2O_2. In comparision, the kinetics of photo-discoloration is faster with $ZnFe_{0.97}La_{0.03}$-600 than with ZnFe-600. Indeed, a complete discoloration was obtained after 110 min and 240 min in the presence of $ZnFe_{0.97}La_{0.03}$-600 and ZnFe-600 respectively, the high photocatalytic activity of the sample was attributed to the addition of La(III). In addition, the study of the possible mechanism of photocatalytic degradation of IC by $ZnFe_{0.97}La_{0.03}$-600 showed that the $HO^{\bullet}$ and h^+ species plays a major role. The material showed high stability after two regeneration cycles with good efficiency.

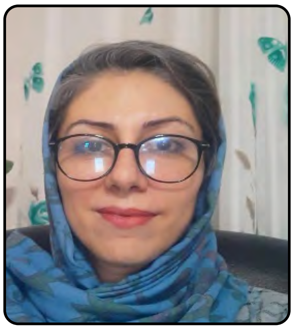
Keywords: LDH, co-precipitation, adsorption, $ZnFe_{0.97}La_{0.03}$-600, photocatalyst, visible light, indigo carmine dye.

Audience Take Away:

- The public will be able to use what they have learned in the role of hydrotalcites containing lanthanum
- The detailed characterization of catalysts was performed.
- The development of systems capable of operating under visible or solar light, which is abundant and free;
- Proposed mechanism of mineralization of the dye
- The catalyst can be used several times

Biography

Dr. Salima Bouteraa, A chemist researcher in inorganic materials chemistry at the Oran-MB University, Algeria with considerable industrial and analytical operations experience gained from working in the industrial and laboratorial sectors. Because her interest in environmental chemistry and chemistry of materials, she is doing her thesis in application of lamellar materials on wastewater depollution, specifically layered double hydroxides by adsorption, bi-adsorption and photodegradation of some dyes. She received her PhD degree in 2021 at the same institution. The scientific production during these years were 4 scientific peer-reviewed articles and 11 conferences.



Elnaz Asghari
University of Tabriz, Iran

Novel non-noble metal-based catalysts for renewable hydrogen production from seawater electrolysis

Hydrogen gas has a great potential for future replacement of fossil fuels. It is used in chemical plants and energy harvesting systems, thus, its production from renewable resources is of great importance. The water electrolysis driven by renewable energy resources such as wind or solar energy is one of the promising strategies to obtain renewable hydrogen gas. Due to the limited water resources the attentions have been attracted to the utilization of other sources such as seawater, brine and wastewater.

The main cathodic reaction in a water electrolyser is the hydrogen evolution reaction (HER); on the anode of a seawater electrolyser, however, there is a competition between the water oxidation (i.e. oxygen evolution reaction or OER) and the chlorine chemistry related oxidation processes especially the chlorine evolution reaction (CER). All these reactions have multi-step mechanisms and thus sluggish kinetics. Pt and Pd-based catalysts have shown the best electrocatalytic performances for HER and the Pt/C electrodes are used commercially for this reaction. The high costs and dissolution of Pt and other noble-metal based (or platinum group metal, PGM) catalysts in seawater are their main challenges. Ni is one of the main none PGM catalysts, however, the performance of these electrodes should be increased with novel nanotechnology and surface engineering methods.

The catalysts used for anode of a seawater electrolyser must also be cost-effective and noble metal-free (Rh and Ru are the best noble metals suitable for catalysis of anodic reactions). Since CER results in toxic and harmful chlorine gas, in most plants (mainly off-shore plants) the preferred anodic reaction is OER. Thus, the anodic catalysts must also be selective to OER. These catalysts must be structural and compositional engineered. The engineered surface defects, oxygen vacancies and using chloride blocking layers on the active catalyst layer are some examples of the recent strategies to prepare high performance, OER selective catalysts for hydrogen production from seawater electrolysis.

Here we would present a short overview on the recent cost-effective catalysts for catalysis of HER and OER. The challenges with seawater electrolysis and recent strategies to improve the efficiency of non-PGM catalysts and increase their stability are also discussed in brief.

Audience Take Away:

- The audiences will learn about the mechanism of HER and OER.
- They will learn about the Volcano plots for catalysis of HER and OER and the recently suggested non-PGM materials and structures.
- The subject is one of the recent most interested topics that many research groups can work on it and expand their research.

Biography

Dr. Elnaz Asghari studied Physical Chemistry at the University of Tabriz, Iran, and received her PhD degree in 2009. She then continued her work at the same department as an assistant professor. Now she is an associate professor and has published almost 30 research articles in SCI journals. Her current research interests are electrocatalysis and electrochemical energy conversion systems, the electrochemical synthesis and electrodeposition of different materials such as inorganic catalysts, optical materials, oxides, chalcogenides and conductive polymers.

Paweł Weroński* and Karolina Pałka

J. Haber Institute of Catalysis and Surface Chemistry, Poland

Roughness spectroscopy of particle monolayer: Implications for spectral analysis of the monolayer image

Surface roughness of particle monolayer is one of its fundamental characteristics, conventionally described in terms of power spectral density. First, we will discuss a general equation for this function and demonstrate its similarity to those applied in the theory of scattering. Specifically, it is a linear function of the squared form factor and static structure factor. The form factor is a Fourier transform of particle height profile and the structure factor is equal to the product of particle number density and Fourier transformed pair-correlation function, increased by one. The relationship suggests that roughness measurements of particle monolayers can be considered as a type of spectroscopy, in a wider sense of the term. Next, we will show that our approach can be generalized to virtually any monolayer image. Therefore, our results provide a framework for a quantitative, cheap, and easy method, based on statistical analysis of the digital monolayer image, for determining the particle pair-correlation function. The approach can be an attractive alternative to standard, expensive methods such as GISANS or GISAXS. The power spectral density provides also quantitative information on key parameters of the system: the particle radius, number density, and dimensions of analyzed area. Therefore, the theoretical model provides also a general framework for an automatic, potentially real-time parametrization of particle monolayers. Unlike in the methods currently used in image analysis, relying usually on individual particle identification, we do not have to localize each of the particles here. Instead, we just need to calculate the Fourier transform of the monolayer image and to least-squares fit the monolayer parameters. We will show that our analytical results are consistent with numerical ones derived for a system with parameters corresponding to typical experimental conditions. We will also demonstrate a practical application of our approach for spectral analysis of a monolayer image found in the literature.

Audience Take Away:

- The audience will be able to use the gained knowledge for statistical analysis of particle monolayer images. After determining the power spectral density of monolayer images with a standard software package for image analysis, the audience will better understand the characteristic variation of the function. The participants will also be able to determine the structure factor and pair-correlation function of the particle monolayers.
- Our preliminary results will help the audience to expand their teaching and research in the field of charactarization of particle monolayers. With further ongoing development, the faculty will be able to use the novel approach for determining key parameters of particle monolayers, such as particle size or surface coverage. This simple method will allow the researchers to increase the accuracy and efficiency of the measurements.

Biography

Dr. Weroński studied Physics at the A. Mickiewicz University in Poznań, Poland, and graduated as MS in 1989. He then joined the research group of Prof. Adamczyk at the Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences (ICSC-PAS). He received his PhD and DSc degrees in 2000 and 2008, respectively, at the same institution. He earned two postdoctoral fellowships: at the Chemical Engineering Department of Yale University and at the Theoretical Division of Los Alamos National Laboratory. He works as an Associate Professor at the ICSC. He has published more than 50 research articles in SCI(E) journals.

Carina B. Maliakkal*, Erik K. Mårtensson, Daniel Jacobsson, Marcus Tornberg, Sebastian Lehmann, and Kimberly A. Dick

Karlsruher Institute of Technology, Germany

Layer growth dynamics in compound nanowires studied by in-situ microscopy

Nanowires are often grown by the vapor-liquid-solid (VLS) mechanism whereby the reactants supplied in the vapor phase dissolves in the liquid metal, supersaturates and eventually precipitates layer-by-layer as a solid nanowire. This liquid alloy is referred to in the nanowire community as a ‘catalyst’ though the exact role of this liquid alloy is still controversial. The exact dynamics of the nanowire is also still unclear. In-situ transmission electron microscope (TEM) during growth of nanowires inside a TEM provides directly interpretable results. Here we discuss compound nanowire growth mechanism studied by in an environmental TEM, using GaAs as a representative example. Au nanoparticles are used to seed the growth.

While the nanowires were growing at different conditions, we measured the particle composition using energy dispersive X-ray spectroscopy.[1] There is significant amount of Ga alloyed into the Au seed particle, but there is hardly any As in the catalyst[1], in agreement with theoretical predictions. This asymmetry in the catalyst composition to the two different components – As and Ga – effects the layer growth dynamics. Growth dynamics in nanowires have two important parts – the nucleation of each layer at the catalyst-nanowire interface followed by lateral growth of the nucleus to a full bilayer. Unlike assumed by most theoretical models of nanowires, and unlike observed in growth of elemental nanowires, the layer completion is not instantaneous.[2] We observe that the Ga flow directly controls the nucleation of each new layer, without a direct effect on the layer completion process. Arsenic on the other hand limits the completion of each nucleated layer. Thus, owing to the difference in solubility of Ga and As in the catalyst it is possible to controlling nucleation and layer growth using precursor flow independently.[2]

An alternate mechanism, where the catalyst used for promoting axial growth of nanowires is a solid, is called the vapor–solid–solid (VSS) mechanism. VSS offers certain advantages compared to the common VLS route, however, it is much lesser understood than the VLS route. The in-situ TEM investigation of VSS growth of compound nanowires has been recently reported.[3]. The layer growth kinetics and dynamics at the wire–catalyst interface are investigated for liquid and solid catalysts under similar growth conditions. The temperature and thermal history of the system are manipulated to control the catalyst phase. The VSS growth rate is comparable or slightly slower than the VLS growth rate. The incubation time for the VSS growth is not necessarily very different from the VLS counterpart. Layer completion time is found to be very similar for VLS and VSS under comparable growth conditions, indicating that the diffusion of reactants through the solid catalyst particle during VSS growth is not the growth rate limiting step. During VLS growth each new layer started only after the completion of the previous layer, while occasions with multilayer growth is observed during VSS.

Audience Take Away:

- Strategy to measure composition of nanomaterials at elevated will be explained.
- A direct comparison of nanowire growth dynamics when two different phases of catalyst (i.e. solid and liquid) are investigated.
- Though nanowires are promising for future technological applications, a deep understanding of the growth process is still lacking. In-situ TEM can provide valuable insights to understand nanowire growth, in turn enabling intentional engineering of nanowire properties.

Biography

Dr. Carina B. Maliakkal recently moved to Karlsruher Institute of Technology as postdoctoral fellow and is working on in-situ TEM investigation during exhaust gas treatment with focus on CO oxidation. Before that she was a researcher at Lund University investigating compound nanowire growth in-situ while the nanowire is growing using TEM. Her PhD research at TIFR, India was based on understanding the growth of III-V semiconductor nanowires.

KEYNOTE FORUM

DAY 02

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28-29 MAR

Gopa Mishra, K. M. Parida, and S. K. Singh*

Materials Technology Department, India

Metal oxide modified silicon carbide nanocomposites

Silicon Carbide has been one of the semiconductors prominently known for its attractive physical and chemical properties for several decades. It continues to be the main driving force for current and future research. Silicon carbide (SiC) exhibits high thermal conductivity, high resistance towards oxidation, high mechanical strength, low specific weight, and chemical inertness. These attributes could lead to SiC-based catalysts becoming widely used new catalytic materials for many years.

The intimate mixture of SiO2 and C in the rice husk (considered agricultural waste) provides an ideal platform for SiC synthesis. A single step has been adopted to prepare SiC directly from raw rice husk in an indigenously developed pot-type extended arc plasma reactor using graphite electrodes. The plasma-produced product was very fragile. The ultrafine SiC could easily be produced by ball milling.

This paper presents the synthesis of different metal oxides (TiO_2, SO_4, WO_3, VPO) modified SiC nanocomposites by various wet chemical methods. The physico-chemical properties of the synthesized materials have been studied by various characterization processes (XRD, FESEM, BET, TEM, XPS, FTIR, UV-Vis DRS, PL, etc.). The catalytic activities of metal oxides promoted SiC have been evaluated towards environment pollution abatement, energy production, and industrially important organic transformation reactions. (i) A series of β-SiC/TiO_2 nanocomposites (5-25 wt%) has been successfully fabricated by a sol-gel process, and the photocatalytic activities of all the β-SiC/TiO2 nanocomposites have been studied for aqueous Rhodamine B (Rh-B) dye degradation under solar light irradiation. (ii) A series of sulfate-modified TiO_2/β-SiC nanocomposite photocatalysts have been fabricated by sol-gel and wetness impregnation method. The photocatalytic activity of the synthesized catalysts has been evaluated toward hydrogen energy production in the presence of visible light. (iii) A series of tungstate-promoted β-SiC catalysts (5-20 wt%) has been tested in liquid phase esterification of acetic acid with n-butanol in a solvent free medium. (iv) A series of VPO/β-SiC composite materials (5-20 wt%) has been successfully fabricated by the wetness impregnation method, and the catalytic activities of VPO/β-SiC composites have been studied in a solvent-free oxidation of methanol using tert-butylhydroperoxide (TBHP) as oxidant.

Biography

Dr. Saroj Kumar Singh obtained M.Tech. & Ph.D. (Materials Science) from I.I.T., Kharagpur. He retired as Professor in AcSIR, Chief Scientist, and Head of Advanced Materials Technology Department of CSIR-IMMT, Bhubaneswar, in 2016. At present, he is working as Emeritus Scientist in CSIR-IMMT, Bhubaneswar. His research specialization areas are Materials Science, Thin films, Plasma Processing of ores, minerals, wastes, nano-materials, etc. He has published more than 270 scientific publications and 18 patents. He has guided ten students for their Ph. D. dissertations and several M.Sc., B.Tech., M.Tech thesis works. He has been adorned with several fellowships and awards, including the BOYSCAST Fellowship, Govt. of India, DAAD fellowship, Venus International Research Awards (Lifetime Achievement) -VIRA 2016 (Specialization – Materials Science & Plasma Processing), etc. He is also an Editorial Board member, Editorial Advisory Board member of Elsevier and Bentham science journals.

J H. Kang, G. N. Ahn, H. Lee, S. J. Yim, S. Lahore, H. J. Lee, H. Kim, J. T. Kim and D. P. Kim*

Pohang University of Science and Technology (POSTECH), Korea

Scalable subsecond synthesis of drug scaffolds by numbering-up 3D-printed metal microreactor

Continuous-flow microreactors enable ultrafast chemistry impossible in conventional batch reactor through the subsecond reaction time control. However, the small capacity of microreactors has restricted the synthesis of pharmaceutical compounds with industrial level productivity. In this work, a scalable subsecond synthesis of drug scaffolds was achieved by a new numbering-up strategy. The compact monolithic 4 numbering-up metal microreactor (4N-PMR) that is embedded with built-in reactors and flow distributors was fabricated by high-resolution 3D SLM printing method. And the 4N-PMR verified successful controlling of highly reactive short-lived aryllithium intermediates at optimal residence time (~16 ms) over a wide range of temperatures and furnished the increased productivity of 12 aryl products in very good to excellent yields (86-98 %). The excellent symmetry of built-in flow distributors of monolithic 4N-PMR afforded nearly same yields as single microreactor within experimental error range. Moreover, 16 numbering-up printed metal microreactor (16N-PMR) was assembled with four 4N-PMRs and external flow distributors (EFDs) to render high productivity of 3 drug scaffolds without significant loss of yield, including precursor of letrozole as an aromatase inhibitor. Highly uniform flow distribution in EFD and 16N-PMR was numerically and experimentally demonstrated for successful scalable subsecond synthesis that is less tolerable to the change of flow rates. The actual isolation of 10 to 20 grams of drug scaffolds for 10 minutes enables the production up to nearly 3 kilograms per day in a single 16N-PMR set. Facile multiple sets in virtue of 3D printing method can meet various scales of drug scaffolds in pharmaceutical industry. Moreover, the modular system would be readily reconfigurable for a variety of scale-up purposes on demand synthesis.

Audience Take Away:

- Unique advantages of microfluidic approach for chemical synthesis
- How to improve the labor-intensive, low-efficient batch process using microreaction technology
- How both engineering and chemistry are integrated to make d synergic effect in synthesis.

Biography

He obtained Ph.D. in chemistry at Temple University in 1991, then post-doctor in University of Illinois at Urbana-Champaign, and back to Korea Research Institute of Chemical Technology at 1993. As he has worked for nearly 30 years at academic institutes, flow chemistry in microreactors become his major field, including a scale-up of API and DDS with automation. He has published >300 peer-reviewed papers and >40 patents and won Academic Excellence Award (2017, Korean Chemical Society), POSTECHIAN of the Year (2016, POSTECH), The Scientist of the Month (2016,NRF) and Yonsan chaired professor of POSTECH.

Byong H. Lee

Department of Microbiology/Immunology, McGill University/AAFC,
Montreal, Canada

Biocatalysis of fermentation derived probiotic enzymes and their commercial applications

Benefits of probiotic bacteria and microbiomes in treating a variety of health conditions, especially digestive-, inflammatory-, allergic-, cancer- and obesity-causing diseases are also bringing this beneficial bacterium into the forefront of mainstream media. However, it is still unclear on their mechanism of action and the use of molecular tools is of paramount important to assess the probiotic properties. Unraveling the probiotic and microbiota mechanisms of action could open a new era for further enhancement of various applications and looking ahead this field holds immense promise for the future in delivering novel biotherapies in different fields. We found the tremendous metabolic activities and high specific enzyme activities in cells of *Lactobacillus* and *Bifidobacterium*, thus we genetically overproduced few probiotic enzymes such as aminopeptidase, esterase/lipase, lactase (beta-gal), bile salt hydrolase, and linoleate isomerase, etc for overproducing bioactive molecules and for positively influencing overall human health by using animal and human models.

Biography

Professor Byong H. Lee is currently a Scientific Advisor at SportBiomics (CA, USA) and Heilenex Pharma Inc. (Toronto, Canada). Byong has worked as Professor (AAFC seconded Chair) in Departments of Microbiology/Immunology and Food Science/Agric Chemistry (1986-2011) at McGill University in Montreal, Canada. He has been an Invited Distinguished Professor in the Department of Food Science and Biotechnology at Kangwon National University and Adviser at MSC Co. Ltd (2014-2019) in Korea. In addition, Byong has also worked as Distinguished Professor in Schools of Biotechnology and Food Science at China Jiangnan University (2011-2014) and Principal Scientist and Head of Biotechnology at Food R/D Center at Agriculture and Agri-Food Canada, AAFC (1982-1986) and Research Director at Sensient Flavor (Former Champlain Industry, 1980-1982) in Canada. Byong received his degrees at the University of British Columbia (MSc, Microbiology/Immunology), McGill University (M.Sc, Food Microbiology) and Laval University (PhD, Food Biotechnology) in Canada. Byong also studied his PhD for two years in Microbiology/Immunology at the University of Pennsylvania/Hahnemann Medical College in Philadelphia (US) as his Canada-US exchange program. Byong spent his sabbaticals as an Invited Professor in the UK (Food Research Institute/U. of Reading, 1991-1992), France (INRA/U. de Bourgone, 1997-1998), Ireland (Teagasc Food Research Centre, 2001-2002) and Korea (Seoul National University, 2007-2008).

Francisco Zaera

University of California,

New nanostructures for increased selectivity and stability in catalysis

One of the major challenges in heterogeneous catalysis is the preparation of highly selective and robust catalysts. The goal is to be able to synthesize solids with stable surfaces containing a large number of specific surface sites designed for the promotion of a particular reaction. New synergies between surface-science studies and novel nanosynthesis methodology promise to afford new ways to design such highly selective catalysts in a controlled way. In this presentation we will provide a progress report on a couple of projects ongoing in our laboratory based on this approach. Platinum-based catalysts have been prepared for the selective trans-to-cis conversion of olefins, with a design based on early surface-science work with model surfaces and quantum mechanical calculations that indicated a particular preference for (111) facets in promoting the formation of the cis isomers. We are currently extending this research by using the concept of “single-site catalysis” with Pt-Cu bimetallics for the selective hydrogenation of unsaturated aldehydes. In a second example, new metal@TiO_2 yolk-shell nanomaterials conceived for both regular and photo-induced catalytic applications have been used to promote CO oxidation at cryogenic temperatures and to suggest that in photocatalysis the role of the metal may not be to scavenge the excited electrons produced in the semiconductor upon absorption of light, as commonly believed, but rather to promote the recombination of the adsorbed atomic hydrogen initially produced by reduction of H^+ on the surface of that semiconductor. New mixed-oxide surfaces are being designed using atomic layer deposition (ALD) as well. Additional examples include the use of “click” chemistry to tether molecular functionality on porous solid materials and design tandem catalysts.

Audience Take Away:

- They will get exposed to the latest nanotechnologies as they are being applied to catalysis;
- A discussion will also be provided on ways to characterize these catalysts;
- Focus will be placed on the need for modern catalysts to be highly selective, and on how to achieve such selectivity.

Biography

Francisco Zaera received his Licenciate and PhD degrees from the Simón Bolívar University (Venezuela, 1979), and the University of California, Berkeley (1984), respectively. He was an Assistant Chemist at Brookhaven National Laboratory (1984 -1986) before joining UCR, where he is presently a Distinguished Professor of Chemistry and Director of the UCR Center for Catalysis. Zaera has authored over 400 scientific articles, and has received multiple international awards, including the ACS Olah and Adamson Awards and a Humboldt Fellowship. He is a Fellow of the ACS, the American Vacuum Society, and the AAAS.

POSTER

DAY 02

10TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

28-29 MAR

Carlos Suárez* and Rogerio de Almeida

National University of San Marcos, Peru

Production of high-quality CuNi thin films using magnetron sputtering

Cu-Ni alloys are widely used in mining and metallurgical work, in the chemical industry due to their high resistance to corrosion, mechanical and catalytic properties. Furthermore, Cu-Ni alloys have received much attention for their thermophysical and magnetic properties and are also used for decorative purposes. They are applied to valves, hardware, condensers and heat exchangers, due to their excellent thermal and electrical properties and are particularly resistant to bio-contamination. CuNi alloys are normally manufactured by electrolytic processes. In recent years, interest in making films using less polluting process than electrolytic baths have increased considerably. However, the commercial electrodeposition of these alloys in cyanide baths as an example produces high quality deposits, but environmental problems arise in the use and disposal of this component. The use of plasma technologies for the deposition of thin films has been studied and, despite being a more complex and costly technology, it has the advantage of generating practically no waste.

There are many techniques to generate plasma. In this work plasma equipment generated by magnetron sputtering will be used. From the bibliographic review, it could be observed that there is not much research on the properties of thin films of binary CuNi alloys produced by plasma technologies. The aim is to investigate thin films composed of metal alloys produced by plasma and to be able to obtain the parameters of the process so that a stable, homogenous and reproducible thin film will be obtained.

We start with the production of an alloy Cu-Ni (70-30) produced by vacuum arc remelting process, so we obtained the targets that are going to be used in the magnetron sputtering, then using a high vacuum magnetron sputtering process with a flux of argon we obtained a Cu-Ni thin film deposited in a glass substrate, finally this thin film is characterized by SEM.

Audience Take Away:

- They can extrapolate the information learn in this presentation so they can apply and replicated in similar alloys for the production of thin films, using magnetron sputtering is going to be a more environmentally friendly process compared to normally use electrolytic baths.
- The audience that are not in touch with this technology can learn a new process for thin film production.
- This is a more environmentally friendly process so the audience can obtain thin films that before were produced by electrolytic baths.
- This is a novel process that, so far, has not been used in this alloy so there is a high potential for new materials production with this technique.

Biography

MSc. Carlos Suárez currently working for his doctor degree in Chemical Engineering in San Marcos University, studied chemistry at The San Marcos University, Perú and graduated in 2013 and in 2015 he started his MSc degree in pontifical catholic university of Perú, having a internship in Dresden Germany for his Ms. Thesis, obtaining the master's degree in Engineering and Material science in 2017. He has constantly been working in Material Science Publishing in 2019 in the polymer Bulletin his first international article. He is currently working in thin film materials.

SPEAKERS

DAY 02

10TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

28-29 MAR

Dr. Haimei Xu

Macquarie University, Australia.

Mesoporous zirconium oxophosphate catalyzed phenylglyoxal conversion

The one-step conversion of α-keto aldehydes to α-hydroxycarboxylic acids and their derivatives using solid acids is of great appeal in biomass utilization. In this work, ordered mesoporous zirconium oxophosphate (ZrPO) catalysts with tunable acidity were prepared and their catalytic performance was evaluated using phenylglyoxal (PG) conversion to ethyl mandelate (EM). The roles of Lewis acid sites (LAS) and Brønsted acid sites (BAS) of ZrPO were investigated by kinetic studies of PG conversion combined with temperature-programmed desorption of ammonia (NH_3-TPD) and solid-state NMR characterizations. It is found that the ratio of LAS to BAS on the ZrPO plays a dominant role in this reaction. ZrPO-0.75-500, with a LAS/BAS ratio of 2.1, was found to be the best catalyst. The reaction pathways, i.e., the direct isomerization of PG to EM by LAS and via the formation of an intermediate hemiacetal by BAS, are therefore proposed. Moreover, the effect of water on the catalytic activity was studied. A moderate amount of water induced either by catalyst pretreatment at the proper temperature or deliberately dosed on the ZrPO materials achieves a maximum catalytic activity. The highest catalytic activity, i.e., 82% of PG conversion and 92% of EM selectivity, was obtained on ZrPO-0.75-500 that was dosed by 15 μmol water per 50 mg of the catalyst. It is concluded that ZrPO with a suitable combination of LAS and BAS is required to efficiently and selectively catalyze the conversion of α-keto aldehydes to α-hydroxy carboxylic acid derivatives. It is feasible, from a practical point of view, to tune the density of LAS and BAS on the catalysts to achieve a better catalytic performance.

Audience Take Away:

- Stable multifunctional solid acid catalysts metal oxides (ZrPO) were fabricated. And their structural features and acidities towards intrinsic activity and selectivity in the transformation of biomass-derived PG via the Cannizzaro reactions were discussed.
- The roles of acidity (density, strength, and types of acid sites) were elucidated, and the reaction mechanisms were therefore proposed.
- These findings could aid the rational design of acid catalytic system in performing multistep cascade processes in one-pot catalytic biomass conversion in the future.

Biography

Dr. Haimei Xu studied Chemistry at Lanzhou University, China and graduated as BS in 2012. She received her master degree in 2015 at Lanzhou Institute of Chemical Physics, University of Chinese Academy of Sciences, China. In 2016, I then joined the research group of Associate Prof. Yijiao Jiang at Macquarie University, Australia. And she received her PhD degree in 2021 at the same institution. Now, she is working on the development of novel mesoporous catalysts for various biomass-derivate carbohydrates conversion reactions and she has published 12 research articles in SCI(E) journals.

Rahat Javaid* and Tetsuya Nanba
National Institute of Advanced Industrial Science and Technology, Japan

Synergistic effect of Ru/CeO_2/MgO catalyst on ammonia synthesis

Ammonia is a potential hydrogen and energy carrier. It has a high capacity for hydrogen. As an energy carrier, ammonia is considered an energy-dense and zero-carbon fuel. Industrially, ammonia is synthesized by the Haber-Bosch process using an iron-based catalyst. The significant drawbacks of this process include the requirement of high temperature (425-600 °C) and pressure (20-30 MPa) conditions as well emission of greenhouse gases. Green ammonia can be synthesized with hydrogen produced from the electrolysis of water using renewable energy. To utilize renewable derived hydrogen, it is required to develop catalysts with higher efficiency at mild reaction conditions. Ru catalysts are known for their higher activity at mild reaction conditions. In this study, Ru/CeO_2/MgO catalysts were prepared with various Ce/Mg molar ratios. CeO_2 and Ru were sequentially deposited on MgO by the impregnation method. The ammonia synthesis activity of prepared catalysts was determined using hydrogen and nitrogen as reactants. Ru/CeO_2/MgO catalyst with Ce/Mg molar ratio 0.1 showed 25% higher ammonia synthesis activity to that of pure CeO_2 supported Ru catalyst. Various characterizations and experiments for measurements of activation energy, ammonia, hydrogen, and nitrogen order were conducted. Relatively higher activation energy and positive hydrogen order were considered the plausible reasons for obtaining higher ammonia synthesis for Ru/CeO_2/MgO catalyst with Ce/Mg molar ratio of 0.1.

Biography

Dr. Rahat Javaid is a Research Scientist at Fukushima Renewable Energy Institute, National Institute of Advanced Industrial Science and Technology (AIST), Japan. Her research interests include synthesis of heterogeneous catalysts and their application to environmental and energy-related fields. She was awarded Gold Medal for getting first-class first position in M.Sc. Chemistry. She earned her Ph.D. degree from Tohoku University, Japan, under the Monbukagakusho MEXT Scholarship. After postdoctoral research experience at Tokyo Institute of Technology, Japan, she obtained the position of Research Scientist at the Fukushima Renewable Energy Institute, AIST. She participated in many national/international conferences and published many research articles.

Ji Wang

Ningbo University, China

The extended galerkin/rayleigh-ritz method for approximate solutions of nonlinear vibration equations

With the wide encounter of nonlinear equations in research activities and practical applications, a search of novel and efficient methods for solving such challenging problems never stopped. In this talk, a novel extension has been made with the popular Galerkin/Rayleigh-Ritz method by integrating the weighted equation of motion or Lagrangian functional over the time of one period of vibrations to eliminate the harmonics arising from the deformation function. A set of successive equations of coupled higher-order vibration amplitudes is obtained, and a nonlinear eigenvalue problem is solved for the frequency-amplitude dependence of nonlinear vibrations of successive displacements. The subsequent solutions of vibration frequencies and deformation are actually consistent with other successive approximate methods such as the traditional harmonics balance method. This is a novel extension to Galerkin/Rayleigh-Ritz method which has wide applications in approximate solutions particularly for vibration problems in solid mechanics. This extended Galerkin/Rayleigh-Ritz method can also be utilized for the analysis of free and forced nonlinear vibrations of structures as a new technique with significant advantages. Application examples are also presented to a wide array of typical nonlinear problems for simple and efficient solutions and procedure.

Audience Take Away:

- Understanding mathematical description of nonlinear problems.
- Knowing some basic methods for solving typical nonlinear problems.
- Learn to use the extended Galerkin and Rayleigh-Ritz methods.

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 bachelor 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 frequent invited, keynote, and plenary presentations in major conferences around world.

Sudip Kumar Das
University of Calcutta, India

Scale-up design for adsorption process

Discharge of toxic heavy metals into our nature causes severe harm. Different plant operation generates heavy metal-bearing wastes, and dyes discharge of these wastes causes various damages to the living beings. Heavy metals and dyes played a significant role as pollutants among the harmful elements because of their high toxicity and high persistence. The adsorption process is an economical and efficient technique used for heavy metal removal.

Various natural bio-adsorbents, agricultural wastes, agricultural by-products, bio-polymers are available at low cost, with good adsorptive capacity. Design of adsorption column using suitable adsorbents for industrial-scale minimizes the operating cost for wastewater treatment which is beneficial for small and medium scale industries of developing countries. The batch study and continuous column study are essential for the scale-up design for industrial purposes.

Experiments were carried out to estimate the sorption capacity of various adsorbents and the effects of various operating parameters such as pH, temperature, adsorbent dose, contact time, column bed depth, influent flow rate, and influent metal ion concentration on the adsorption process. Different kinetic models were applied to the experimental result to investigate the process breakthrough curve and best model, further used for scale-up designing.

This study proposes a novel methodology of scale-up design for both batch and continuous operation, and obtained results suggest that selected adsorbents could be used further for industrial wastewater treatment.

Audience Take Away:

- In the developing countries, i.e., 3rd World countries, exist a large number of small and medium-sized industries, discharge heave metals and dyes in their wastewater
- These wastewater is discharge in drain, is directly flow into the nearby water bodies or agricultural fields, thus polluted it and ultimately enter into the food chain
- These industries does not have sufficient fund to treat their wastewater
- The use of agricultural waste materials as adsorbent shows a potential removal of heavy metals or dyes
- Thus the use of waste materials is an example of circular economy, and also for collection of these materials has some job potential to the rural areas

Biography

Dr. Sudip Kumar Das is currently Professor and Former Head in the Department of Chemical Engineering, University of Calcutta. He has completed his Ph.D. and M. Tech. in Chemical Engineering from the Indian Institute of Technology, Kharagpur, and graduated from Calcutta's Chemical Engineering and Chemistry Hons. From the University of Calcutta He is also actively engaged in research related to different fields of Chemical Engineering, like single and multiphase (gas-liquid) flow through pipelines and piping components, multiphase flow through coils, fluidization and inverse fluidization, wastewater treatment technology, heavy metals, and organic pollutants removal from wastewater, Process Plant Safety, Computational fluid dynamics, artificial neural networks, and machinable glass-ceramics. He has published 1 book, 15 chapters, more than 250 papers in National and International journals, and presented many invited lectures at the Conferences. He has guided 20 Ph.D., 38 M.Tech. and more than 80 B. Tech. students. He has been a reviewer for more than 125 National and International journals. He was recipient of Indian National Science Academy Visiting Research Fellowship award 1999-2000, Research Ratna Award 2019 for best researcher in Environmental Engineering, The Bharat Joyti Puraskar 2018, Indira Gandhi Gold Medal Award 2016, The Best Citizen Award 2015, Dr. Radhakrishnan Gold Medal Award – 2015, 2014, Outstanding Faculty Award 2015, The Best Citizen of India Award – 2015, Bharat Gaurav Award 2014, best paper presentation award several times in International/National Conferences. He is member of Refrigeration and Air Conditioning Sectional Committee, ME 03, Bureau of Indian Standard, also in professional societies like, Indian Institute of Chemical Engineers (life), Institute of Engineers (Fellow), IEEE, Indian Association for Air Pollution Control (life), Indian Chemical Society (Fellow), Millennium Institute of Energy and Environment

Management (life), International Congress of Chemistry and Environment (Fellow). He acted as the Head of the Chemical Engineering Department, University of Calcutta, 2010-2012, 2017-2019. He also served as Hony. Secretary 2006-2007, 2014, 2018 and Hony. Treasure 2005, 2011-2013 in the Indian Institute of Chemical Engineers. He also served as Hony. Treasure 2017 to till date in Indian Chemical Society. He also acted as Chairman, Calcutta Regional Centre, Indian Institute of Chemical Engineers, 2012-2014. Hony. Secretary and Hony. treasure for several years in the Calcutta Regional Centre, Indian Institute of Chemical Engineers.

Prince Kumar Gupta, Arvind Kumar Yadav*, Krishna Nand Singh

B. R. D. P. G. College, India

Visible light triggered β-allylation of indoles using baylis-hillman bromides

A facile regioselective β-allylation of indoles has been accomplished employing Baylis-Hillman bromides as allyl source under visible light photoredox catalysis in the presence of $Ru(bpy)_3Cl_2.6H_2O$ and blue LED.

Audience Take Away:

- Use of photoredox catalysis to functionalize Baylis-Hillman adduct.
- Application of photocatalysis to replace halogens fron arenes and alkyl halides.

Biography

Arvind Kumar Yadav was born in Ghazipur, U.P., India. He received his M.Sc. degree (2010) in chemistry from the University of Allahabad, India. In the same year, he joined the research group of Prof. L. D. S. Yadav as a PhD student. He has qualified twice for a Junior Research Fellowship (JRF) in the National Eligibility Test (NET) of CSIR-UGC in 2010 and 2011. His research is focused on organic synthesis via Photoredox catalysis. He received his PhD degree in 2016 and worked with Prof. K. N. Singh (BHU, Varanasi) for two year (2017-2019). To 19 march 2019 he joins BRD PG College, Deoria as assistant professor and still working there. He has published more than 32 research articles in SCI(E) journals.)

Jyoti Waikar, Pavan More*

Institute of Chemical Technology, India

Complete oxidation of CO and propene as model component of diesel exhaust and VOC using manganese oxide supported on octahedral (AlO_6^{3-})-Ce^{3+}

The complete oxidation of propene and CO as model components of diesel engine exhaust and VOC has been investigated on series of Ce doped $MnOx/Al_2O_3$ catalysts. The optimized $MnOx/Al_2O_3$ doped with 0.05 mol Ce showed higher CO and propene oxidation activity at 200 oC and 215 °C respectively. The physicochemical properties of catalysts were analyzed by using XRD, RAMAN, NMR, H2-TPR, HRTEM, and XPS techniques. The formation of Mn_3O_4 and Mn^{4+} species were observed on the catalyst surface. 27Al Solid-state NMR showed formation of octahedral $[AlO_6^{3-}]$-Ce^{3+} species, which was responsible for the donation of oxygen required for CO and propene oxidation. The formation of adsorbed oxygen and oxygen vacancies were observed on the catalyst surface due to the synergistic interaction between Mn, Ce, and Al[1,2]. The HRTEM results showed formation of well dispersed Mn over Al-O-Ce, which facilitate the proton abstraction required for the activation of hydrocarbon. The mechanistic and kinetic aspects of CO and propene oxidation on catalyst surface have been reported in detail.

The $MnO_x/0.05Ce$-$0.45Al_2O_3$ showed facile redox properties of Mn_3O_4 and MnO_2. The well-dispersed manganese oxides and Ce on Al_2O_3 support lead to increase in distortion and consequently oxygen vacancies, which eventually increases the mobility of oxygen from bulk to surface of the catalyst[3]. The increase in Ce concentration causes the Mn agglomeration, which shifts the catalytic activity towards higher temperature. However, coating the catalyst on the monolith and their investigation under realistic conditions is the challenge and would be the next step of the research work.

Audience Take Away:

- For abatement of VOCs and CO emission from automobiles the non-noble metal-based catalyst system like Ce doped $MnOx/Al_2O^3$ has shown relatively low temperature activity.
- It shows effect of support (Al_2O_3) modification on CO and Propene oxidation activity.
- After Ce doping in $MnOx/Al_2O_3$ generation of different active sites, active O-species and structural defects required for low temperature oxidation.
- The improvement in low-temperature oxidation activity of CO and Propene was observed due to the strong synergistic interaction of Mn-Ce, enhancement of redox properties of Ce (Ce^{3+}/Ce^{4+}), formation of surface oxygen vacancies and availability of active oxygen species (O^-, O^{2-}, O^{2-}, etc.)
- The formation of oxygen vacancies is responsible for the activation of gaseous oxygen at a lower temperature.

Biography

Dr. Pavan More Studied M. Sc (Analytical Chemistry) at the Garware college, Pune university.He then joined as a Q. C. Chemist in Prophyla Biologicals Pvt. Ltd. Pune, 2007-2008. He received his Ph. D. degree in Chemistry from CSIR-National Chemical Laboratory, Pune, India in 2010 – 2015. During his PhD (May-July 2011, May-July 2012, June-July 2015) he worked in Lille University France under "International Associated Laboratory Program", between CNRS, France and CSIR, India collaboration. He is presently working as "Assistant Professor in Micro analysis" in the Department of Chemistry at Institute of Chemical Technology (UDCT), Mumbai (Oct. 2015). He has published 20 research articles in SCI(E) Journals.

Mridusmita Barooah
National Institute of Technology, India

High performance gas separation studies by membrane technology

Global warming, a subject of increased emphasis in the recent years, is caused by the emission of greenhouse gases such as CO_2 in the atmosphere. Greenhouse gases (GHGs) trap the heat radiating from the surface of earth when solar energy is being transmitted through the atmosphere thus increasing the global surface temperature. As a result of global warming, melting icebergs in polar oceans is causing the sea level to rise globally. The Intergovernmental Panel on Climate Change (IPCC) has predicted that the sea level will rise by 0.09 to 0.88 meters from 1990 to 2100, which is a matter of serious concern. CO_2 which is the primary anthropogenic greenhouse gas, accounts for 77% of the human contribution to the greenhouse effect in recent decade (26 to 30 percent of all CO_2 emissions). Carbon capture and storage (CCS) as a major strategy is being used to reduce GHGs emission. There are three methods for CCS: pre-combustion capture, oxy-fuel process, and post-combustion capture. Among them, post-combustion capture is the most important one because it offers flexibility and it can be easily added to the operational units. Conventional separation techniques such as absorption, cryogenic distillation and adsorption have huge applications. However, advanced technologies such as membrane separation technology have advantages of less energy consumption, light weight, space efficiency and compact modular design over these conventional techniques. Hence, membrane technology serves as clean, compact, energy management alternative thus amplifying its future scope as a very efficient technique for industrial application. The first idea of membrane separation dates back to 1980's with major contributions by separex, generon and cynara. The performance of a membrane can be measured based on its permeability (Barrer) and selectivity. Different types of separation mechanism include molecular sieving, knudsen diffusion, solution diffusion and the more recent facilitated transport mechanism. Based on the materials used, membranes can be broadly classified into (1) Organic membranes, (2) Inorganic membranes, and (3) Mixed matrix membranes. Organic or polymer membranes are the most widely used commercial membranes in gas separation due to its advantages of low cost, high mechanical stability and efficient separation efficiency.

The constraint of this membrane came to be popularly known as Robeson's upper bound limitation. In the Robeson's plot, the selectivity was plotted as a function of CO_2 permeability (Barrer). However, for large-scale application of gas separation membranes high CO_2 permeance along with high selectivity plays a pivotal role. Also, organic membranes are restricted by low thermal, mechanical and chemical stability. Inorganic membrane normally exhibits high separation ability and operates at fairly high temperatures. However, the long-term application of these membranes is restricted by its high cost and brittle nature. Some common examples of inorganic membranes used for gas separation application includes zeolite and silica membranes. Another major class of advanced membrane material is mixed matrix membranes (MMM), developed by researchers in the mid 1980's. These membranes combine the synergistic effect of both polymeric and inorganic materials. In this work, we will discuss in detail about the membranes available along with its recent advances in the field.

Audience Take Away:

- This article provides a comprehensive review with respect to the utility of membranes (constituting a bulk and a filler scattered phase) towards CO_2 separation. A thorough analysis was carried out with respect to membranes and their ability to enhance the CO_2/N_2 gas transport properties.
- This study provides alternate advanced fabrication methods to achieve membranes with high performance in gas separation.
- The high-end separation technology provided opportunity for large-scale gas separation operation and a very viable approach to be replaced with the conventional separation technology in terms of physico-chemical property enhancement and gas separation performance.

Biography

Dr. Mridusmita Barooah did her graduation in Chemical Engineering from Assam Engineering College, Guwahati, Assam in 2012. Thereafter, she worked as Project Scientist in DST sponsored projects, Government of India from CSIR-North East Institute of Science and Technology, Jorhat and Indian Institute of Technology (IIT) Guwahati. She then joined the research group of Dr. Bishnupada Mandal, Senior Professor, Department of Chemical Engineering, IIT Guwahati. She was awarded her PhD degree in 2019. Her PhD topic was, “Development of CO2 selective mixed matrix membrane for CO_2 separation.” She worked in National Institute of Technology (NIT), Arunachal Pradesh as Assistant Professor from July 2019 and has taught core subjects in Chemical Engineering which include Mass Transfer, Chemical Reaction Engineering, Chemical Process Technology, Process Instrumentation, Chemical Engineering lab. She is currently working as Assistant Professor, NIT Warangal, Telangana, India. She has 4 International publication of research article and attended many International and national conference along with workshops.

Farzin Asghari Sana*, Menemşe Gumusderelioglu
University of Medical Sciences, Iran

Boron doped nano hydroxyapatite: Antibacterial and synergistic effect with β-lactame antibiotics

Nowadays, synthetic biomaterials are extensively employed in the manufacture of medical devices and implants. Here, we studied on the development of a novel antimicrobial nanocomposite against a wide spectrum of bacteria including multi-drug resistance (MDR). This is why, we considered to produce boron-doped nano-hydroxyapatite (B-nHAp). In our groups' previous studies bone-like nano hydroxyapatite (n-HAp) and B-nHAp were synthesized. In this study, we considered that, B-nHAp with antibacterial and β-lactamase inhibitory characteristics provides an interesting approach to inhibit adherence and growth of bacteria. Moreower, synergistic effect of B-nHAp/β-lactam antibiotic combinations extends its spectrum against MDR pathogenic bacteria with safe biocompatibility and appropriate tissue interactions as well as their nontoxicity in-vitro toward odonteoblasts and mesenchymal stem cells.

In-vitro antimicrobial activities of nHAp and B-nHAp was investigated by Disk Potentiation Tests, Double Disc Synergy Test, Agar Dilution Method and Etest methods according to the recommendation of the Clinical and Laboratory Standards Institute. In this study, Escherichia coli, American Type Culture Collection (ATCC) 25922, Staphylococcus aureus ATCC 25923, Enterobacter cloacae ATCC 1143 (control strain for the Ampc disk test: strong positive), Klebsiella pneumoniae ATCC1144 (control strain for the Ampc disk test: weak positive), Klebsiella pneumoniae ATCC 700603 (control strain for extended-spectrum β-lactamase) were used. As β-lactam antibiotics, ampicillin, ceftriaxone, ceftazidime, ceftazidime/clavulanic acid, amoxicillin, amoxicillin/clavulanic acid, cefotetan, cefotaxime and cefoxitin were selected.

The results denoted that B-nHAp showed antibacterial activity against gram positive and gram-negative bacteria. As due to the β-lactamase inhibitory properties of B, B-nHAp showed synergistic effect when used in combination with β-lactame antibiotics and increased the effectiveness of antibiotics in all tests. However, nHAp showed no antimicrobial activity against tested microorganisms. In the light of these results, we concluded that B-nHAp nanocomposite developed by our group can be used in various dental and orthopeadic implant materials during manufacturing.

Biography

Farzin Asghari Sana was born on October, 1979 in Urmia, Iran. He received PhD degree and postdoctoral studies in nanomedicine from nanotechnology and nanomedicine Institute of Hacettepe University, Turkey. His research is in the field of Nano biomedicine agents for targeting, sensing, Imaging and Drug Delivery applications. Sana's work has garnered awards from the 10th. Nanoscience and Nanotechnology Conference (NanoTR-10), İstanbul, Turkey. He has published more than 10 papers in reputed journals and he has been postdoctoral researcher in Urmia medical science university. He also Established Lotus Nanomedicine R&D Company at Urmia University of Medical Sciences, Iran (2019).

Dr. Davood Fathi
Tarbiat Modares University, Iran

Catalysts in water-splitting

Although many catalysts have been proven worthy to accelerate chemical reactions, there is still the challenge of finding a more efficient and optimized catalyst; thus, it is crucial that researchers learn about various compounds. In recent years, due to the shortage of energy, water-splitting solar cells that directly convert solar energy into chemical energy have attracted growing attention. In order to achieve maximum performance of these cells, catalysts are used to speed the hydrogen evolution reaction (HER), and oxygen evolution reaction (OER) and generate hydrogen fuel.

In a photo-electrochemical (PEC) water-splitting cell (Figure 1), catalyst plays an important role in improving the photoinduced electron and hole separation/transportation, works as the active site to previously mentioned reactions, decreases the probability of photo-corrosion and increases the chemical stability of photoelectrodes. As the reaction in PEC water-splitting cells will happen on the photoelectrodes' surface, surface-decoration with catalyst is needed. To promote the reaction, perovskite oxides are considered great visible-light-active electrocatalysts which consist of a huge variety of compounds. Besides the fact that finding the efficient material as a catalyst is the main issue, figuring out new methods to optimize the catalysts' performance matters as well. It is also important to consider catalysts and cocatalysts to be earth-abundant and cost-efficient.

In my proposed presentation, I will discuss how using an efficient catalyst will benefit the outcome results of different chemical reactions, optimizing new methods over conventional methods to develop convenient and frugal catalysts, and innovative process technologies to use catalysts as particles with different morphologies or layers.

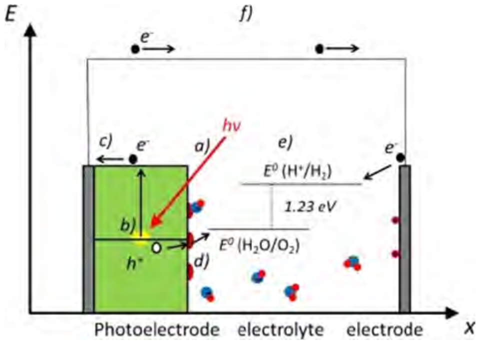

Figure 1. Scheme illustrating the main phenomena involved in photoelectrochemical water splitting, where a photoanode is immersed in an aqueous electrolyte. a) light-matter interaction, b) electron-hole pair generation, c) charge separation and transport, d) catalysis and e) the water-splitting reaction, and f) photocurrent associated with the photoelectrochemical (PEC) water splitting.

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, 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.

**Rommel Hans Ortiz Guzmán* and
Antonio Ramiro Jesús Bueno Lazo**

National University of San Marcos, Peru

Evaluation by simulation of the reactor design to obtain urea from natural gas

Urea is the fertilizer with the highest domestic consumption in agriculture; however, currently Peru is imported mainly from countries such as Russia, China and Algeria. The Peruvian State should promote investment in urea production from methane volumes from proven natural gas reserves from the Camisea fields; In this way, imports would be reversed, generating various benefits for the country: an increase in the Trade Balance, an increase in the economic and commercial development of the area where the plant is installed, and job creation. In the present research work, the design and characterization of the reactor of a urea production plant from natural gas was proposed, comparatively analyzing three commercial processes currently in operation: Stamicarbon, Snamprogetti and Toyo. The ASPEN PLUS software was used as a simulation tool, selecting the SR-POLAR thermodynamic model, which is suitable for the high pressure and temperature conditions of urea synthesis. In addition, the model contains extensions that allow a precise description of the phase and chemical equilibria and other thermodynamic properties; like enthalpy. There are two main reactions that develop in the urea synthesis process; the first reaction, which occurs in the liquid phase, converts ammonia and carbon dioxide into ammonium carbamate, this reaction is very exothermic and fast; chemical equilibrium is easily achieved under reactor operating conditions. The second reaction, which is the decomposition of the ammonium carbamate formed in urea and water, also occurs in the liquid phase and is endothermic, its speed is slow and equilibrium is not normally reached in the reactor. To carry out the simulation and subsequent comparison of the three urea production technologies, we will start from the same feed of ammonia (37,851 Kmol /day) and carbon dioxide (18,989 Kmol /day) for the three cases. For the design of urea synthesis reactors, plug flow reactors of the same size (diameter 2.3 m and length 29 m) were designed, but with different operating conditions and with a different configuration of equipment. The results are graphs that illustrate the variation of the length of the reactor with temperature, the residence time with the variation of the length of the reactor and the variation of the conversion with the residence time for each patent. The results presented are part of the doctoral research project sponsored by the National Fund for Scientific, Technological Development and Technological Innovation (FONDECYT), nowadays PROCIENCIA.

Keywords: urea, natural gas, ammonium carbamate, reactor, petrochemical, process engineering, process simulation, ASPEN PLUS

Audience Take Away:

- Understanding of the main reactor operating parameters of each urea production patent, for easier handling in process simulation.
- The research may be expanded by the group of researchers who wish to deepen the analysis of any variable of interest.
- The research turns out to be of a practical nature, since it evaluates the comparison of the energy efficiency of the 3 reactors of each urea patent, which can be proposed as a case study at the undergraduate or graduate level.
- Optimize the design precision of a urea production reactor under certain conditions.

Biography

Msc. Ortiz studied Petroleum & Natural Gas Engineering and Chemical Engineering at the National University of Engineering, Peru and graduated as Msc in Petroleum & Natural Gas Engineering in 2019. Currently, he is studying the fifth semester of the Doctorate in Chemical Engineering at the National University of San Marcos, Peru; with a comprehensive scholarship, granted by FONDECYT (PROCIENCIA) - World Bank. The title of his doctoral thesis is “Evaluation by Simulation of the Most Efficient Process for Obtaining Urea from Natural Gas”, which will be supported in June 2022.

Farid Aiouache

Lancaster University, United Kingdom.

Relevance of synergetic approaches in intensifying catalytic reactors

Intensifying chemical reactors by development of an efficient synergy between the reactor and catalyst is leading to non-negligible saving in capital and operating costs of chemical plants while meeting requirements over conversion, selectivity and energy consumption. Recent achievements in developments in the topic of multifunctional catalytic reactors by combination of the chemical reaction with momentum, heat and mass transports in a single chemical unit are presented through a number of examples, including among others, hybrid catalytic reaction and separation, local catalyst deactivation in real flow system and multiphase flow in engineered packing type of internals. In the first example, the etherification of tert-amyl alcohol with ethanol was carried out in a catalytic reactive distillation column inserted by a pervaporative zeolite NaA membrane tube. The design has shown alleviation of azeotropes of H_2O-reaction components mixtures and a gain of 10% in tert-amyl ethyl ether yield. In the second example, local deactivation of the preferential oxidation of CO was investigated in real flow reactor by three-dimensional modelling of flow and experimental tomography where the profiles of deactivation were found sensitive to the rates of deactivation, heat transfer by dispersion and intra-particle mass transfer at both reactor and packing pore scales. For instance, elevated deactivation was seen close to the wall due to a preferential flow circulation and progressed at the exteriors of the catalytic particles, particularly over the regions in contact with the convective flow. This presentation brings attention to relevance of accessing to real-time data of concentration, temperature and flow velocity, as well as relevance of the space scales by in-situ sensing. It also emphasizes the multidisciplinary approach when dealing with the simultaneous design of catalyst and catalytic reactor.

Keywords: catalytic process intensification, multifunctional reactor, multiscale design, in-situ sensing, engineered catalytic packing

Audience Take Away:

- Process intensification is innovative strategy to design reactive processes while looking at multiple aspects associated with reducing heat conception, by-products, unit size and catalyst load while promoting sustainable practices. The audience will appreciate relevance of innovative techniques to access to data while reactors are in operation along with prediction by modelling and design of conditions, which are not affordable to reproduce experimentally.
- Since the theme of the conference is about CCET, the audience will appreciate in the daily laboratory operations the fact that designing a catalyst and reactor is regarded as multidisciplinary subject where sub-subjects should be investigated simultaneously. A number of worked examples will be presented which could be taken further depending on their research interests. These examples are not final solutions but would contribute to solutions that can simply design of multifunctional catalytic reactors. The design by process intensification is intended to promote conversion, selectivity under less raw material and energy uses

Biography

Dr Farid Aiouache is Senior lecturer at Lancaster University since November 2012 after working as Lecturer at Queen's University Belfast (2006-2012) and Project engineer for a year in the oil and gas industry (CUB Engineering, Calgary, Canada, (2005–2006). He was full time Postdoctoral Fellow at Ecotopia Science Institute, Nagoya University, Japan (2003–2005) and a part-time Research Associate at the National Industrial Science and Research Institute, Japan, (2003–2005). During his postdoctoral work, he was involved in a pioneering work on spatially resolved NIR/IR imaging for heterogeneous reactions. He gained his PhD in Chemical Engineering (Nagoya University, 2000-2003) for a work on reaction and transport rate effects on pervaporative reactive distillation efficacy. Prior to his PhD project, he was Research Visitor at Nagoya University, chemical reaction engineering laboratory, 1999-2000, and was involved in a research area on multifunctional reactors (membrane reactors and reactive distillation). He holds a research background in oil and gas industry, reaction engineering applied to multifunctional reactors and process intensification for green chemical design. Currently, He is carrying out research projects in 3D modelling of catalytic processes, spatially resolved spectroscopic tools for 3D observations of fluid flow, mass and heat trends in chemical processes using lasers and tomography techniques applied to reactors, adsorbers, fuel cells, batteries, etc). Other subjects under developments are sustainable separation processing using green solvents, rational use of CO2 (separation, conversion and storage), bio-wastes conversion to liquid and gaseous fuels, bio-catalytic recovery of valuable metals from e-wastes, catalytic stripping for nuclear waste waters processing, reactive waste ashes for biodigestates processing into fertilizers. He has published over fifty peer-reviewed papers.

Mohammed M. Bettahar
Lorraine University, France

The hydrogen spillover effect fundamental aspects

In this paper we examine the controversy over the hydrogen spillover effect (HSPE) on metal catalysts supported on non-reducible oxides. We propose that hydrogen spiltover species would consist in H/OH pairs, produced by an interfacial dehydroxylation then diffusing over the support by a thermodynamically neutral H/OH exchange mechanism and not by a H atom hopping process, as generally believed. The hydrogen atoms of the H/OH pairs may be consumed in a hydroconversion reaction or desorb as H_2, giving rise to $/O^{2-}$ pairs (where denotes an oxygen vacancy) which, in turn, may further incorporate H atoms for subsequent hydrogenations or hydrogen storage. H/OH and $/O^2$ constitute conjugated pairs in the hydrogen spillover effect.

Biography

Mohammed M. Bettahar held his PhD degree in Physical Chemistry (Paris, 1975). He worked for the CNRS as Attaché de Recherche (Thiais) and Research Director (Caen). He pursued his career as Full Professor in Algiers (1980) then in Nancy (1995). He is Professor Emeritius in Lorraine University since 2015. Main research topics are related to Nanomaterials and Catalysis (Selective Hydrogenation or Oxidation, CO_2 or CH_4 transformations, Hydrogen Storage). Currently his research focuses on Nanomaterials for Biofuels and Chemicals fabrication.

Kaustubh Laturkar*, Kasturi Laturkar
Michigan State University, US

Analysis of the ethanol and benzene extractive distillation using p-xylene as solvent in a cape-open simulator

An analysis of the extractive distillation and solvent recovery processes for the separation of ethanol and benzene from its azeotropic mixture using p-xylene as a solvent through Cape-Open steady-state simulation is presented. A case study is conducted using a two-column distillation system, where the first column was used for the extraction of ethanol, while the second column was used to recover pure benzene and the solvent. This recovered solvent is then reinjected into the first column. The results indicated that p-xylene is a reliable solvent for the separation ethanol-benzene azeotrope and can distill pure benzene with a high recovery of the solvent during the process.

Keywords: extractive distillation, ethanol, benzene, p-xylene, cape-open simulator

Audience Take Away:

- Simple distillation methods cannot separate azeotropic mixtures. These components are separated using extractive distillation. A diagram illustrating a T-xy plot of ethanol and benzene is presented which explains why the components cannot be separated by conventional techniques.
- The mathematical model used for extractive distillation is based on equilibrium stage models and represents all the material and energy balances (MESH) used in the simulated model.
- An extractive distillation and solvent recovery case study is analyzed, the simulation is completed using an open-source Cape-Open Simulator to give accurate results. Temperature profile and concentration profiles across the extraction column and the solvent recovery column are plotted and analyzed.

Biography

Mr. Kaustubh Laturkar is currently working as an engineer at the Facility for Rare Isotope Beams which is a US-DOE project in Michigan after having completed his M.S in chemical engineering from University of Florida and B.E. in Chemical Engineering from Panjab University, Chandigarh, India. He has more than 8 years of experience working in the field of process engineering, refinery operations, utility systems design and operation with a special focus on design and commissioning of engineering systems.

Tshepo D. Dipheko*, Vladimir V. Maximov, Mohamed E. Osman, Evgeny A. Permyakov, Alexander G. Cherednichenko, Victor M. Kogan

Poeples’ Friendship University of Russia, Russia

Ethanol dehydrogenation over carbon supported (K)(Co, Ni, Fe)MoS_2-based catalysts

Utilizing renewable resources to synthesize fuels and high-value chemicals is a pivotal step for the chemical industry, given the limited nature of global natural gas and petroleum reserves. Due to the economic viability of large quantities of ethanol, it has been used to synthesize a variety of value-added chemicals that complement existing markets for petrochemical products. This leads to a decrease in reliance on oil supply, which has direct economic and geopolitical implications. Herein, ethanol dehydrogenation was studied over mono-, bi- and trimetallic-carbon-supported (K)(Co, Ni, Fe)MoS_2 catalysts. Across all catalysts, ethyl acetate was synthesised at a high quantity. The effects of catalyst textural properties on catalytic activity were studied and found to be substantial. It is established that catalysts with a large proportion of microporous structure are more active in the production of liquid products than those with a probable mesoporous structure. Both the morphology of molybdenum disulfide crystallites and the catalytic activity in the synthesis of oxygenated hydrocarbons are affected by the support material. The average length and stacking number of MoS_2, as well as the dispersion, were calculated. In all the reactions tested, the turnover frequency (TOF) rose as the average length increased and the dispersion decreased. The conversion of ethanol is expected to proceed on MoS_2-based catalysts while taking into consideration the support’s type and the reaction atmosphere’s effects. The impact of catalyst acidity on product distribution and conversion was evaluated; it was discovered that, although acidity had no direct effect on total conversion, it did influence product yields.

HRTEM microscopy, UV spectrum analysis of pyridine adsorption, scanning electron microscopy, X-ray photoelectron spectroscopy, and N_2 physisorption was used to evaluate supports and catalysts. The reactions were carried out under helium reaction atmospheres in a fixed-bed reactor.

Audience Take Away:

- Supported transition metal sulfides, such as (K)(Co, Ni, Fe)MoS_2, as a viable catalyst for ethanol dehydrogenation.
- The effect of the textural features of the catalyst, namely the surface area and volume (micropores and mesopores), on the synthesis of oxygenated hydrocarbons.
- The influence of active phase composition on catalytic activity is being investigated with the goal of controlling the ratio of liquid products to hydrocarbons.

Biography

Mr Tshepo Dipheko studied Chemistry at North-West University in South Africa and graduated in 2016 with a Master of Science. He subsequently continued his PhD studies at the Peoples’ Friendship University Russia in collaboration with Zelinsky Institute of Organic Chemistry, Russian Academy of Science. He is now pursuing a PhD in Chemistry Sciences. His doctoral research now focuses on the synthesis of oxygenated hydrocarbons from CO/H_2 and direct-ethanol conversion over supported transition metal sulfides catalysts, specifically supported (K)(Co, Ni, Fe)MoS_2-based catalysts.

Ozcan Koysuren
Ankara University, Turkey

The effect of iron doping on the photocatalytic efficiency of SiC nanofibers and their composite with polyaniline

Organic dyes in the wastewater stream is hazardous to the aquatic life and the terrestrial life. Photocatalytic activity is one of the most appealing process to convert harmful organic dyes into harmless small molecules in the presence of the UV light or sunlight. The photocatalytic activity of SiC nanofibers were studied in the context of the present study and it was aimed to improve their photocatalytic efficiency through doping with iron atoms. In addition to doping, SiC nanofibers were compounded with a conducting polymer, polyaniline. Under the sunlight or the UV light, valence band electrons of SiC are excited to the conduction band, forming photoexcited electron-hole pairs. SiC exhibits high recombination rate of the photoexcited charge carriers. To suppress the recombination rate of the photoinduced charge carriers, SiC was doped with iron atoms and/or compounded with polyaniline. SiC was doped with iron atoms though the wet impregnation technique. Polyaniline/SiC composites were prepared by in situ chemical oxidative polymerization process. The photocatalytic activity of SiC and its composite with polyaniline was evaluated through analyzing the degradation of a model dye, methylene blue, under UV light irradiation. The photoinduced electrons of SiC may be trapped by Fe atoms, suppressing the recombination process. On the other hand, polyaniline may accept the photoexcited holes of SiC and transfer its photoinduced electrons to SiC, reducing the recombination rate. Both effects enhanced the photocatalytic activity of SiC. Polyaniline composite, including 15 wt.% of doped SiC nanofibers, exhibited the highest photocatalytic degradation efficiency of almost 22% after 300 min. of UV light irradiation. Iron doped SiC and its composite with the conducting polymer could be considered as a promising photocatalyst to remove organic dyes from the wastewater.

Audience Take Away:

- SiC is a new example for photocatalyst. Its application potential was studied in this study and will be presented in the conference.
- Compounding the photocatalyst with a conducting polymer is an alternative method to reduce the recombination rate of the photoinduced charge carriers. The composite application also enhance the reusability of the photocatalyst.
- Application of photocatalytic degradation in the wastewater treatment is also new topic. The audience coul study on different photocatalyst for the wastewater treatment purpose.
- Doped SiC and polyaniline/SiC composite could be considered as a promising photocatalyst to remove organic dyes from the wastewater.

Biography

Dr. Ozcan Koysuren received his B.S. degree from Middle East Technical University (Ankara, Turkey) in 2002 and Ph.D. degree from the same University in 2008. Dr. Koysuren started his academic career as a research assistant in the Chemical Engineering department of Middle East Technical University in 2002. He is currently Associated Professor in the Energy Engineering department of Ankara University (Ankara, Turkey). Dr. Koysuren has published 23 research articles in SCI(E) journals.

Ashiff Khan*, Dr. A.Seetharaman, Dr. Abhijit Dasgupta

Saudi Aramco, Saudi Arabia/ SP Jain School of Global Management, Australia

Adoption of big data by global chemical industries

Big Data is making tremendous changes in various sectors of the economy. Chemical engineering can get the advantage of accelerating their processes, increasing the efficiency of plants by accurate projects. The chemical industry is just starting to realize the importance of a large amount of data that they own to make the right decisions and to support their strategies. They need to train the chemical engineers about the understanding of data science, command over coding, and strong quantitive aptitude. There are various big data tools available in the market which can make the integration easy by providing one platform for the collection and arrangement of information extracted from big data. This paper will focus on the list of big data tools, competencies necessary to make the investment for big data adaption, and skills. To achieve this objective government, academia, and industry need to collaboratively work together to overcome all present and future challenges.

Biography

Ashiff Khan is having 19 years of experience in oil & gas, environment, energy, chemicals, water treatment, and metallurgy. He is currently working in Saudi Aramco handling Process Engineering, Capital Projects, and Master Plans. His bachelor's degree is in chemical engineering. He also has three post graduations; 2 in management and one in data analytics, two master's degrees; MBA and Law, 5 international certifications along with Chartered Engineer and Professional Engineer Certifications. He has 5 publications and 3 filed patents in the US. Ashiff also holds PhD.h.c and is currently doing a master's in data science and doctorial studies from SP Jain school of global management, Australia. He is also Session Chair in International Petroleum Technology Conference (IPTC)-2022

Morgan Donnard
CNRS – University of Strasbourg, France

Captodative enamides: From controlled syntheses to original heterocycles

Enaminals are valuables building blocks in organic synthesis as they open the door to a wide range of more complex structures such as polyfunctionalized heterocycles or act as precursors of unconventional α and β amino-acids for instance. Noteworthy, both regioisomers (α or β enaminals) are appealing as they allow access to different molecular edifices. If β-enaminals, being valuable push-pull building blocks, have been well studied in the past, α-enaminals, having this time a captodative character, have been much less investigated and remain really complex to obtain, especially if you target tri- or tetra-substituted scaffolds with complete control of the regio- and stereo-chemistry. During the past few years we have developed diverse methodologies based on carbonylation and silylation reactions on ynamides to obtain versatile enaminal derivatives. Notably these methodologies are highly stereo- and regio- controlled. Among the reactions that will be introduced, we will present the first examples of regiodivergent hydroformylation of alkynes which are totally controlled by the nature of the ligand used. In addition we will also introduce the controlled synthesis of various silylated enaminal-derivatives as well as their post-functionalization leading to a wide scope of original and valuable building blocks. Nicely, these new compounds open the door to rapid and efficient syntheses of original heterocycles.

Audience Take Away:

- How to control efficiently, thanks to the catalytic conditions, the difunctionalization of ynamides.
- How to control the dual character (electrophilic & nucleophilic) of captodative enaminals.
- The potential of captodative enamines as building blocks in organic synthesis

Biography

Morgan Donnard obtained his PhD in organic chemistry in 2008 under the supervision of Pr. Jacques Eustache at the Ecole Nationale Supérieure de Chimie in Mulhouse (ENSCMu). He then joined the group of Pr. Jonathan Clayden in Manchester as Post-Doctoral Research Associate where he stayed 2 years. At the beginning of 2011 he came back to France for a second post-doctoral stay in the team of Dr. Nicolas Blanchard (ENSCMu) . In 2012 he was offered a CNRS Research Associate (Ass. Prof.) position at the university of Strasbourg. He obtained his habilitation in 2019.

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