8TH EDITION OF GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

SEPTEMBER 27-28, 2021

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CAT 2021
BOOK OF ABSTRACTS

8TH EDITION OF GLOBAL CONFERENCE ON

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SEPTEMBER 27-28, 2021

Theme:

Exploring the advances and challenges in Catalysis and Chemical Engineering

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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 CAT 2021

Magnus Group with gratification and privilege announcing its "8th Edition of Global Conference on Catalysis, Chemical Engineering & Technology"(CAT 2021), an Online Event scheduled during September 27-28, 2021 with the theme "Exploring the advances and challenges in Catalysis and Chemical Engineering." The main aim of CAT-2021 is to provide interaction between Chemistry experts, Pharma industries, R&D department, Young Researchers, Ph.D. scholars, and other professionals in the areas of Catalysis and Chemical Engineering around the world to share about their research studies and new innovations in the field. You can increase your professional skills and discuss the practical challenges encountered and the solutions adopted.

KEYNOTE FORUM

DAY 1

8TH EDITION OF
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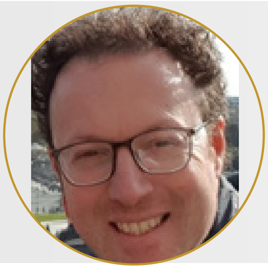

Eugenio Meloni*, Marco Martino, Vincenzo Palma
University of Salerno, Italy

Electrification of chemical engineering: A new way for intensifying chemical processes

The European Union, through the SET-Plan, aims to reduce greenhouse gas emissions by 20%, to have a 20% share of energy from low-carbon energy sources and to have a 20% reduction in the use of primary energy by improving energy efficiency by 2020, with a long-term ambition to reduce emissions by 80-95% by 2050. In the way of Process Intensification, the European Commission promoted the electricity-based processes: so, low-carbon electricity can be used for heat generation and/or steam generation in electric boilers replacing natural gas fired boilers (Power-to-Heat). This route is already considered or even operated by large chemical producers, because it can be flexibly employed as demand-side management measure to use low-cost intermittent power supply from renewables. Due to the substitution of natural gas it constitutes a low-carbon measure.

The use of electricity in power-to-heat applications or hybrid boiler concepts switching between natural gas and electricity-based heating provides several advantages. Electricity based heating has a fast response time and can therefore flexibly be used to valorise intermittent surplus supply of renewable electricity. This way, chemical industry can offer an active contribution to the demand side management and enhanced flexibility of the power sector, and on the other hand chemical industry can benefit from periods with low electricity prices. This can be perceived as an element of industrial symbiosis between the chemical industry and the power sector.

Audience Take Away

- The presentation could allow the audience to view Chemical Engineering in a new point of view, by identifying the limiting step of a process and consequently generating alternatives in order to implement an innovative process.

Biography:

Eng. Eugenio Meloni studied Chemical Engineering at the University of Salerno (Italy) and graduated in 2001. He then joined the research group of Professor Vincenzo Palma at the Department of Industrial Engineering of the same University, as research fellow in the field of Catalysis and Industrial Chemistry. His research involves the formulation, preparation, characterization and testing of structured catalysts for (i) soot abatement emitted by diesel engines or bio-mass combustion plants, and (ii) the intensification of different catalytic processes, also by means of alternative energy sources. He published 62 research articles on international peer reviewed journals, with h-index 16.

Miroslaw Szukiewicz*, Adrian Szalek, Elzbieta Chmiel-Szukiewicz
Rzeszow University of Technology, Poland

Optimization of experiments for heterogeneous reactor processes

The study of chemical kinetics is concerned with the measurement and interpretation of the rates of chemical reactions in the so-called process window. It tracks how quickly, the transition from an initial to the final states of reaction occurs and what compounds are formed. This know-how is necessary to commercialize any reactor process, it helps to determine proper temperature and concentration of substances, amounts of desirable products and by-products produced that is helps designing of chemical reactors and optimization experimental conditions. The necessary condition of correct design and optimization is precision of mapping of the influence of process variables (usually: pressure, temperature, concentrations, etc) on the rate of the process. Kinetic studies can link with determination of reaction mechanism, so they can give a deeper insight into process nature. Further analysis will be presented for two heterogeneous hydrogenation processes namely hydrogenation of propylene and hydrogenation of carbon dioxide on nickel catalysts.Let's accept that expenditure of money, time, and other resources can be treated as a total cost of the kinetic research. Kinetic studies are tedious and resulting expensive. For heterogeneous reactor processes, many authors recommended a full research plan (FRP) as a method of determination of the kinetic dependences. FRP assumes that for all process variables the process window is divided on the grids and for each combination of the variables the rate of the process is determined experimentally. This idea is costly, especially for many process variables and the wide process window. For instance, for the first considered here process there are three process variables (temperature, total flow and propene concentration) and number of necessary measurements (NoM) is equal to 49. Designing of experiments (DoE) is one of the most powerful quality improvement techniques for reducing process variation and enhancing investigation effectiveness. It helps to reduce number of experiments that is a cost reduction without or with small precision reduction. To show how simple and efficient this manner of planning experiments is, we propose the application of factorial-design method (FP). This technique speeds up the problem solution by permitting evaluations to be made before completing all experiments. Additionally, it also indicates the relative importance of process variables and possible interactions. The most often DoE method applied in heterogeneous catalysis basis on the FP.Since heterogeneous processes areusually highly nonlinear full factorial plan (FFP) or 3kfactorial plan (3kFP) are used; however the 3k design predominates. 2k factorial plan are not used. The goal of the work is presentation of steps taken to determine a kineticequation of the mentioned hydrogenation processes, application of DoE method sand verification of results. We show that application of factorials of mixed levels -factors at two and three levels - (MFP) helps to the further reduction of costscomparing with the FFP and the 3kFP. For instance, the FFP for the first considered here process includes 27 measurement points, while the MFP –only 8. Experimental verification confirmed the correctness of the concept.

Audience Take Away

- The results of work help to reduce costs of experimental work by reduction of the number of experiments by application of Design of Experiments methods. In the area of heterogeneous catalysis, we show that remarkable reduction of costs is possible in spite of the fact that those processes are highly non-linear.
- The research results can be easily expanded to other areas and can help to reduce numbers of experiments, and, of course, costs. The specific characters of other processes should be considered.

- The method presented help make the job more efficient.

Biography:

Dr Szukiewicz studied Chemical Engineering at the Rzeszow University of Technology (RUT), Poland and graduated as MS in 1986. He then joined the research group of Prof. Petrus at the Department of Chemical and Process Engineering, RUT. He received his PhD degree in 1995 at Cracow University of Technology. Furthermore, he obtained DSc (Habilitation) from Lodz University of Technology in Chemical Engineering in 2009. Since 2009 he works as a Professor in the Department of Chemical and Process Engineering (RUT). His main research interests are chemical reactor engineering and mathematical methods in chemical kinetics and engineering.

SPEAKERS DAY 1

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Iryna Antonyshyn*,Yu. Grin, A.M. Barrios Jimenez, U. Burkhardt, S. G. Altendorf, R. Schlogl

Max-Planck-Institut fur Chemische Physik fester Stoffe, Germany

Intermetallic $Hf_2B_2Ir_5$ as OER electrocatalyst

The transition from fossil fuels to renewable energy sources requires multiple solutions, among which the water electrolysis will play an important role. Considering proton-exchange-membrane (PEM) electrolysis with its advantages as a route for hydrogen production, the kinetics of both electrode reactions should be sufficient for large-scale application. However, at current stage the slow kinetics of anodic oxygen evolution reaction (OER) limits the overall efficiency of PEM electrolyzer and requires active and stable OER electrocatalyst. Additionally, the harsh oxidative conditions of OER restrict the catalyst choice to noble metals and their oxides. The implementation of intermetallic compounds (IMCs) as electrocatalyst materials introduces the possibility to modify the electronic state of the active centers (influence on OER activity) and realize the combined scenario of the chemical bonding through complex atomic interactions in IMC (contribution to electrode stability).

Based on the chemical bonding analysis, the orthorhombic structure of ternary compound $Hf_2B_2Ir_5$ has cage-like character [1]. The structural units B_2Ir_8 form the anionic covalently bonded framework and hafnium cations occupy corresponding 14-vertices B-Ir cages. The hafnium atoms are positively charged (+1.83), whereas B and Ir possess negative charges (B: -0.19, Ir: -0.66). These features of chemical bonding are reflected in the chemical behaviour of $Hf_2B_2Ir_5$ under OER conditions and have influence on the OER activity of this material. The prominent initial OER activity of $Hf_2B_2Ir_5$ is accompanied with the suppressed dissolution of Ir (compared with Ir anode), revealing the enhancement of the material stability in case of IMC. The long-term operation at current densities of 100 mA cm-2 for 246 h reveals the continuous improvement of OER activity with time, which can be explained by the"team"OER activity of Ir-terminated surface of $Hf_2B_2Ir_5$ and *in situ*-formed IrO_x particles as a catalyst of 2nd generation. The covalent bonding in the Ir-B framework hinders the massive Ir dissolution and leads to the long-term bulk stability of $Hf_2B_2Ir_5$ material. The electrochemical data are supported by comprehensive bulk- and surface material characterization of the electrode after electrochemical experiments. The assessment of this material at different scales and different states highlights that $Hf_2B_2Ir_5$ is self-optimizing stable OER electrocatalyst.

The presented results are relevant, because: investigation of the ternary compound $Hf_2B_2Ir_5$ as a new OER electrocatalyst explores the "OER electrocatalyst" library and contributes to our knowledge about the catalyst behaviour under harsh oxidative conditions of OER; they highlight the advantages of using intermetallic compounds with well-defined crystal structure and special features of the chemical bonding as OER electrocatalyst; the comprehensive understanding of relations between crystal structure/chemical bonding of IMC and (electro)catalytic performance can be a powerful tool for future catalyst development and/or optimization.

Biography:

Dr Iryna Antonyshyn studied Chemistry at Ivan Franko National University of Lviv (Lviv, Ukraine) and received her diploma in 2006. In 2006–2011 the scientific work on PhD thesis "Interaction of gallium and antimony with transition (V, Mn) and rare-earth (Y, La, Ho) metals" under supervision of Dr. Stepan Oryshchyn was carried out. During this period, she earned DAAD scholarship and joined the group of Prof. Juri Grin in Max-Planck Institut für Chemische Physik fester Stoffe (Dresden, Germany) for 10 months (2008–2009). After successful PhD defense in 2011 she joined the same group as postdoc and from 2019 Dr. Antonyshyn is group leader at MPI CPfS. The chemical properties of intermetallic compounds and their application in the field of heterogeneous catalysis and electrocatalysis are the main research interests of Dr. Antonyshyn.

Wojciech Snoch, Dawid Wnuk, Tomasz Witko, Jakub Staroń, Andrzej J. Bojarski, Maciej Guzik

Polish Academy of Sciences, Poland

Biocatalysis in search of effective anticancer agents – A novel sugar esters based on polyhydroxyalkanoate monomers

Bacterial polyhydroxyalkanoates (PHA) are natural polyesters synthetized in unfavorable environmental conditions to store and reuse carbon source inside a microbial cell. They are also a rich source of valuable intermediates that can be chemically modified in numerous ways and used in biocatalytic reactions. This is possible due to the 3-*R*-hydroxyl and carboxyl groups of the PHA monomers. One example of such use is a synthesis of fatty acid sugar esters (SFAE) catalyzed by fungal immobilized lipases (e.g. *Canadida anctrctica* lipase B - CalB, *Thermomyces lanuginosa*) in anhydrous conditions. Since the 1970s, scientists have demonstrated anticancer properties of SFAE and continuously investigate how modifications of the hydrophobic component affect cancer cells and enhance their therapeutic potential. However, no other group used PHA monomers as such component so far. During the presentation I will bring the audience closer not only to cancer statistics but also need to search for novel anticancer agents and therapies. A process of synthesis, obtainment and manufacturing of PHA polymers in order to produce hydroxyacids will also be described. I will show possibility of introducing trifluoroethyl groups into PHA monomer molecules selectively. Further, I will explain how these modified and unmodified PHA monomers are used for the synthesis of sugar esters using immobilized lipases, and what molecules have cytotoxic properties against Du145 prostate cancer cells and HTB140 skin melanoma. I will discuss why these molecules are interesting in search of new anti-cancer therapies and their prospective application to enhance the effectiveness of other therapies.

This work was supported by:

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InterDokMed project no. POWR.03.02.00-00-I013/16

Audience Take Away

- The audience will learn how to perform fed-batch cultivation leading to bacterial polyhydroxyalkanoates and produce monomers in order to obtain valuable synthons for biocatalysis.
- Listeners will find out what fungal lipases one can use to synthetize sugar fatty acid esters based on polyhydroxyalcanoates monomers.
- Audience will know how one can selectively introduce fluoroethyl moieties into hydroxyacid molecules using free 3-R hydroxyl group and which parameters, conditions are crucial to get desired products.
- Why one can consider sugar fatty acid esters as anticancer agents and what is their potential to support commonly used anticancer drugs.
- The participants will be able to expand their knowledge about anti proliferative compounds.
- Knowing conditions of my reactions they will be able to perform reaction of esterification using their molecules which possess –OH and -COOH groups.
- The audience will be able to apply newly described way of protection 3-R-OH group of hydroxyacids to try different types of modification in their laboratories.

Biography:

Wojciech Snoch studied biology at Jagiellonian University, Poland, graduated as MS in 2012. After the graduation he became a laboratory worker at Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences (PAS) for next eight months. In 2013 he was organizing a new laboratory at Faculty of Chemical Engineering and Technology of Cracow University of Technology. Then in 2015-16 he worked as a biotechnologist at Petroster- a company specialized in bioremediation of soil using fungal and bacterial consortia. Since 2016 he is doing doctoral thesis under dr Guzik and Prof Szaleniec at PAS.

G. Satishkumar
Vellore Institute of Technology, India

Sustainable heterogeneous catalysts for arylation of arenes via C-H and C-O bond activation

Selective cleaving and functionalizing C-H, C-O bond in organic chemistry still remains a great challenge due to its weakest reactivity. Transition metal catalysts played a significant role in constructing various organic molecules through C-C coupling by activating the C-H and C-O bond. However, the need for ligands and additives are inevitable for homogeneous catalysts to accomplish the good yield and selectivity. On the other hand, heterogeneous catalysts do not find widespread application in organic transformations involving C-H and C-O bond activation due to its poor catalytic activity. Thus, an effective heterogeneous catalyst for challenging organic transformations besides possessing its advantages must have distinct active sites like its homogeneous counterpart. Here we show Fe and Al grafted over mesoporous silica SBA-15 as sustainable, efficient heterogeneous catalysts towards arylation of arenes. 8wt%Fe/SBA-15 has proven as efficient heterogeneous iron catalyst for direct arylation of biphenyl methane C(sp^3)-H and benzene C(sp^2)-H. Selective extraction deposition (SED) technique was adopted to graft iron easily over the mesoporous support SBA-15 using LaFeO3 as an iron precursor. The adopted SED technique is highly successful to graft 8wt% iron without forming iron oxide particle into the mesopores of SBA-15. It could be successfully recycled for 5 cycles. In the same way, alumina grafted SBA-15 catalyst demonstrated excellent catalytic activity towards the construction of diarylmethane using aryl boronic acid and 2-naphthalene methanol as reactants. It was observed that the presence of Brønsted acid sites (originates by incorporation of Al in the silica framework) and Lewis acid-base sites together over the support is critical to catalyzing the above reaction with 79% isolated yield. The catalyst was successfully recycled 5 times. In another study, iron grafted over 10wt% alumina coated SBA-15 (AlSBA-15) through SED technique demonstrated excellent redox catalytic activity like homogeneous iron catalyst in arylation of benzene with 74% biphenyl yield without additives. Alumina act as a solid-state ligand to polarize the electrons of Fe(III) grafted over them through its Lewis acid property. The catalyst performed successfully for 7 cycles.

Audience Take Away

- Fabrication of heterogeneous catalysts for challenging organic transformations involving C-H and C-O activation. Nature of the catalytic sites required at the surface of the heterogeneous catalysts to accomplish high catalytic activity like homogeneous catalysts.
- Immobilization of two or more functionalities over mesoporous supports at the appropriate distance, which is difficult or impossible to achieve in solution, to catalyze consecutive reactions by cooperative effects.

Biography:

Dr G Satishkumar is an Assistant Professor (Senior) in the Department of chemistry, SAS, VIT, Vellore since 2010. He has completed M.Sc Chemistry and Ph.D at Anna University, Chennai. He was previously working as a visiting Scientist in KIST, University of the Negev, Israel. His current research has focus on designing sustainable heterogeneous catalysts for various challenging organic transformation and recalcitrant pollutant degradation. He received funded projects from DST and Indo-Israel bilateral programme. He has published his South Korea. Latter, as a post-doctoral researcher in the Blechner center for industrial catalysis and processing, Ben-Gurion research work in reputed catalysis Journals.

Kong Fei Tan*, Armando Borgna, Mark Saeys
Curtin University Malaysia, Malaysia

Enhancing the stability of Co Fischer -Tropschcatalysts with boron promotion

Fischer-Tropsch synthesis (FTS) converts synthesis gas, a mixture of CO and H2, into various hydrocarbon products. Co catalysts are supported on various inert materials to increase their dispersion. They are preferred for FTS because of their good hydrocarbon selectivity, high CO conversion, and low water gas shift activity. Natural gas and gasification of coal is traditionally the preferred route for FTS to produce high quality hydrocarbons. However, with increasing environmental regulations, feed stocks obtained via gasification of biomass appears to be an excellent alternative for FTS. This shift towards sustainability and more carbon neutral processes is desirable for producing various hydrocarbons deemed essential for human civilisation.

Nevertheless, supported Co catalysts are known to deactivate under realistic FTS conditions, and it is hence desirable to improve the stability of Co catalysts. A number of deactivation mechanisms have been investigated and proposed, including sintering and oxidation of the metallic Co catalyst by product water. Nevertheless, the work of Tan et al in Journal of Catalysis showed that carbidic and graphitic coke can deactivate Co catalyst under realistic conditions. To improve the resiliency of Co catalyst towards carbon deposition, Tan et al used promoted Co catalyst with boron. Their study elucidated how boron doping can enhance Co catalyst against carbon deposition in the Journal of Catalysis, both from molecular modelling and reactor studies.

In this oral presentation, the relative stability of various forms of deposited carbon and the effect of boron on the carbon deposition mechanism will be discussed using periodic Density Functional Theory (DFT-PBE). To confirm the first principles based predictions, a series of Co catalyst promoted with various concentrations of boron were synthesized, characterized and tested in a fixed bed reactor under realistic FTS conditions.

Audience Take Away

- FTS can be deactivated with carbon deposition under realistic operating conditions of 220 – 2400C with H2/CO syngas ratio of 2. This discovery can help scientists and engineers to plan effective ways to regenerate Co catalysts or enhance its stability against carbon deposition.
- Ab-initio modeling can be extremely useful to design an effective promoter to enhance the stability of Co catalyst used in FTS. Additionally, deploying theoretical modeling not only speeds up the screening of potential promoters, but also reduces experimental risks.
- The effectiveness of boron as a promoter to Co catalyst is elucidated both from ab-initio molecular modeling and reactor studies. The amalgation of both disciplines allows designing catalyst from theory and accruing its tangible benefits in realistic FTS conditions.

Biography:

Adrian Tan is presently the Senior Engineering Project Manager at Roc Oil. He serves in Curtin University as Adjunct Professor and has a parallel appointment to PETRONAS University of Technology as Advisor. He read his PhD in NUS, Singapore majoring in Fischer-Tropsch Synthesis under the guidance of Prof. Mark Saeys from the University of Ghent, Belgium and Dr Armando Borgna from ICES, Singapore. Prior to his PhD, Adrian completed his MSc in Biomolecular Engineering through a joint MIT and Singapore initiative. Adrian is also a practicing engineer and holds a Fellow status with IChemE, UK.

Dr. Pavan Manohar More
Institute of Chemical Technology, India

Complete oxidation of propene using Cu/Ce/Hydroxyapatite: Effect of preparation methods

Propene is one of the component present in diesel exhaust and volatile compounds emitted from various sources. The mitigation propene emission can be done by using catalytic oxidation. It is one of the efficient method compared to the other methods. Pt/Al2O3has been used a commercial catalyst. However, due to the higher cost low hydrothermal stability and low activity at lower temperature non-noble catalyst were preferred for oxidation of propene. Bimetallic catalyst like Cu and Ce supported on Hap could be better and cheaper alternative for complete oxidation of propene.

The active component modification of Cu/Hap catalyst by Ce was prepared by successive deposition and co-precipitation method, and investigated for propene oxidation as model component of diesel engine exhaust and VOC. The Cu0.4/Ce0.1/HAp catalyst prepared by successive deposition showed 50% conversion (T50) at 267 °C whereas Cu0.4-Ce0.1/HAp catalyst prepared by coprecipitation method showed T50 at 287°C. Furthermore, Cu and Ce concentration has been optimized using successive deposition method. The catalyst modified with 0.4 mol Cu and 0.1 mol Ce deposited on HAp showed T50 at 267 °C, whereas 0.5 mol of Cu deposited on HAp showed T50 at 290 °C. All catalysts were characterized by PXRD, BET, Raman, XPS, ATR-FTIR, H2-TPR, FESEM, and HRTEM techniques. The formation of facile CuOx, P-O species with more Ce3+ and adsorbed oxygen were observed in Cu0.4/Ce0.1/HAp catalyst. These species facilitate the low temperature activation of propene and consequently increases the rate of propene oxidation.

Audience Take Away

- The completed work helps to understand the active components role and their effect to enhance the VOCs oxidation at lower temperature.

Biography:

Dr. Pavan More studied Msc at University of Pune and complete his PhD at CSIT-NCL, Pune, India in 2015. He then joined institute of Chemical Technology, Mumbai, India as Assistant Professor. He is working on selective oxidation of hydrocarbons into valuable chemicals and complete oxidation of pollutants using catalysts. He has over 15publicationsin national and international peer reviewed journal.

Wilfried G. Kanhounnon*,Guy Sylvain Atohoun, Jean-François Paul, Michael Badawi

Université d'Abomey-Calavi, Bénin

DFT study of catalytic hydride oxygenation of furan and derivatives on different metallic edge of MoS_2

Biomass is a sustainable feedstock expected to replace the fossil fuels in energy production. Biomass derivative oils contain however a high amount of oxygenated compounds. This is disadvantageous for the direct utilization of bio-oil as transportation fuels since these oxygenates confer them a low chemical and thermal stability, a low energy value and a high viscosity. It is then important to diminish considerably the amount of oxygenates in bio-oils to optimize their utilization. Catalytic upgrading of pyrolysis oils is one of the processes used to reach this target. Phenolic compounds widely studied in the literature but also furanic compounds are among the most representative oxygenated molecules of bio-oils. In line with previous studies, we investigated furan and two of its derivatives (methylfuran and benzofuran) hydrodeoxygenation on the metallic edge of MoS_2, through a periodic DFT modeling. The adsorption site considered is a vacancy created under hydrogen pressure on the metallic edge. This catalytic site has been chosen because It is stable under HDS and HDO conditions and seem to be good potential active site for hydrodoxygenation reaction. The hydrodeoxygenation mechanisms of molecules have been calculated and the influence of substituents groups on the furanic has been highlighted. For furan and methylfuran, the rate determinining step is the formation of water molecule during the vacancy regeneration while the concomitant addition of H and dissociation of the second C-O bond is the limiting step for benzofuran.

Audience Take Away

- How reactions mechanisms, difficult to be obtained experimentally, can be be elucidate by means of theoretical modeling.
- How hydrodesulphurization catalysts can be used for hydride oxygenation.
- Results will provide idea of how to modify catalysts to enhance hydride oxygenation process.

Biography:

Wilfried G. Kanhounnon obtained his PhD in quantum chemistry since 2016 in the University of Abomey-Calavi in Benin. He obtained a position of assistant professor in the University of Abomey-Calavi in 2017. Since 2020, he is a senior assistant professor of universities of CAMES. Dr KANHOUNNON co-authored around 12 research articles in scientific journals of large and high quality audience and participated to three master and one thesis supervision. He has academic partnership with many countries (France, Ivory Coast …).

Sujoy Bandyopadhyay
Indrashil University, India

Conjugated porous polymers: Potential testbed for platinum free electro-catalysis for oxygen reduction reaction

Background: Starting from the grand old activated charcoal to zeolites, porous materials have been utilized for environmental and technological benefits for mankind. Of late, porous organic polymers (POPs) have emerged as a new class of functional materials with applications ranging from gas adsorption, gas/liquid separations, catalysis, light harvesting, energy storage to chemo/biosensing.

Objective: A combination of porosity and π-electron conjugation leads to the development of a new field of conjugated porous polymers (CPPs) and utilization of platinum free electrocatalysis for oxygen reduction reaction.

Methods: In this context, we have synthesized a monomer of 2, 3-bis (4-bromophenyl) pyrido[3,4-b] pyrazine, and fabricated CPP in the form of solid powder, which is not soluble in common organic solvents.

Results: The synthesized polymer CPP was characterized by solid state 13C (CP-TOSS) NMR spectroscopy and Fourier transform infra-red spectroscopy (FTIR) spectra. The CPP polymer is an excellent catalyst for oxygen reduction reaction.

Conclusion: We created a conjugated porous polymer using 2, 3-bis (4-bromophenyl) pyrido[3,4-b] pyrazine. We utilized the polymer as a heterogeneous catalyst to reduce oxygen. DFT simulations revealed a precise mechanism for the four-electron ORR. The oxygen molecule may decompose on the closest pyrazine site, converting N=O to N-OH. Also, fewer densely packed structures have a smaller free energy of the ORR steps.

Biography:

Sujoy Bandyopadhyay earned his bachelor's degree in 2010 from the University of Burdwan. In 2012, he got his MS from Vidyasagar University. IISER Bhopal earned a PhD degree from IISER in 2018. He did his postdoctoral research at Hanyang University. He is now an assistant professor at Indrashil University. The research is primarily focused on the creation of novel porous organic polymer molecules and the investigation of their multifunctional application.

Tudor Spataru*, Petru Spataru, Igor Povar, Francisco Fernandez
Columbia University, USA

The mechanism of the vitamin B12 active forms catalytic processes in human body

For decades Methionine Synthase process has been considered as an energy barrier process by research community. Nevertheless, the in-vivo Methionine Synthase process can, in principle, run unlimited number of its turnovers without side effects and products. This requires two valid conditions for this process: a) the Methionine Synthase process reactions are running without energy barrier; b) the minima of the energy of the Methionine Synthase process reactions correspond to the products formation at each Methionine Synthase process threshold. CASSF(13,13) approximation has been used for Methionine Synthase process mechanism determination in this research. We have proved that the in-vivo Methionine Synthase process is of full effectiveness, meaning that all reactions are running without energy barrier under influence of the studied process substrate and that the minima of total energy Methionine Synthase reactions correspond to the products formation at each Methionine Synthase process thresholds. This is the first time that this biochemical phenomenon is completely solved. The Co-C bond cleavage and hydrogen transfer from the substrates to the 5’- deoxy-5’-adenosyl ligand are considered the triggering reactions of adenosylcobalamin cofactor dependent bio-chemical processes by international research community for decades. Moreover, these two reactions have not been distinguished and separate from each other by experimental data up to now. We have proved that the triggering reaction e. g. the Co-C bond cleavage of the in-vivo adenosylcobalamin dependent bioprocesses is of full effectiveness, meaning that is running without energy barrier under influence of the studied processes substrates and that the minimum of total energy of Co-C bond cleavage reaction correspond to the full Co-C bond rupture. We also have shown the transfer of the hydrogen from the substrates of the studied bio-processes to 5’- deoxy-5’-adenosyl ligand of the adenosylcobalamin cofactor and the Co-C bond cleavage are closely connected concerted reactions, which cannot be separate from each other and that the hydrogen transfer from substrates of the adenosylcobalamin dependent bioprocesses has a tunneling nature and is energetically convenient. Our data show that, the Co-C bond cleavage is favoring the hydrogen transfer from the substrate to 5’-adenosyl radical, and vice versa.

Audience Take Away

- The audience will be able to know that the in-vivo Methionine Synthase process is of full effectiveness, meaning that all reactions are running without energy barrier under influence of the studied process substrate and that the minima of total energy Methionine Synthase reactions correspond to the products formation at each Methionine Synthase process thresholds. This is the first time that this biochemical phenomenon is completely solved.
- This research that other faculty could use to expand their research or teaching the Co-C bond cleavage and hydrogen transfer from the substrates to the 5’- deoxy-5’-adenosyl ligand are considered the triggering reactions of adenosylcobalamin cofactor dependent bio-chemical processes by international research community for decades. Moreover, these two reactions have not been distinguished and separate from each other by experimental data up to now. And the triggering reaction e. g. the Co-C bond cleavage of the in-vivo adenosylcobalamin dependent bioprocesses is of full effectiveness, meaning that is running without energy barrier under influence of the studied processes substrates and that the minimum of total energy of Co-C bond cleavage reaction correspond to the full Co-C bond rupture.

Biography:

Professor Tudor Spataru studied Chemistry at the Cishinau State University, Republic of Moldova and graduated Thesis in 1972. He then joined the research group of Prof. Bersucher at the Institute of Chemistry, Moldovien Academy of Sciences . She received her PhD degree in 1985 at the same institution. A long time is an Associate Professor at the Department of Chemistry, Columbia University and Profesor at Natural Sciences Department, Hostos Community College. Published more than 100 research articles in SCI(E) journals.

Ozlem Alptekin*, Emre Karaoglan
University of Cukurova, Turkey

Transferase enzymes used in drug synthesis

Transferase enzymes catalyse the transfer of different functional groups of a donor molecule to another molecule. In drug synthesis, they are especially used to obtain enantiomerically pure drug intermediates. This kind of chemoenzymatic synthesis is used to improve unfavourable conditions of traditional chemical syntheses. Unlikely chemical syntheses, chemoenzymatic syntheses are more efficient, faster, more affordable, more effective, and environmentally friendly. For this purpose, the number of studies of researchers about chemoenzymatic syntheses is increasing day by day.

In this presentation about transferase enzymes that are obtained from various sources to be used in chemoenzymatic syntheses were evaluated. Glycosyltransferase and transaminase enzymes are investigated in detail. Glycosyltransferase enzymes were used to obtain derivatives of vancomycin which is an antibiotic. Transaminase enzymes were used in the synthesis of rivastigmine which is a drug used in the treatment of Alzheimer's disease, steroid, and steroid derivatives, levetiracetam which is an anticonvulsant drug, sitagliptin which is an anti diabetic medication and glasdegib which is an inhibitor of SMO (Smoothened). Studies in the literature have been examined in detail in terms of parameters such as general properties of used enzymes, reaction medium, the yield obtained as a result of synthesis, conversion, and enantiomeric excess rates in these studies.

Audience Take Away

- The audience will learn about some transferase enzymes that play a critical role in the enzymatic synthesis of various drugs and drug precursors.
- There may be an alternative synthesis route that can be applied in the laboratory to the person working in the synthesis of drugs and drug-derived compounds.
- It may be an important opportunity for her/him to recognize transferase enzymes.
- She/He can use this knowledge both theoretically and practically.
- Due to its catalytic importance, it may be causing the investigation of new types of transferase enzymes.

Biography:

Dr Alptekin studied Department of Chemistry at the Cukurova University, Turkey and graduated as MS in 2003. She received her PhD degree in 2009 at the same institution. After four years she obtained the position of an Assist Professor at the Faculty of Pharmacy at Cukurova Univetsity. She has published more than 14 research articles in SCI(E) journals and 530 over cites.

Dr Nivedita Sharma*, Nisha Sharma
Dr Y S Parmar University of Horticulture & Forestry, India

Microbial hydrolytic enzymes - power house of green fuel

The world is facing a reduction of global fossil fuels resources, like petroleum, natural gas, or charcoal, while energy requirements are progressively growing up. Fossil fuels should be replaced, at least partially by biofuels once the current fuel supply is suspected to be unsustainable in the foreseen future. In fact, the search for sustainable alternatives to produce fuel and chemicals from non-fossil feedstocks has attracted considerable interest around the world, to face the needs of energy supply and to response to climate change issues. Alternative resources of energy are being explored in order to reduce oil dependence and increase energy production by exploring non conventional renewable sources. Among them, biomass possesses a potential target for fuel and power production. Thus biomass can efficiently replace petroleum-based fuels for a long term. Apart from direct food chain items, lignocellulosic woody waste is preferred due to its easy availability and abundance in nature.

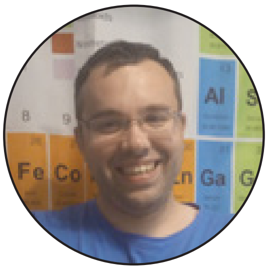
Lignocellulosic waste consists of three main components: cellulose, hemicellulose and lignin which make about 50% of the total biomass in the world. Enzymatic hydrolysis of lignocellulosic biomass is considered as a key step for generating fermentable hexose and pentose sugars from lignocellulosics which in turn are converted to ethanol as biofuel. These hydrolytic enzymes viz. cellulase, xylanase and laccase are produced by specialized microorganisms- bacteria and fungi. The conversion of biomass into bioethanol not only will accomplish the demand for energy resources but also have positive effects on the environmental and socioeconomic position of the world.

Audience Take Away

- Globally, there is a great expectation regarding huge transformation in fuel industry. Biofuels have become of special interest to replace conventional fuels partially/ fully in near future. Thus hydrolytic enzymes of microbial origin are the key players for green fuel based biorefineries to make the process cost effective and economical. A powerful role of enzymes will definitely create interest amongst the audience.
- Audience will be benefitted in a multiple way through this talk as it will cover all the important aspects of industrial process i.e. isolation, screening of robust enzyme producing strains, their identification, enzyme production, optimization of environmental parameters, purification and application for hydrolysis of complex carbohydrates to saccharify and convert woody waste to 2nd generation bioethanol.
- This lecture will try to tackle the constraints/ bottlenecks of bioconversion process with novel scientific solution for commercial feasibility in biobased industries.

Biography:

Dr Nivedita Sharma is working as Professor and Head in the Department of Basic Sciences, Dr Y S Parmar university of Horticulture and Forestry Nauni, Solan (H.P.) –India. She has about 26 years of teaching and research experience in Microbiology discipline. She is actively involved in the research area of enzymes, biofuels, probiotics, functional foods and neutraceutical. She has guided many MSc and PhD students. She has published more than 200 publications in International and National journals and Proceedings. She is an active organizing committee member for seminars, conferences, workshops of the department and university. She is the recipient of many National and International awards. She is the member of many prestigious societies.



Michael Badawi
University de Lorraine, France

Ab initio tools for upgrading of biomass and production of biofuels

Pyrolysis of lignin, derived from lignocellulosic biomass, produces bio-oils with high oxygen content (20-45 wt.%). These bio-oils can be upgraded by hydro deoxygenation (HDO), a thermal catalytic process under H2 pressure, to obtain more valuable oxygen-free products.Thus, we combine theoretical and experimental techniques to elaborate, characterize, and test innovative HDO catalysts. Among different catalysts and supports, iron supported on silica proves an optimal selectivity/activity with low deactivation rate. Different amorphous silica surfaces having various silanol densities (7.2, 5.9, 4.6, 3.3, 2, 1.1 OH/nm2) have been considered. DFT calculations show negligible CO competition on phenol adsorption over those surfaces, which make them more favorable than conventionally used CoMoS supports. Among them, the one with 3.3 OH/nm2 appears to exhibit the highest selectivity for the direct C-O bond cleavage with less water competition effect.

Then single iron atom catalysts (SACs) supported on mesoporous silica were elaborated following the Sol-gel mechanism using non-ionic (P123) and metallic (CTAF) surfactants as porogens. Tuning the P123/CTAF molar ratio enables to control the iron loading, as well as the silica structural properties, Fe-impregnated and Fe/Cu impregnated catalysts were tested for guaiacol HDO conversion and results proved that Fe-Cu have a better performance (90% conversion, 70% phenol selectivity) than pure Fe catalysts since incorporation of Cu facilitates the reduction of Fe(III) species.

We will also show how protonated zeolites and mesoporous silica with optimized silanol density can be used to purify the bio-oils obtained by selectively remove the residual phenol from the feed.

Audience Take Away

- How theoretical modeling can guide experimental work, especially synthesis of materials.
- How theoretical modeling can explain experimental catalytic results, and help to improve the processes.
- Concrete examples of catalytic applications will be shown: from predictive DFT modeling to the optimization of catalysts and conversion results.

Biography:

Michael Badawi, 40 years old, is Associate Professor in the Laboratory for Physical and Chemistry Theories (LPCT), CNRS - University of Lorraine, in France. His research focus on the in silico design of materials for environmental applications and energy production from biomass using modern atomistic simulation techniques such *asab initio* molecular dynamics. He currently manages several projects (PIA, FEDER, PHC) in connection with industrial (BASF, ArcelorMittal, EDF) and academic partners from many countries (Germany, Slovakia, Morocco, Tunisia, Lebanon, Chile). He supervised 2 post-doc and 7 PhD. He is co-author ofmore than 100 publications and 90 communications.

Petru Spataru*, Alexandru Visnevschi, Oxana Spinu, Igor Povar, Francisco Fernandez, Tudor Spataru
Academy of Sciences of Republic of Moldova

The influence of temperature and presence of organic sulfur R-S-H on the separation degree of organic solids from wastewater

In the technology of separation of organic solids from wastewater, there are several ways of combining activated sludge, produced under technological aeration conditions, with primary sediment, obtaining different results depending on the ambient temperature, so the natural climatic conditions. At the same time, the sedimentation dynamics depends directly on the temperature. As the usual summer temperatures do not exceed thirty degrees, the bio-coagulation process takes place, which ensures about 5% concentration by gravitational sedimentation. Using flocculants, dispersed systems can be processed/concentrated/dehydrated by centrifugation. However, in the temperature range 40-45oC, under thermo-mesophilic conditions, a separation process takes place not by sedimentation, but by well-contoured flotation. In the conditions of dehydration of organic solids in sediment processing, the temporary, short-term reduction of the smell of organic residues is recently used by treating them with inhibitory preparations, which link organic sulfur with the general formula *R-S-H*, in which *R* is an organic radical. The above-mentioned treatment aims to replace hydrogen from organic sulfur compounds of the general formula R-S-H with an organic radical, which makes it possible to reduce the odor of organic residues in biological treatment. Experiments through laboratory simulations show that the replacement of hydrogen with a radical leads to a decrease in the flotation effect within the thermo mesophilic separation process. Thus, the lack of R-S-H compounds leads to the decrease of gaseous microbubbles that ensure the flotation process. In this way the flotation conditions are ensured by the thermo mesophilic temperature regime and the presence of organic sulfur compounds with adjacent hydrogen.

Audience Take Away

- Both scientific researchers and students will know how (a) the ambient temperature and (b) the activity of R-S-H compounds influence the stimulation of the processes of separation of organic solids from wastewater in the process of urban wastewater treatment.
- Scientific researchers will find out (a) how at some ambient temperatures a synergistic process is prioritized, and at temperatures that differ by only 10 -15 degrees Celsius, a different type of process is prioritized; (b) how R-S-H compounds stimulate the formation of gas bubbles which cause the change for separation processes from gravitational to flotation sedimentation. The related knowledge in the field of processing of organic solids residues from urban wastewater is useful for both researchers and students. Specialists in the field of wastewater treatment technologies will learn new methods to streamline the processes of dehydration of organic solids.

Biography:

Dr Spataru studied Chemistry at the Chișinau State University, Republic of Moldova with a bachelor’s thesis in the field of nuclear magnetic resonance in 1977.In 1995-2013 employee of the National Institute of Ecology Dh D Chemistry since 2011. From 2013 until today senior scientific researcher then (2016) coordinating scientific researcher in the Laboratory of Physical-Chemical Methods of Research and Analysis Has published more than 80 research articles in SCI(E) journals.

Seda Cetindere
Gebze Technical University, Turkey

BODIPY dyes in light driven catalysis

Due to population growth and rising industrialization, the global energy demand will increase significantly over the coming decades. Amongst several alternative energy schemes, hydrogen has been considered as one of the most promising candidates to provide sustainable, carbon neutral energy on a global scale. Therefore, the light-driven production of hydrogen from aqueous media using homogeneous or heterogeneous multicomponent catalysts is considered one of the most urgent areas of sustainable energy research to provide hydrogen as energy carrier and chemical feedstock. Suitable catalysts for the light-driven hydrogen evolution reaction (HER) must combine high catalytic activity, high stability and long operating times with economical viability and availability on a global scale. The production of solar hydrogen requires multi-functional systems that combine light absorption, charge separation, and catalytic conversion. One promising approach is the combination of all required functions into one molecular or supra molecular photo sensitizer–catalyst dyad. The visible light-driven HER by covalent photo sensitizer-catalyst dyads is one of the most elegant concepts in supra molecular homogeneous solar energy conversion. For hydrogen production, a deep understanding of the chromo phore and catalyst is crucial in building an efficient system. While many current studies focus on noble-metal-based photo sensitizers (e.g. ruthenium or iridium complexes) and catalysts (e.g. rhodium, platinum or palladium complexes), there is an urgent need to expore noble-metal-free alternatives. One promising photo sensitizer class are boron-dipyrromethene (BODIPY) dyes which are ideal photo sensitizers and feature high molar absorptivities, tunable absorption and emission energies, and high fluorescence quantum yields. In addition, they can be chemically functionalized and thus linked to catalytically active species. The aim of this research is to provide fundamental concepts for the design of high-efficiency sunlight-driven homogeneous HER catalyst systems which bring together high catalytic performance with a completely noble-metal free design based purely on earth abundant components.

Audience Take Away

- The aim of this talk is to provide fundamental concepts for the design of high-efficiency sunlight-driven homogeneous HER catalyst systems which bring together high catalytic performance with a completely noble-metal free design based purely on earth abundant components.
- As such, the system will provide new design principles to demonstrate how efficient light absorption, charge separation and catalytic hydrogen production can be combined in one molecular component.
- Catalytic, photo physical and mechanistic studies will form the basis for a detailed understanding of the catalyst performance and catalyst limitations.
- Based on these insights, this research aims at providing optimized materials design routes which could lead to improved, technologically relevant HER catalysts.

Biography:

Dr Seda Cetindere is a research assistant of Chemistry Department at Gebze Technical University. She received her BSc degree from Abant Izzet Baysal University Department of Chemistry in 2006. She completed her MSc and PhD in 2017 at Gebze Technical University in Chemistry Department. She completed her post-doctoral research at Ulm University Institute of Inorganic Chemistry I (Materials and Catalysis) in 2019. Her research interests are inorganic-organic hybrid materials for photocatalysis, polyoxometalates, BODIPY dyes and phosphazenes chemistry. Dr. Cetindere has co-authored in SCI, SCI-expanded journal articles, book chapters and conference papers and has taken part in many national projects.

Silviya Boycheva*, Denitza Zgureva, Hristina Lazarova, Margarita Popova

Technical University of Sofia, Bulgaria

Development of cost-effective catalytic systems for total oxidation of VOCs by utilization of solid fuel combustion by-products

Coal-based energy production still plays a leading role worldwide, growing in a number of fast-developing countries. The European Union's strategy for the next decade is to limit the burning of coal, but the number of incinerators and gasifiers for municipal waste continues to increase rapidly. The combustion of coal and household municipal waste generates a solid by-product from the thermal modification of the mineral components contained therein, the so-called ash that is disposed or utilized. The utilization of coal ash for the production of building materials is based on the self-cementing properties at high lime content and on the pozzolanic reaction at significant presence of alumina silicates, and is well studied and widely applied in practice. National and international standards for the classification of coal ash as a construction raw material have been introduced while the development of technological solutions for the recovery of ash from municipal waste is still pending. A solution also awaits the fertilization of huge quantities of already deposited coal ash and the restoration of soils. The application of the concept of circular economy in production, including energy generation, requires a minimum consumption of raw materials and maximum utilization of by-products in terms of efficient energy consumption. This requires the development of efficient and smart approaches to waste recovery by converting them into products with high practical and environmental benefits. The present study aims to utilize coal ash to develop cost-effective and highly active catalytic systems for the total oxidation of volatile organic compounds (VOCs). Coal ash usually contains more than 70 wt. % alumina silicates and the other components are mainly oxides of alkali, alkaline earth and transition metals. The content of iron oxides in the form of hematite, magnetite or maghemite, as well as of iron ions incorporated in alumina silicates, usually varies between 5 and 15 wt% and depending on the type of coal can reach even higher concentrations. This composition of coal ash allows it to be processed into zeolite-like materials by simple alkaline conversion, as alumina silicates form the structural framework of the zeolite phase, and iron oxides and other metal particles from the source ash are evenly distributed in the zeolite matrix, forming active catalytic centres. These self-assembled catalytic systems of porous support and active centers show high efficiency toward total oxidation of VOCs comparable to that of platinum group metal catalysts (PGMs), which are extremely expensive and PGMs are in critical supply worldwide. Coal ash catalytic systems (CACats) were obtained by two-stage alkaline conversion and ultrasonic homogenization of the reaction mixtures. They are characterized in terms of phase composition of the zeolite matrix, morphology, surface properties and thermal stability, and the state and distribution of iron oxide components. An additional modification was applied by wet impregnation technique with copper or cobalt oxides to improve their catalytic properties. The thermal and dynamic functions of catalytic oxidation of CACats to model VOCs and competitive catalysis in VOCs mixtures were studied. Total oxidative destruction of VOCs was achieved with a sharp decrease in the process temperature below 500 C.

Acknowledgements: This work was financially supported by the National Science Funds, Ministry of Education and Science of R. Bulgaria under contract DN 17/18 (2017).

Audience Take Away

- Utilization of solid waste from fuel combustion in environmental protection systems in the context of circular economy Conversion of fly ash from coal combustion into cost-effective catalytic systems.
- Application of dual-function systems derived from wastes as reliable and cost-effective catalysts for total oxidation of volatile organic compounds and carbon capture.
- The current study will focus on technologically viable opportunities for recovery of solid waste with high aluminosilicate content for development of cost-effective catalysts with significant effect in environmental protection.
- The present research provides technologically accessible practical solutions to severe environmental problems;
- The research is multidisciplinary and is based on a number of modern techniques for characterization of new materials and research of their applications;
- The developments can be applied in theoretical and practical training of students and graduates;
- The study is of interest to companies that implement environmentally friendly technologies for integrated pollution prevention in their industries.

Biography:

Assoc. Prof Dr Eng Silviya Boycheva is a lecturer at Technical University of Sofia, Bulgaria. Graduated as chemical engineer in 1995, attained PhD degree in 2002 and academic rank Associate Professor in 2012. S. Boycheva is specialized in the University of Kassel, Germany (2003-2005,2007,2009,2011) and Research centre ENEA-Casaccia, Rome, Italy (2005,2006,2007). Supervisor of above 30 diploma thesis works; author of a book "Systems and devices for environment protection in thermal energy plants" (2011) and of over 140 scientific publications; involved in more than 25 research projects; member of Humboldt Union in Bulgaria. Research fields: water chemistry, utilization of combustion by-products, carbon capture, sensors, composite films, etc.

E Kweinor Tetteh* and S Rathilal
Durban University of Technology, South Africa

Application of biophotocatalytic system for CO_2 mitigation in anerobic biogas production

With the rapid increase in global energy consumption and depletion of natural resources, economic assessment of photo -bioreactor technology in wastewater settings for water and energy (biogas) production comes as an essential drive for global sustainability development. Thus, recovering biogas and other valuable resources from wastewater treatment is foreseen as the centre for bio-based circular economy. In this study, an integrated Biophotoreactor (BP) systems incorporated `with titanium dioxide magnetite (2g of Fe-TiO2), activated sludge (450 mL) and wastewater (350 mL) were developed. A techno-economic analysis was carried out to evaluate the performance and economic viability of the integrated systems for the consideration of wastewater treatment, biogas production and carbon footprint improvement. With a working volume of 0.8L and headspace of 0.2L, the BP system was operated at mesophilic temperature of 35oC for a hydraulic retention time of 30 days, was operated under two UV-light bulbs (T8 blacklight - blue tube, 365 nm, 18 W, Philips, Netherlands). Above 65% of chemical oxygen demand (1600±16.2 mg/L), Total Kjeldahl Nitrogen (76 ±6.4 mg/L), total solids (135 ±12 mg/L) and volatile solids (94±6.8 mg/L) contained in the wastewater were removed by the BP at a pH of 6.5. The cumulative biogas estimated were 1125 mL/d and was successfully fitted on a modified Gompertz kinetic model. The the BP system energy assessment resulted in 2.04 kWh/L produced from the breakdown of the organic matter. Assuming 78% of the biomethane produced was used to power the UV-lights, the carbon emission reduction estimated was 464.37 kgCO2/kwh. Synergistically, the results of the integrating photocatalysis in biological system is viable for biogas production and wastewater purification. Therefore, the prospects of adapting this technology into the wastewater settings has sustainable tendency for both energy and wastewater reuse.

Keywords: Anaerobic digestion, biogas, biomethane, magnetic nanoparticles, wastewater, renewal energy

Audience Take Away

- Synthesis of magnetized photocatalyst and its application is highlighted.
- Valorization and treatment of wastewater biologically is presented.
- Adding value to the wastewater economy is discussed.
- Mitigation of CO2 emission in the wastewater settings.
- Reinforcing this finding in the wastewater settings has good prospects for industrialization and commercialization with reusable of photocatalyst.

Biography:

Emmanuel Kweinor Tetteh is a doctoral researcher with Green Engineering and Sustainability Research Group under the same department and supervision of Prof Sudesh Rathilal. His research focus aimed to develop magnetic photocatalyst for wastewater abatement and CO2 methanation from biogas. He also holds many accolades to his name, key among them being the ENI Award for the Young Talent from Africa, in a ceremony presented by the President of the Italian Republic, Sergio Mattarella. As a young researcher, he has authored and co-authored more than 30 peer reviewed journal papers, book chapters with google citations of 250 and h-index 10

Riheb Mabrouk, Hacen Dhahri, Hassane Naji
University of Monastir, Tunisia

Lattice boltzmann simulation of metal foam porosity effects on phase transition phenomenon in a latent heat storage device

This paper performs a numerical evaluation of the geometric structure of metal foam such as pore density (PPI; number of pores per inch) and porosity effect on melting and solidifying phenomena heat transfer in an open-ended rectangular porous channel (metal foam) contained a phase change material (PCM: paraffin) under forced convection. The local thermal non-equilibrium condition (LTNE) is manifested between phases (thermal field) and the Darcy-Brinkman-Forchheimer model (DBF) for dynamic field. Governing equations are simulated using the thermal single relaxation time (T-SRT) lattice Boltzmann method (LBM) at the representative elementary volume (REV) scale. In this work, the lattice Boltzmann equations (LBE) are based on the D2Q9 model. Fluid flow and the fluid and solid temperatures were simulated via three distribution functions. The effects of metal foam PPI (10 £ PPI £ 30), porosity (0.7 £ e £ 0.9) and Reynolds number (200 £ Re £ 400) on melting (charging) and Solidifying (discharging) phenomena were investigated. Outcomes are presented for the local thermal non-equilibrium parameter and the entropy generation rate for the selected parameters range. Previously, to validate our in-house code, a comparison with other available cases in literature was done. Results show that among the different features of metal foam such as thermal conductivity and porosity, the decrease of the latter and the increase in Re speeds up the melting phenomenon under the unsteady, forced and laminar convection. However, a decrease of PPI for high porosity (=0.9) gives a minimal LTNE value during charging case (melting), but during discharging process (solidification), an increase of PPI for lower porosity (=0.7) decreases the LTNE parameter whatever Re number.

Audience Take Away

- The system presented in this work is an exchanger heat that stores thermal energy. The objective of this study is:
- Analyze and find a range of parameters that makes good storage conditions. Find the ideal conception of a heat exchanger calculate the global energetic and exergetic efficiencies.

Biography:

Riheb Mabrouk is a PHD student at the National Engineering School of the Monastir/ Monastir University. Her research focus on thermal energy storage in porous media using the Boltzmann method. She has published four papers in International Journal of Heat and Mass Transfer, International Communication in Heat and Mass Transfer, energies and processes.

Guray Yildiz
Izmir Institute of Technology, Turkey

Pyrolytic production of biofuel intermediates in the presence of zeolites: A focus on continuous operations

Renewable energy sources principally used for power and heat production (wind, solar, etc.), are not suitable for the production of conventional fuels and raw materials (e.g. petroleum-based chemicals) currently used in the existing industries. To continue the production of chemicals and (transportation) fuels, and to contribute to the sustainability of the current petrochemical-based economy, biogenic resources (e.g. biomass, MSW) should be utilized.Pyrolysis has been considered as a viable thermochemical conversion technology for the production of fuel intermediates, chemicals, and heating sources from the aforementioned resources. The outcome of a pyrolysis process depends on several factors related to the type and the properties of the biogenic feedstock and to the reactor, process conditions, and intended application of the final products. By carefully tuning those, a pyrolysis process can be designed for the maximized production of a liquid product, viz. fast pyrolysis bio-oil (FPBO). For specific applications of FPBO, like in diesel or gasoline engines, or as an intermediate bio-based feed material in the existing petroleum refineries, a certain degree of upgrading including the (partial) removal of oxygen and cracking of the oligomers is required. For this purpose, zeolite-based heterogeneous catalysts can be utilized. This can be achieved by (partially) replacing the heat transfer material by a solid catalyst (in situ). Besides, the primary pyrolysis vapors can be catalytically reformed in a separate catalytic reactor (e.g. fixed or trickle bed) just after the fast pyrolysis reactor (ex situ vapor phase upgrading, i.e. ex situ VPU). The presence of the catalyst favors oxygen removal via decarbonylation (CO rejection), decarboxylation (CO2 rejection) and dehydration (H2O removal) reactions. VPU induces vapor phase reactions that cause a change in oxygen functionalities and oxygen concentration, alleviate the acidity, and increase the calorific value of the produced liquid product. Hence, such a liquid biofuel intermediate becomes more similar in chemical composition to current conventional fuels.On the operational side, however, continuous bench- and pilot-scale testing with zeolite-based catalysts have shown poor results: de-oxygenation of the pyrolysis vapors appears to go along with a progressive reduction in organic liquid yield. Apart from any control over the catalyst activity, selectivity and lifetime, the other critical issue is in the process design which is complicated by the rapid catalyst deactivation through coke formation and catalyst poisoning by thefeedstock originated minerals.Hence, for a successful implementation of technology, the translation of laboratory results to viable process concepts and pilot plant trials by addressing key issues like the most suitable processing mode, reactor technology, and the way of heat integration of the process are needed.The objective of this talk is to focus on the research and development advances and trends in the field of pyrolytic production of biofuel intermediates in the presence of zeolites based on precisely selected literature studies. The spotlight will be on research aiming at optimal catalytic process conditions, reactor technologies, and the end product properties. The final goal is to come up with a clear picture on how to realize this technique at a commercial/industrial scale.

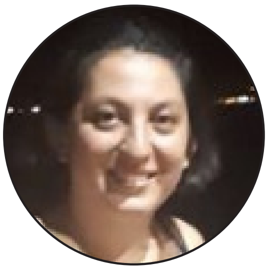
Audience Take Away

- This talk will help researchers to brainstorm in designing more effective catalysts capable of handling complex feedstocks in pyrolysis conditions.

- Macro-scale applications of catalysts and their effective utilization in a process are as important as the synthesis of catalyst, and their micro-scale experimentation and related analyses. Hence, this talk will provide important insights for the catalyst scientists, as it will discuss catalyst-specific requirements for a successful implementation of these specific catalysts (zeolite-based) at a commercial-scale operation. The information that will be given in this talk will propose practical solutions to the problem of catalyst deactivation during pyrolysis; this could simplify or make a catalyst designer's job more effective.

Biography:

Dr Guray Yildiz is a chemical engineer specialized in pyrolysis technology, particularly in the design, development and optimization of pyrolysis reactors/processes. After receiving his PhD degree from Ghent University (Belgium) in 2015, he worked as a postdoctoral research associate in Ghent University and a visiting postdoctoral fellow in Iowa State University of Technology (USA). Currently, he works as a tenure track professor on waste-to-energy, thermochemical energy conversion systems and renewable fuels in Izmir Institute of Technology (IZTECH, Turkey). Dr. Yildiz has over 30 academic records and acts as a reviewer for several journals listed in Web of Science.



Ece Kilic
İskenderun Technical University, Turkey

Picoplankton under the influence of climate change

Anthropogenic activities like greenhouse gas emission, land use change and deforestation alter the dynamics of atmosphere. Ecological life in the marine environment depends on the balance between atmosphere and ocean; so, variations in the climate cause changes in the chemical and biological equilibrium of oceans. Sea surface warming, ocean acidification, alterations in nutrient cycles and available nutrients influence the picoplankton dynamics. Some functional groups like cyanobacteria may become beneficial; while, some others like calcifies may negatively impacted. Eventually, marine microorganisms will adapt to the new control mechanisms of changing world. Therefore, predicting the future responses of picoplankton to the climate change will help marine biologist to understand the marine dynamics. This study was aimed evaluate the picoplankton responses to the impacts of climate change in the Mediterranean Sea.

Audience Take Away

- This talk will help researches to understand the ecological balance of Mediterranean Sea.
- This talk will help researches to evaluate the balance between biological and chemical components of marine systems.
- This talk may help researches to get inspiration from marine ecosystem.

Biography:

Dr Ece Kilic was graduated from Environmental Engineering department of Middle East Technical University at 2014. Since then, she has been working at İskenderun Technical University, Water Resources Management and Organization Department as a research assistant. She studied biological and chemical indicators of surface water quality in MS and graduated in 2017. She studied marine biology in her doctoral thesis and received her PhD in 2021. She published many articles in several peer-reviewed journal and participate several symposiums worldwide.

Francesco Nocito*, Angela Dibenedetto, Michele Aresta
University of Bari, Italy

Biomass-derived molecules valorization: from furfural to 2, 5-furan dicarboxylic acid using a two-step oxidation/carboxylation process

Biomass-derived oxygenate-species can be considered an alternative to fossil resources derived chemicals. Among them furfural, that can be easily produced from xylose dehydration over acid catalysts, has received great attention as precursor of commodity chemicals. In this paper we present a two-step process for the conversion of furfural into 2,5-furan dicarboxylic acid (FDCA) that can replace fossil sourced phtalic acid used for the production of polyesters such as polyethene phtalates (PET). Polyethene furoate–PEF, has the right properties for being converted into fibers, films and packaging materials. The highly selective synthetic procedure is based on two steps, namely: i) a heterogeneously catalyzed aerobic oxidation of furfural to furoic acid in water and ii) the direct carboxylation of the latter to 2,5-FDCA. In the first step, furoic acid is obtained with 20% yield and 100% selectivity using low cost mixed metal oxides (MMO) as catalysts: both the unreacted reagent and the catalyst are recovered and re-used in subsequent cycles to improve the conversion [3]. In the second step, furoic acid is converted into 2,5-furan dicarboxylic acid in presence or absence of CO2 [4]. A key copper-di-furanoate intermediate has been synthesized and fully characterized that is able to promote the carboxylation at C5 of furoic acid affording 2,5-FDCA with 98% yield and 100% selectivity. The recovery and recycling of metal species make this process quite useful for synthetic purposes.

Acknowledgements

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Audience Take Away

- What is the importance of using renewable materials compared to fossil sources?
- Use of lignocellulosic biomass in the preparation of bioplastics
- Market and technological differences between the use of C5 and C6 sugars
- CO_2 valorization

Biography:

Dr Nocito graduated in Inorganic Chemistry and received his PhD degree in Chemical Science at the Bari University, Italy. He then joined the research group of Prof. Aresta and Prof. Dibenedettoin the field of Catalysis, CO2conversion and renewable sources valorization.He also worked as Chemist and Plant Manager for a wastewater treatment industry (2012-2017).

Dawei Chen
Research Institute of Petroleum Exploration, China

Gas generation mechanism of interaction between organic matter and water in high evolution stage

In this paper, a comparative simulation experiment of bitumen, crude oil and kerogen samples under water and no water conditions was conducted to study the mechanism of the interaction between highly evolved organic matter and water.

The results show that:

1. The participation of water improves the yield of natural gas from the pyrolysis of high evolution residual organic matter.
2. The participation of water delays the cracking of ethane and propane, resulting in low drying coefficient of natural gas and delayed reversal of carbon isotope, which inhibits the generation of natural gas at low temperature.
3. The participation of water can provide hydrogen source, promote the further cracking of high evolution residual organic matter macromolecules at high temperature stage, and promote the generation of natural gas.

Audience Take Away

1. The gas generation mechanism of residual organic matter in deep, ultra deep and high evolution stages is established.
2. The gas generation mechanism of highly evolved organic matter water interaction was studied.
3. The existence of water may be an important factor in the downward extension of the lower limit of crude oil pyrolysis gas in the reservoir.

Biography:

Dawei Chen received a master’s degree from the University of the Chinese Academy of Sciences in 2020, and then studied for a doctorate at the Research Institute of Petroleum Exploration & Development. He studied organic geochemistry under Professor Jian. Li.

Binitha N Narayanan*, Sowmya Bala subramaniam
University of Calicut, India

Eco-friendly preparation of copper oxide/graphene nanocomposites and their Fenton like activation of persulphate for the degradation of 4-chlorophenol

Facile preparation of graphene in an eco-friendly manner and development of its composites for enhanced catalytic performance is one of the main targets of researchers. Green synthesis of copper oxide/graphene nanocomposites are performed here by a simple hydrothermal treatment of copper precursor with an aqueous dispersion of graphene prepared by ball-milling graphite with sucrose and their application as catalysts in the Fenton like degradation of 4-chlorophenol using ammonium persulphate is investigated. The structure and morphology of the prepared copper oxide/graphene systems as well as the characteristics of the active sites responsible for the catalytic activity are analyzed through various characterization techniques. XRD analysis reveals that the prepared system contains Cu mainly in the form of CuO together with a minor amount of Cu2O as active sites responsible for the catalytic activity. More or less uniform distribution of copper oxide nanoparticles over graphene support and the homogeneity of the prepared samples were obtained by performing FESEM analysis and selected area mapping analysis. The uniformity in size and the spherical nature of the copper oxide nanoparticle that is decorated on the graphene sheets are visible from the TEM analysis. XPS analysis confirmed the existence of strong bonding interaction between Cu and graphene which further favoured the formation of the effective nanocomposite. The activity of the prepared systems in treating wastewater containing 4-chlorophenol is proved from the high efficiency of copper oxide/graphene nanocomposites in the Fenton like degradation of 4-chlorophenol. 100% of degradation of 1 mM 4-Chlorophenol (50 ml solution) is observed when using the best CuO/graphene nanocomposite under the selected reaction conditionsof 0.05 g of the catalyst with 0.02 g of APS in 3 h reaction time.

Audience Take Away

- A facile preparation of graphene is presented here, which is eco-friendly and an alternate means of graphite oxide assisted routes of graphene.
- The composite preparation with CuO is possible in aqueous medium which is an additional advantage even though the prepared graphene is of less defective nature.
- Audience can explore the method of preparation of graphene for the design of various composites of graphene in aqueous medium. These kinds of graphene preparation enable the use applications of graphene to variety of fields since there is no stringent or hazardous conditions in material preparations. Even a UG student can execute the method easily and in a safe manner if there's the availability of a ball mill. Since the yield is also high, there is the possibility of upgradation and industrial scale up.

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 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 doneone-year postdoctoral fellowship (2008-2009) supervised by Prof. Dr Zahira Yaakobat the Department of Chemical and Process Engineering, National University of Malaysia, Malaysia. She has published more than 60 research articles in SCI(E) journals.)

KEYNOTE FORUM

DAY
2

8TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

SEP 27-28, 2021

CAT 2021

Nikolaos C. Kokkinos
International Hellenic University, Greece

Process Simulation of in situ Catalytic Fuel Upgrade in Aqueous Media

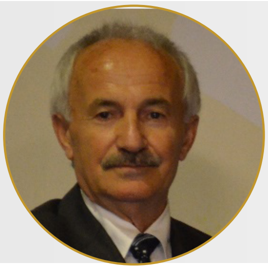
Homogeneous catalysis in refinery processes is rare, mainly due to the separation difficulties that emerge. Thus, the very many benefits of the homogeneous catalysis are still kept apart from the petroleum industry. In the present research work, a successful application of heterogenized homogeneous catalysis was implemented taking into advantage its pioneering benefit that is the efficient and convenient recovering of the catalyst. To that end, homogeneous catalysis is introducing to the downstream petroleum industry efficiently and effectively. The effects of partial hydrogen pressure and reaction temperature in biphasic hydrogenation of a hydroformylated fuel catalyzed by water-soluble Ru/TPPTS complex, which was produced in situ by adding $RuCl_3 \cdot xH_2O$ catalyst precursor to TPPTS (TPPTS = $P[m\text{-}C_6H_4SO_3Na]_3$, trisodium salt of m-trisulfonated triphenyl phosphine), were thoroughly examined. Furthermore, the chemical process has been modeled and simulated based upon cubic equations of states (CEOS) modifications employing PR78 CEOS, Twu's alpha function and vdW mixing rules. $RuCl_3$/TPPTS catalytic system proved to be an effective catalyst for fuel upgrading process with particularly high conversion of the hydroformylated fuel (98.9%). Taking into consideration the complexity of the substrate composition and the groundbreaking features of the proposed fuel upgrading chemical process, the simulation model managed to develop a complete phase behaviour of the fuel as well as to achieve an adequate AARD from the experimental data; giving the opportunity for a scale-up study of the process. The final upgraded fuel could probably replace from the refinery blended gasoline pools the toxic gasoline ether oxygenates (GEOs) such as ethyl tert-butyl ether, methyl tert-butyl ether, tert-amyl methyl ether, with an in situ and an environmentally benign catalytic process.

Audience Take Away

- Heterogenation of homogeneous catalysts and taking advantage of their pioneering benefits.
- Chemical process modeling and simulation on complicated substances for an effective scale-up study.
- Verification and validation of the chemical process model.
- A comprehensive phase behavior of the fuel during hydrogenation reaction.
- Influence of partial hydrogen pressure and reaction temperature in the activity of the catalytic system.

Biography:

Dr Nikolaos C. Kokkinos is Associate Professor at the Department of Chemistry of the School of Science of the International Hellenic University (IHU), Greece. He is the Program Director of MSc in Oil and Gas Technology at IHU. He is in charge of Process Simulation in Petroleum and Natural Gas Engineering Laboratory at IHU; and he holds a researcher position in the Division of Petroleum Forensic Fingerprinting (PFF) at Hephaestus Advanced Laboratory. Dr Kokkinos has more than 80 peer-reviewed publications in international scientific journals and conference proceedings. His research interests among others include applied catalysis and process modelling and simulation of complex substances.



Osman Adiguzel
Firat University, Turkey

Lattice reactions and chemical factors governing shape reversibility 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, due to the shape reversibility and capacity of responding to changes in the environment. 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 thermoelasticity. These alloys have dual characteristics called thermoelasticity and superelasticity, from viewpoint of memory behavior. Shape reversibility is governed by lattice reactions and some chemical factors, like atomic bonds, internal friction and lattice vibration. Lattice reactions are two successive crystallographic transformations, thermal and stress induced martensitic transformations. Thermal induced transformation occurs along with lattice 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. 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 lattice twinning and detwinning reactions play a considerable role in shape memory effect and superelasticity. Thermal induced martensitic 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 ternary alloys exhibit shape memory in β-phase field. Lattice invariant shear and twinning is not uniform in these alloys, and cause to the formation of long period layered martensitic structures with lattice twinning on cooling. 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, and this result refers to the rearrangement of atoms in diffusive manner.

Audience Take Away

- Shape memory alloys are multifunctional materials and used as shape memory devices from biomedical to every field of engineering.

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 already been working as professor. 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 as 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.

magnus Group

SPEAKERS DAY 2

8TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

SEP 27-28, 2021

Faridul Islam*, Jianglong Yu
The University of Newcastle, Australia

Microwave-assisted synthesis and structural investigation of coal-derived few-layer graphene via a catalytic graphitization process

Few-layer graphene was synthesized via microwave-assisted catalytic graphitization due to its increasing demand and wide applications. The microwave irradiation temperature at a set holding time played a key role in synthesizing few-layer graphene. The highest degree of graphitization and a well-developed pore structure was fabricated at 1300 °C using a 10% iron catalyst for 20 min. A high-resolution transmission electron microscopy analysis confirmed that the fabricated few-layer graphene consisting of 2–7 layers. In addition, the 2D band at 2700 cm−1 in the Raman spectrum indicated the presence of graphene layers. The Raman mapping also represented the catalyst loaded sample was homogeneously distributed and displayed a few-layer graphene sheet. The highest I2D/IG value indicated a few-layer graphene sheet. The few-layer graphene growth process was induced when iron oxide was reduced to metallic iron. The graphene nucleation and growth occurred via the dissolution-precipitation mechanism of bituminous coal and catalyst droplets. Finally, the synthesis of graphene using the traditional heating method takes around two weeks and over the higher temperature at 3000 °C. While the microwave graphitization required only 20 min and was much faster than the traditional heating method, moreover, the few-layer graphene precursor, i.e. coal, was abundant and inexpensive material. This technique assists in developing a cost-effective and environmentally friendly few-layer fabrication method using a coal-based carbonaceous material.

Audience Take Away

- The audience will quickly convert disordered carbon to ordered carbon structure by drawing an instrumental setup.
- The structural investigation of the few-layer graphene using the Raman mapping and spectrum assists in learning to identify a few-layer sheet.
- Application of few-layer graphene in lithium-ion battery assist in boosting up the energy sector.

Biography:

Faridul Islam obtained his Master's degree in Applied Chemistry and Chemical Technology in 2008, Bangladesh. He is a researcher in the Department of Chemical Engineering, School of Engineering, The University of Newcastle, NSW 2308, Australia. He started his carrier as a Scientific Officer in Bangladesh Council of Scientific and Industrial Research (BCSIR), Bangladesh, from 2010 to now. He has 11 years of research experience. His research is focused on the fabrication of few-layer graphene from coal-based carbon materials for energy storage. He studied the fundamental aspects of the few-layer graphene mechanism via catalytic graphitization under microwave heat treatment. Faridul's actively involved in many research projects of coal-derived advanced carbon nanomaterials for energy storage applications. He has published more than 25 peer-reviewed articles in leading journals.

Wang Xiaosheng*, Li Ranjia, Yu Changchun
China University of Petroleum-Beijing, China

Improving catalytic activity and stability over mordenite for dimethyl ether carbonylation: Effect of selective acid sites removal

Dimethyl ether carbonylation reaction over Mordenite has gained many attentions due to its mild reaction conditions and high product selectivity. However, Mordenite still suffered from short lifetime and poor stability. In this report, we summarized our work on improving catalytic activity and stability over Mordenite for dimethyl ether carbonylation by selective removing the acid sites that were responsible for coke deposition. Taking advantage of the protection effect of the template molecules, we successfully removed the acid sites located inside the 12 member-ring channels by post alkaline or acid treatment. To investigate the modification effect of post treatment to the structure and acid sites, the obtained catalysts were characterized by XRD, N_2 adsorption-desorption, SEM, ^{29}Si NMR, ^{27}Al NMR, NH3-TPD and FTIR. The characterization results showed that the crystallinity of all samples decreased while specific surface area and pore volume increased to some extent. Certain amount of Si species and Al species were leached out during the treatment process, thus leading to the formation of mesopores and macropores. The protective effect of templates to the strong acid sites in the 8 MR and micropores were remarkable. Without the presence of templates, part of the micropores would be destroyed and the strong acid sites would largely be removed. Over the samples that had been post treated with templates inside the micropores, the carbonylation performance still remained the same and the single-pass lifespan gradually extended due to the enhanced mass transfer efficiency and decreased acid sites in the diffusion paths. The side reactions were largely inhibited and the amount of coke deposition also decreased, which demonstrated that retaining the templates during the post treatment was an effective way to enhance the DME carbonylation performance and suppress the coke deposition during the carbonylation process at the same time.

Audience Take Away

- Carbonylation reaction provides a new way for ethanol production from syngas via heterogeneous reaction.
- It was possible to enhance the catalytic activity and stability of Mordenite for the carbonylation reaction by post treatment.
- Mesopores and macropores were formed Strong acid sites were protected by templates in the post treatment process.
- The coke deposition and side reactions were suppressed over the modified MOR catalysts

Biography:

Dr. Wang Xiaosheng studied Chemical Engineering and Technology at China University of Petroleum-Beijing (CUPB) from 2007-2018. After obtaining his Bachelor and Master's degree, he joined research group of Prof. Xu Chunming at 2014. After obtaining his Ph.D degree at 2018, he got a position of Lecture in CUPB. His main research interests mainly focused on the high value utilization of syngas, including higher alcohol synthesis (HAS), ethanol synthesis from DME carbonylation and olefin synthesis from DME. He has published 15 research articles in SCI(E) journals.

Marita Pigłowska*, Beata Kurc
Poznan University of Technology, Poland

Natural carbon materials for sodium-ion batteries

Sodium-ion cells turn out to be a breakthrough compared to lithium-ion cells due to the similar amount of storage energy and much lower price and ease of production compared to lithium-ion cells. Sodium-ion batteries not only replace lithium with one of the most popular earth elements, but also give real hope for completely getting rid of cobalt from the electrodes. When working on the effectiveness of these cells, the world of science is currently focusing on electrode materials. Many biomaterials can be used in the negative half-cell in both lithium-ion and sodium-ion batteries. The form of the material turns out to be a limitation - when processing carbon materials of polymer origin, e.g. polysaccharides are the so-called hard coal. Hard carbon differs from soft carbon in that it will never graphitize, so it cannot be used instead of graphite in a lithium-ion cell. Due to the spread of green chemistry, waste materials are used to obtain hard coal, which increases the biodegradability of the cell and also facilitates its recycling and allows you to get rid of waste from the paper, agricultural, food industries and so on. The aim of this work is to show the natural carbon materials used in sodium-ion cells in order to obtain efficiently operating batteries. The submitted work presents the use of biomaterials as electrode materials, and their functioning and structure are tested using physicochemical and electrochemical techniques. Using materials of natural origin increases the biodegradability of the cell, contributes to spreading the slogan of green chemistry, and also achieves high specific capacities after many charge-discharge cycles.

Audience Take Away

- It is important topic for people who wonder if it is possible to avoid using flammable lithium-ion cells in constructions such as electric vehicles.
- It lets people see which carbon materials are appropriate for sodium-ion cells compared to lithium-ion cells.
- This topic could be used in automotive industry, as green chemistry aspect, in electrochemical studies, kinetics and catalysis. This provide a practical solution to a problem that could simplify or make a designer's job more efficient. It gives the improvement of the accuracy of a design of more biodegradable sodium-ion battery and also information to assist in this problem.
- Combining practical knowledge with theory (learning and working in a laboratory has a very big impact on our lives).

Biography:

Eng. Marita Pigłowska (graduated in 2021), current master student of Composites and Nanomaterials at Poznan University of Technology. In her scientific carrier she published 9 articles in international reviewed journals. She took part in 2 international conferences (presented topics: flammability of lithium-ion cells (she won the prize for the best student oral presentation) and use fuel cells and batteries in automotive industry). In 2019 she became the winner of the 2nd place in Hydrogen Competition in Poland. In 2021 she won the Veolia contest for the best engineering thesis and took part in Summer School of Veolia.

Md Nurul Islam Siddique
University Malaysia Terengganu (UMT), Malaysia

Influence of supplementary nutrients on methane generation from anaerobic fermentation of agricultural waste: Viability & Fertilizer recovery

Different substrates processed together might be the enhancement of needs for the organisms drew in with anaerobic digestion. In the current work, the effect of supplements on the co-digestion of cultivating substrates was assessed. An extra enhancement plan which expects a critical occupation in the anaerobic digestion was used at three stages: 37 °C, 40 °C, and 50 °C. Results exhibited that at 37 °C by the utilization of enhancements, biogas production accomplished 1.38-times that of control. Additionally, 40 °C without supplements addressed a fascinating philosophy as a result of the incredible usage of this mid-temperature that had been found huge (56 % of VS end and 8.4 L-biogas). The anaerobic co-digestion at 50 °C exhibited that biogas production surpassed 11.3 L with supplements and that mL-CH_4/g-VS were 1.24-times that achieved for the system without extra enhancement. Results for each temperature exhibit that the enhancement course of action adds to co-digestion. Also, 37 °C was the most utilized temperature on the advanced scale and had the best impact on the utilization of enhancements during the anaerobic process. Recovery of sludge was 0.09 m^3 sludge/m^3 substrate and the recovery of water was 0.86 (m^3 sludge/m^3 substrate) from the digester. The processed sludge can be utilized as compost and the water can be utilized for irrigation purposes. The time needed to recapture the investment was seen as 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 CO2. 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. He has published more than 40 research articles in ISI journals.

Jesus Gonzalez Cobos*, L. Han, I. Sanchez-Molina, S. Giancola, S.J. Folkman, J.R. Galán Mascaros
Institut de Recherches sur la Catalyse et l'Environnement de Lyon, France

Formate electrooxidation using cobalt hexacyanoferrate as non-noble metal catalyst

One of the biggest challenges currently facing humankind and the scientific community is the energy production and consumption without the use of fossil fuels. Big efforts have been invested in creating technologies that enable closed carbon or carbon neutral fuel cycles, decreasing CO2 emissions into the atmosphere. Formic acid/formate (FA) has attracted increasing interest as a liquid fuel over the last half century, giving rise to many studies seeking for efficient catalysts for FA electrocatalytic oxidation in fuel cells. However, the FA oxidation catalysts are typically based on Pt or Pd, which are prone to catalytic deactivation by adsorption of intermediate species (e.g., CO). We propose the use Co–Fe Prussian Blue derivative (CoFePB), which is one of the first heterogeneous noble-metal-free catalysts reported for the electrooxidation of small hydrocarbon molecules. Importantly, the catalyst showed a very high tolerance against surface poisoning during the reaction, as supported by the cyclic voltammetry and electrochemical impedance spectroscopy data. The remarkable selectivity, stability, and high current density of CoFePB, in contrast to state-of-the- art catalysts based on platinum-group metals, open new oportunities in the search for inexpensive earth-abundant materials for oxidation of organic molecules either for use in liquid fuel cells or for selective organic molecule sensors. Focusing on fuel cell applications, although the currently obtained onset potential must be further decreased, CoFePB can be already implemented in a formate fuel cell using a strong enough oxidant, i.e., stronger than oxygen, which is the typically employed oxidant in fuel cells. As a proof-of-concept, an aqueous direct formate fuel cell configuration has been developed using CoFePB as a formic acid oxidation catalyst coupled with carbon felt as a cathode, Ce4+ as oxidant, and anolyte and catholyte solutions working at basic and acidic pH conditions, respectively. With a maximum power output of 8.6 mW cm-2, this is the first example of a fully noble-metal-free direct formate oxidation fuel cell.

Audience Take Away

- This presentation will show the results obtained in a set of electrocatalytic tests performed under different conditions (reactant concentration, pH, temperature), which have been addressed to study the formate oxidation reaction but could be implemented for many other electrocatalytic reactions.
- Two different kinds of classical electrochemical cells will be described: a three-electrodes cell employed for fundamental studies under anode-potential control, and a two-electrodes cell emulating a fuel cell configuration.
- Along with the electrochemical tests, the developed product analytic techniques will also be described, which are actually useful for faradaic efficiency quantification, but not commonly implemented in electrocatalytic tests reported in literature.
- The results obtained with the proposed CoFePB catalyst may give new ideas to the audience in the search for unexpensive and abundant materials for fuel cell applications.

Biography:

Dr. J. González-Cobos studied Chemical Engineering at University of Castilla-La Mancha, Spain, and graduated as MS in 2011. He obtained the PhD decree in 2015, at the same university, under the supervision of Prof. J.L. Valverde and A. de Lucas-Consuegra. Then he worked for four years in the group of Prof. J.R. Galán-Mascarós at Institute of Chemical Research of Catalonia, Spain, and, since 2020, he is working at Institut de Recherches sur la Catalyse et l'Environnement de Lyon, France, in the group of Prof. P. Vernox. His main subject areas are heterogeneous catalysis, electrocatalysis and energy.

Ashanendu Mandal
University of Calcutta, India

Adsorptive removal of phenol from wastewater using low-cost adsorbents

Phenol being toxic in nature needs to be removed from wastewater before its discharge. This research therefore aims for removal of phenol from its aqueous solution through adsorption process. Four bio-adsorbents such as guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and four industrial waste adsorbents such as rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina have been used in this research work. The surface characterization of the adsorbents were carried out by SEM, XRD, FTIR and BET analyzers. The phenol removal percentage by the adsorbents were investigated through batch experiments with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum removal percentage was obtained as high as 97.50%. The experimental results were used for kinetic study which showed that the pseudo-second order was best fitted for all adsorbents except red mud and the adsorption mechanism was supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggested that Freundlich isotherm model was best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm was best supportive for rice husk ash and clarified sludge respectively. The thermodynamics study successfully revealed the spontaneity, randomness and endothermic / exothermic nature of the adsorption process for each adsorbent. The adsorption experiments were also performed with the real industrial wastewater collected from a coke oven plant. The innovative ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient was also studied which established that the experimental and predictive data were within the allowable range. The scale-up designs and the safe disposal of used adsorbents were studied for examination of their commercial applications. The regeneration of the adsorbents were studied using distilled water and ethanol solution separately to find out their regeneration efficiency. The research however concludes that all the adsorbents are effective for phenol removal and therefore can be considered for circular economy.

Biography:

Ashanendu Mandal has been an energy professional for more than 34 years. His work for ONGC in offshore and onshore oilfields includes commissioning, modifications, safety, operations, artificial lifts, pressure maintenance, EOR and planning. In addition, Mr. Mandal has more than 10 years' experience in marketing of upstream and downstream products. He has participated in oil and gas events in more than 17 countries as a speaker, panelist, roundtable moderator or session chairman. He has few publications in Chemical Weekly. He is an M.Tech in Chemical Engineering and MBA in Finance, and now pursuing his Doctorate in University of Calcutta.

Pranita Rananaware, Parimal Pandit, Aviva D'Souza, Mahaveer . Kurkuri, Varsha Brahmkhatri*

Jain University, India

Surface engineered; noble metal nanoparticle incorporated natural diatom biosilica catalyst for oxidation of D-glucose

Diatoms, unicellular photosynthetic algae that occur in all water territories on earth. Their cell walls are composed of amorphous biosilica also called frustule. They exhibit nanoporous to microporous and macroporous patterning that is specific to particular species. Attributable to their highly porous structure, diatom biosilica is a promising renewable material for various applications such as catalysis, drug delivery systems, and bio-photonics. These are highly potent siliceous materials these days due to excellent biocompatibility, low cost and ease of surface modification. Catalysis is an important technology for industrial production of chemicals and various biotechnological reactions. Heterogeneous catalysis is particularly advantageous because the separation of the catalyst from the reaction products is effortless and easy. Therefore, the exploration of more suitable catalyst supports has become ever more vital over the last few decades. Diatom biosilica can be a suitable candidate as catalyst support material due to its porous structure and also naturally available for sustainable catalytic solutions. In the current work, the properties of diatom (Aulocoseira sp.) were surface functionalized with thiol groups and decorated with silver and gold nanoparticles. Diatoms biosilica (DE) as catalyst supports and two series of synthesized catalysts DE-SH-AuNP and DE-SH-AgNP were characterized by various spectroscopic techniques such as FT- IR, SEM, EDAX, XRD and BET surface area analysis. DE as catalyst supports and the synthesized catalysts DE-SH-AuNP and DE-SH-AgNP were investigated for oxidation of D-glucose to D-gluconic acid. D-gluconic acid is an important chemical intermediate in the pharmaceutical industry, food industry and also useful in paper and concrete production. Diatom biosilica showed very high nanoparticle-loading (AgNP and AuNP) capacities with a homogeneous nanoparticle distribution. The catalysts exhibited higher activity in for oxidation of D-glucose.

Audience Take Away

- The current presentation will cover the brief introduction about the naturally occurring diatom basilica and its applications in catalysis. It will be useful for scientists working in the field of inorganic Chemistry, materials chemistry, nanotechnology and catalysis.
- Additionally, the presentation will be very beneficial for the industries that are continuously looking for the new materials to develop new nano-catalyst systems for industrial processes.

Biography:

Dr. Varsha Brahmkhatri studied Chemistry at The Maharaja Sayajirao University of Baroda, Gujarat, India, and graduated as M. Sc. in 2007. She received her PhD degree in 2013 at the same institution. She then joined the research group of Prof. Hanudatta S. Atreya at the Indian Institute of Science, Bangalore, India. After three-year postdoctoral fellowship at IISc Bangalore, she obtained the position of an Assistant Professor at the Centre for Nano and Material Sciences, Jain University, Bangalore. She has published 25 research articles in SCI(E) journals. She is member of National magnetic society (NMRS) of India and Society of Materials Chemistry (SMC), BARC, Mumbai, India. Her research interests include design and fabrication of nanomaterials and Bio inspired materials for catalysis.

Pragati Shukla *, S. Manivannan, D. Mandal
Bhabha Atomic Research Centre, India.

Packed and Fluidized beds for elemental mercury adsorption

Mercury is one of the most hazardous air pollutants [1- 2]. Due to high vapour pressure of mercury under ambient conditions, exposed mercury may lead to significant mercury air vapour concentration in working atmosphere. The disadvantages associated with the available treatment technologies as well as strict environmental regulations have led to search for environmentally friendly, low-cost and efficient processes for the removal of mercury from liquid as well as air [3]. In recent years, considerable attention has been given to remove mercury through adsorption process using different adsorbents [4,5]. Adsorption experiments can be performed in packed and fluidized beds both. This work focuses on packed and fluidized bed operations for elemental mercury adsorption for various mercury adsorbents. Both the systems have their own advantages. Generally, fluidization is an engineering principle in which a particulate matter in a solid-like condition is brought into a fluid-like condition. Various benefits of fluidization have been reported in literature[6].Fluidized bed provides better gas–solid contact, improved heat and mass transfer, uniform temperature distribution, low pressure drop, etc. [7]. The minimum fluidization velocity is an important parameter for the process design, regulation, and operation of the fluidized bed system. Also, it can be easily measured and controlled during experiments [8]. This work provides an insight to design complete experimental setup for both packed and fluidized beds. It also explains the operational difficulties associated with both type of beds for various self synthesized sorbets . Effect of varying various process parameters shall also be explained. Particle distribution in packed bed and fluidized bed is pictorially represented in figure1. Actual packed bed setup for testing various sorbents has been shown in figure2.

Audience Take Away

- An insight to “Design and operation of packed and fluidized beds for elemental mercury adsorption” will be provided.
- Synthesis & Characterization of various elemental mercury adsorbents will be discussed.
- Technical challenges and competing methods in sorbent synthesis and adsorption operation will be addressed.
- Researchers working in material synthesis, adsorption studies and equipment design shall be benefitted.

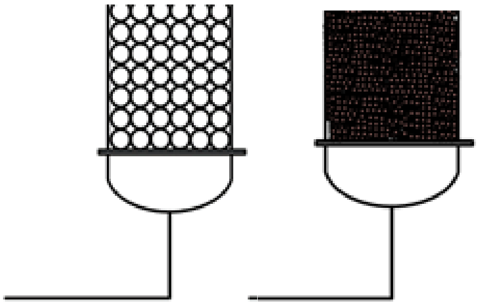


Figure1: Sorbent distributionin Packed and fluidized bed

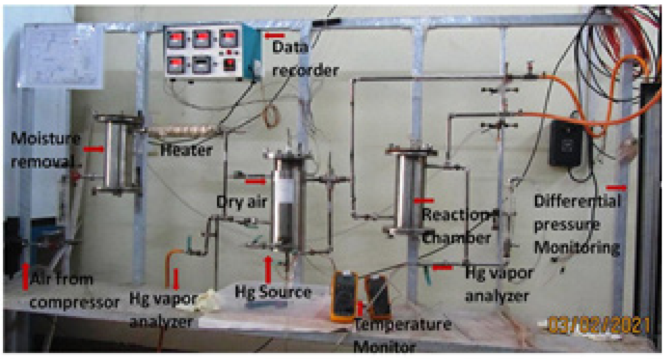


Figure2: Packed bed Experimental facility

Biography:

Ms Pragati Shukla is a Scientist at Bhabha Atomic Research Centre, DAE India with a rich experience of more than a decade in fields like material synthesis, material characterization, adsorption, carbon nano tubes, waste management, process development, modeling & simulation. Her recent work involves synthesis of various hybrid materials mercury detection and adsorption having silica, Carbon nano tubes or zeolite as base material with doping of various metals, non metals & bacteria. She also has expertise in material characterization using DMA, SEM, TEM, DRUV, FTIR and XRD techniques. She has also developed the facilities for testing of synthesized materials in packed, fluidized or packed fluidized beds. She holds a Masters degree in Chemical Engineering and pursuing her PhD in same domain. She has published/presented her work in reputed journals, book chapters, technical reports, conferences and webinars. She is also a reviewer for various international peer reviewed journals.

Mridusmita Barooah*, Bishnupada Mandal
Department of Chemical Engineering, NIT Warangal, India

Enhancement of CO_2 performance with incorporation of amino-functionalized filler in mixed matrix membrane

Mixed matrix membrane for gas separation is an advanced technology for the cost effective fabrication of high performing defect-free membranes. Compared to the conventional membranes, mixed matrix membrane prove to be effective for cleaner energy production, natural gas purification and CO_2 capture from flue gas systems. This class of membranes, provide synergistic effect on the functional integration of organic matrix (performing within the trade-offs of Robeson's plot) and inorganic filler materials (performing beyond the Robeson's plot based trade-offs). The broad domain of MMM research and development devotes towards selection of appropriate materials, defect-free inexpensive fabrication techniques and characterization for simulated and real world application scenarios. The efficient large-scale uses depend comprehensively on the development of highly compatible polymer-filler interface without any defects or interfacial voids. Usually, its observed that for poor phase boundary interaction, the CO_2 separation performance shows declined results. To address this issue, addition of modifying agents plays a pivotal role in improving the gas transport performance (CO_2 permeability as well as CO_2/N_2 selectivity). A critical discussion on the fillers used and its consecutive modification has been discussed in detail in this following work. The influence of these material on the overall physicochemical property of the membrane material has been discussed in detail.

Audience Take Away

- This article provides a comprehensive review with respect to the utility of MMMs (constituting a bulk and a filler scattered phase) towards CO_2 separation. A thorough analysis was carried out with respect to the filler particles in the MMM and their ability to enhance the CO_2/N_2 gas transport properties.
- This study provides alternate advanced fabrication methods to achieve MMMs with high performance in gas separation.
- Modifying agents have been added to improve the physico-chemical properties of the membrane. As indicated, the size, shape and porosity of the filler particles significantly influence the gas separation characteristics of the MMMs. Characterization studies concluded that the functionalization agents improve the membrane performance.
- 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 CO_2 selective mixed matrix membrane for CO_2 separation." She is working in National Institute of Technology (NIT), Arunachal Pradesh as Assistant Professor from July 2019 upto present. She has been teaching core subjects in Chemical Engineering which include Mass Transfer, Chemical Reaction Engineering, Chemical Process Technology, Process Instrumentation, Chemical Engineering lab. She has 4 International publication of research article and attended many International and national conference along with workshops.

Jianying Ouyang*, Chang Guo, Zhao Li, Jianfu Ding and Patrick R. L. Malenfant

Security and Disruptive Technology Research Center, National Research Council, Canada

Enrichment of sc-SWCNTs for thin film transistor and gas sensing applications

Purification and enrichment of semiconducting single-walled carbon nanotubes (sc-SWCNTs) will be reported and discussed. Conjugated polymer extraction (CPE) process was developed and it was found that a trace amount of polar solvents was able to boost the enrichment yield drastically. We provide insights on CPE by demonstrating that a conjugated polymer having a hydrophobic backbone and hydrophilic side chains provides near full recovery (95%) of sc-SWCNTs using a multi-extraction protocol. This polymer, poly(9,9-bis(2-(2-(2-methoxyethoxy)ethoxy)ethyl)fluorene-alt-pyridine-2,5) [P(FEt3M-Py-2,5)] was designed and synthesized in our laboratories. The resulting hydrophilic SWCNT dispersions demonstrate long-term colloidal stability, making them suitable for ink formulation and high-performance thin-film transistors (TFT) fabrication. As a result, the enriched sc-SWCNTs demonstrated application in high-performance fully ink-jet printed TFT [ACS Nano 2018, 12, 2, 1910–1919]. We also developed a novel indigo-fluorene-based copolymer (PFIDBoc) that has been designed to selectively enrich sc-SWCNTs with excellent purity (>99.9%) yet contain a latent function in the form of a tert-butoxy (t-BOC)-protected amine that can be later revealed and exploited for carbon dioxide gas sensing. The enriched sc-SWCNTs demonstrated TFT-based CO2 gas sensing application with up to ~5.4% sensitivity between 400 and 2000 ppm in air with a relative humidity of ~ 40% [ACS Sensors 2020, 5, 2136-2145].

Audience Take Away

- Nanomaterials are important for many advanced applications. The quality of these materials is the key to achieve the high performance of various devices. Here I will go through a few examples to illustrate systematic investigation on various parameters would lead to well controlled enrichment of sc-SWCNTs. The audience will be able to use what they learn from this presentation to optimize their nanomaterials.
- Such detailed research should benefit other researchers to expand their research or teaching. It will provide a systematic way to assist others in a materials-related development problem.
- The materials structure-property relationship will be demonstrated. This should benefit others to fabricate high performance devices with high quality nanomaterials.

Biography:

Dr. Jianying Ouyang graduated from National University of Singapore in 2003 with a PhD degree in Polymer Chemistry. She continued her research in City University of New York from 2003-2004. In 2005, she joined National Research Council Canada in Ottawa as a visiting fellow, dedicating to synthesis and characterization of semiconducting nanocrystals (quantum dots). In 2008, she was hired as a research officer and continued her research in quantum dots aiming for photovoltaics, bio-imaging, and photodetectors. In recent years, she also dedicated to purification and enrichment of single walled carbon nanotubes used for thin film transistors and gas sensors. She has published ca. 50 research articles in SCI journals.

Carlos Alonso Lopez Gordillo*, F. Pola-Albores, J. Conde
Universidad de Ciencias y Artes de Chiapas, Mexico

PVOLED electrical simulation and analysis using CdSe quantum dots as an active layer

Organic photovoltaics (OPs) have been notably developed in the last years, OLED technology is now on the market in devices such as smartphones and flat screens. On the other hand, organic solar cells (OSC) are been used in buildings and cars as solar windows and even in clothes to charge small batteries. The possibility to combine OSCs and OLEDs had been explored. This device, besides absorbing ambient light was also capable of reuse part of the light emitted by the OLED and recycle it and lower power consumption in the device. However, several materials were used for its implementation and expensive deposition techniques, which generates higher fabrication costs. In 2012 was developed OSC with 66% transparency using AgNW as transparent cathode and spin-coating deposition. Due to OSC's low efficiencies, hybrid devices have been studied, the combination of organic and inorganic materials to increase efficiencies and lifetimes. An advantage of organic technology is that it requires very thin layers of material which allows the deposition of several layers without compromising the transparency of the device. It has been reported implementations of 4 OSC in tandem structure. In this work, we use the software Silvaco to simulate the electrical behavior of a hybrid Solar Cell/OLED device in tandem structure adding CdSe quantum dots as an active layer (donor/emissive) and transparent contacts for lowering power consumption in display applications. We achieved a theoretical 20% power consumption reduction using a AM 1.5 spectrum in the simulation.

Audience Take Away

This work will help you to:

- Understand PVOLED electrical behavior
- Use Silvaco Software to simulate tandem hybrid devices
- Add new information about PVOLED devices
- Use the simulation as a solid base to design new physical devices

Biography:

MS Carlos Lopez graduated in electronics and automation control at Innstituto Tecnológico de Tuxtla Gutiérrez, México in 2013. He joined the research group of nanophononics and materials at Centro de Investigaciones en Optica (CIO) in Leon, México contributing with a research in white light OLEDs using quantum dots in 2014. He graduated as MS in 2020 in materials and renewable energy systems leading a project of tandem PVOLED devices. In 2019 he was named operation manager in the south of México at Valefab International, contributing also as a design and manufacturing engineer, selling and designing new technologies for solar luminaries and other solar solutions.

Orlando Elguera
Instituto de Química (IQSC), Peru

Review of research topics for scaling-up of sonochemical reactors (Sono-Reactors)

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

Julia Muller-Hulstede*, Henrike Schmies, Dana Schonvogel, Peter Wagner, Alexander Dyck and Michael Wark
DLR – Institute of Engineering Thermodynamics, Germany

Pt-free Fe-N-C catalysts for the ORR in HT-PEMFC – Investigation of carbon black- based Fe-N-C and commercial Fe-N-C

High-temperature proton exchange membrane fuel cells (HT-PEMFCs) are promising candidates for the sustainable conversion of chemical into electrical energy with the option of utilizing sustainable fuels like green methanol. The use of methanol is beneficial if no hydrogen infrastructure is available and only possible due to the high operating temperature of 150-180 °C that increases the catalyst tolerance towards fuel impurities like CO. However, due to the partial deactivation of the Pt catalysts by phosphates in HT-PEMFC, high loadings of Pt with up to 1 mg cm-^{2} on both electrodes are necessary in HT-PEMFCs.[1] Thus, the increasing Pt price limits a further commercialisation of HT-PEMFCs. Therefore, platinum group metal (PGM)-free catalysts are under investigation as replacement for the scarce noble metals. Promising candidates are Fe-N-C materials consisting of Fe-N sites which are incorporated into a graphitic carbon network.In this presentation an overview of Fe-N-C synthesis, characterisation and application in HT-PEMFC will be given. A carbon support-based synthesis with carbon blacks like Black Pearls® as matrix for Fe-N sites will we presented. Furthermore, physical characterization in terms of X-ray photoelectron spectroscopy (XPS) for analysis of surface elemental content and transmission electron microscopy (TEM) images with energy dispersive X-ray spectroscopy (EDS) for evaluation of the elemental distribution will be shown.[2] Next, activity data acquired with a rotating-ring disc electrode of a Black Pearl-based Fe-N-C and a commercial Fe-N-C from Pajarito Powder, which is fabricated through a sacrificial support method, will be compared. The commercial catalyst shows a slightly higher mass activity at 0.8 V of 2.2±0.4 A g^{-1} compared to the Black Pearl-based Fe-N-C with 1.1 ±0.1 A g^{-1} (Figure 1a).

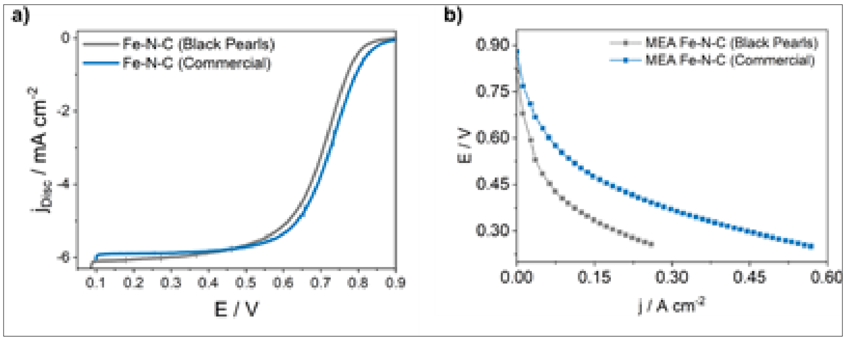


Figure 1: a) ORR polarization curve in 0.1 M HClO4 with a scan rate of 5 mV s-1 at a rotation rate of 1600 rpm with a catalyst loading of 400 µg cm-2 and b) polarization curve of HT-PEMFC MEAs at 160 °C with H2/O2 operation with H2 = 1.5 and O2 = 9.5 and compression of 0.75 MPa.

Finally, the application of the previous mentioned Fe-N-Cs in HT-PEMFC as cathode catalyst will be presented, showing significantly higher performance for the commercial Fe-N-C (Figure 1 b). These performance discrepancies can be attributed to differences in the catalyst's activity on the one hand but are also evoked by the structure of the gas diffusion electrode, on the other hand. This talk will highlight our past work on Fe-N-Cs and the challenges to overcome with a catalyst able to compete with Pt/C.

Audience Take Away

- Mandatory properties of carbons for support-based Fe-N-C catalyst synthesis
- Analysis of activity, selectivity and stability of Fe-N-Cs
- Challenges in application of Fe-N-C as cathode catalyst in HT-PEMFC

Biography:

Julia Müller-Hülstede studied chemistry at the Carl-von Ossietzky University of Oldenburg, Germany and graduated as M. Sc. in 2018. In her bachelor thesis which was in cooperation with NEXT ENERGY – EWE Research Center for Energy Technology she investigated the platin nanoparticle deposition on carbon black and reduced graphene oxide as ORR catalysts. The master thesis was written at Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM in the field of fiber reinforced plastics. Since 2018 she is a PhD candidate at the Carl-von Ossietzky University of Oldenburg, Germany working at German Aerospace Center, Institute of Engineering Thermodynamics in Oldenburg. The PhD work focusses on activated Biochar based Fe-N-C catalysts for the oxygen reduction reaction in HT-PEMFC.

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POSTERS

DAY 2

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CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

SEP 27-28, 2021

CAT 2021

G. Yergaziyeva*, N. Makayeva, J. Shaimerden , M. Telbayeva, K. Dossumov
Institute of Combustion Problems, Kazakhstan

Study of the possibility of using catalysts based on iron-ore concentrate in the decomposition of methane

Known catalysts containing iron ores as an active component, for example, in the oxidation of sulfur dioxide; processing of carbon-containing raw materials to obtain liquid and gaseous products, etc. One of the main advantages of such catalysts is the low cost of their production, which is especially important for large-scale production. Therefore, studies on the use of readily available iron ores for the production of catalysts and the use of the products of their processing as catalysts are promising. To study the catalytic function of the iron ore concentrate, the methane decomposition reaction was selected. The catalytic decomposition of methane is a promising technology for the production of hydrogen and nanocarbon without emissions of carbon oxides (CO, CO_2), and at the same time is a promising replacement for steam reforming of methane to produce hydrogen. The obtained hydrogen can be used in the field of electronic, metallurgical, synthesis of fine organic chemicals and aerospace industries. Nanocarbon obtained as a by-product in the decomposition of methane, due to its unique properties, is used in various industries: from oil and coal mining to the automotive industry. The study of the catalytic activity of iron ore concentrate in the decomposition of methane was carried out on a laboratory flow-type installation in the temperature range of 500-850 ° C, at atmospheric pressure. Methane was fed in a nitrogen flow at a rate of $W = 4980\ h^{-1}$. Analysis of the reaction products was determined by chromatography. The results of the study showed that methane begins to decompose on iron ore concentrate starting from 550 ° C with a conversion of 0.5%. The highest methane conversion of 20.4% is observed at a reaction temperature of 850 ° C, hydrogen with a concentration of 0.4% is formed in the reaction products. The data obtained indicate that iron ore concentrate can be used as a catalyst for the decomposition of methane, however, it requires an improvement in catalytic activity and further research.

Biography:

Yergaziyeva Gaukhar is a candidate of chemical sciences, works in the field of catalysis and petrochemistry. The main scientific direction of research is the study of the mechanism of action and the development of new catalysts of directed action for the processing of hydrocarbon raw materials (methane, propane-butane, benzene, ethanol), obtaining valuable products (synthesis gas, hydrogen, maleic anhydride, etc.).

K. Dossumov, G. Yergaziyeva*, S. Azat, M. Mambetova, K. Askaruly
Institute of Combustion Problems, Kazakhstan

Conversion of ethanol over copper catalysts on rice husk

Copper-containing catalysts have shown good activities for ethanol dehydrogenation to acetaldehyde. Acetaldehyde is one of the most important aliphatic chemicals. It can be used as a raw material for production of acetic acid, acetic anhydride, ethyl acetate, butyl aldehyde, crotonaldehyde, pyridine and many other products. Main industrial method of obtaining acetaldehyde is oxidation of valuable ethylene in presence of aqueous solutions of chloride of expensive palladium and copper. This technology is characterized by the formation of a number of toxic chlororganic by-products, as well as dissolved in large quantities of water, acetic acid and croton aldehyde. Recently, against the backdrop of stricter requirements for environmentally friendly technologies and desire to get rid of oil dependence, interest in process of acetaldehyde synthesis by ethanol dehydrogenation increases again. In addition, it is worth noting the importance and value of hydrogen obtained in the process of catalytic dehydrogenation of ethanol along with acetaldehyde. However in order to create a competitive technology for the production of acetaldehyde from ethanol it is necessary to develop an effective catalyst. Activity and selectivity of these catalysts depend on the physical and chemical structure of active components. Dispersion of the metal over the support is an important factor. In our work the copper catalysts supported on rice husk. Rice husk is the predominant by-product in the milling process of domestic agriculture. It is usually either burned or discarded, resulting not only in resource wasting, but also in environmental pollution. As a consequence, especially in the prevailing field of material science, it makes sense to prepare rice husk (RH), which is composed of extremely amorphous silica. Silica from rice husk was obtained via hydrochloric acid leaching treatment. Silica produced from RH at a temperature of 500 to 650 °C with a calcination time of 2.5 to 6 h is predominantly amorphous, while crystallinity is achieved when the calcination temperature rises above 700 °C. Copper catalyst supported on rice husk was prepared by mixing copper nitrate and rice husk. These samples were dried in at 723 K for 3 h. Catalyst activity tests in ethanol conversion were carried out with an automated flow catalytic unit. Results showed that the ethanol is selectivity converted to acetaldehyde when the reaction temperature is between 523-573 K. Ethanol conversion is found to be dependent of calcination temperature of RH and Cu loading.

The results of the work may be of interest to scientists in the field of catalysis and materials science. The fundamental difference between the works is that silicon oxide obtained from rice husk is used as a carrier for copper catalysts.

Biography:

Yergaziyeva Gaukhar is a candidate of chemical sciences, works in the field of catalysis and petrochemistry. The main scientific direction of research is the study of the mechanism of action and the development of new catalysts of directed action for the processing of hydrocarbon raw materials (methane, propane-butane, benzene, ethanol), obtaining valuable products (synthesis gas, hydrogen, maleic anhydride, etc.).

Christian Wulkesch*, Constantin Czekelius
Heinrich-Heine-Universität Düsseldorf, Germany

A mild and simple approach to the a-perfluoroalkenylation of aldehydes by photocatalysis using phosphines

Per-fluorinated compounds are a substance class of increasing interest. The unique characteristics of molecules with fluorine substituents with regard to lipophilicity, solubility, chemical reactivity strongly affect biochemical processes such as binding ability and metabolic stability. Therefore, a lot of pharmaceuticals or agrochemicals are (per)fluorinated and the research on methods for introducing fluorine into organic molecules selectively is a steadily growing field. A well-known approach for perfluoroalkylations are photocatalytic radical reactions using ruthenium or iridium complexes as photocatalysts. Lately, it was found that by irradiation of blue light on electron donor acceptor (EDA)-complexes of phosphines and perfluoroiodoalkanes generation of electrophilic perfluoroalkyl radicals also occurs efficiently. Those radicals easily react with double bonds such as alkenes or alkynes. In this work the aim was to react perfluoroalkyl-radicals with the electron-rich double bond of an enamine, which is previously formed from an aldehyde and an imidazolidinone organocatalyst. After perfluoroalkylationrapid elimination occurs leading to enals with tetra-substituted, (per)fluorinated double bonds. These highly electron-deficient structure motifs are rare in literature so far and can be obtained in a single synthesis step straight from the aldehyde. There is no need of transition metals, heating, inert conditions or large excesses of reactants, rendering this reaction economically and ecologically particularly favourable. The tolerance of functional groups is high, leading to different perfluoroalkenylated enals in moderate to good yields. Surprisingly, other carbonyl groups, like esters and even ketones, stay untouched. Furthermore, the aldehyde functionality was tested towards further reactions such as their reduction to the corresponding allylic alcohols or their reactivity towards nucleophiles.

Audience Take Away

- The synthesis of perfluoroalkenylated aldehydes is presented. This compound class incorporating an extremely electron-deficient C=C double bond has rarely been reported so far.
- The synthesis of tetrasubstituted, fluorinated double bonds of enals is achieved in a one-step synthesis using a combination of organocatalysis and photocatalysis. This is a very efficient catalyst system and may give new ideas for further reactions or application of these compounds.
- Using phosphines as photocatalysts under mild reaction conditions can replace transition metals for perfluoroalk(en)ylation reactions.
- A new self-built 3D-printed photoreactor is presented.

Biography:

Christian Wulkesch studied chemistry at the Heinrich-Heine-University Düsseldorf, Germany and graduated as M.Sc. in 2019. He joined the research group of Prof. Czekelius where he is in his 2nd year of PhD. His research focuses on asymmetric catalysis and the synthesis of fluorinated compounds.

Aliyah Abdullah Alsharif*, Ivan Kozhevnikov, Elena Kozhevnikov
Department of Chemistry, University of Liverpool,

Dehydroisomerisation of α-pinene and limonene to ρ-cymene catalysed by metal oxides in the gas

ZnO catalyst is demonstrated to be an efficient, noble-metal-free catalysts for one-step dehydroisomerisation of α pinene and limonene to ρ-cymene in the gas phase. This is an example of the use of heterogeneous catalysis for the conversion of renewable feedstock into value-added chemicals. The reaction was carried out in a fixed-bed reactor at 370 °C to yield 90% of ρ-cymene at 100% α-pinene conversion. The proposed reaction mechanism involves acid-catalysed α pinene isomerisation followed by dehydrogenation of ρ-cymene precursors. ρ-Cymene can also be produced by dehydroisomerisation of limonene occurring through double bond migration on acid sites followed by dehydrogenation on metal sites. Limonene dehydroisomerisation reaction was conducted at 250 °C which produced 100% ρ-cymene with 100% limonene conversion. The catalysts showed stable performance for over 24 hours.

Audience Take Away

- Importance of ρ-cymene and how to produce it catalytically from renewable feedstock. Proposed mechanism for both of α-pinene and limonene dehydroisomerisation. The most important characterisation of applied metal oxides.

Biography:

Aliyah Abdullah Alsharif is a 2nd year PhD student in the University of Liverpool, UK. She received her MS in 2015 from King Saud University KSU in Saudi Arabia. Then she obtained a scholarship to study for a PhD in the UK. She joined research group of Prof. Ivan Kozhevnikov at the University of Liverpool.

Ivaylo Slavchev
Bulgarian Academy of Sciences, Bulgaria

Facile and effective amide bond formation through direct acylation of inactivated esters

Amide bond is arguably the most fundamental functionality in organic chemistry. Yet, new strategies are always needed to meet the contemporary synthetic challenges. Classical methods, using coupling agents, metal catalysts or harsh reaction conditions become less and less favored due to reasons, such as atom economy, energy efficiency and the implementation of green synthetic processes. A very promising approach is the direct coupling of inactivated esters and amines in mild conditions, in the presence of a strong base. The method is inexpensive, due to the affordability of the inactivated esters; it does not require toxic metal catalysts or auxiliary reagents; it often works at room temperature; the reactions are generally fast and with good yields. Our interest in the exploration of the direct acylation of amines with inactivated esters is based on some weaknesses in the current state of this research. The existing literature suffers from non-systematic approach; fractionalized data, lack of diversity in the used substrates without a complete overview of the reaction's scope and limitations. Virtually there are no reports of unsuccessful experiments, which can create a misconception that the reaction is universal towards all esters and amines. There are no attempts to find a practical application i.e., the implementation of the new reaction setting for the synthesis of a valuable commercial or scientific products. We therefore report a comprehensive study of over 85 reactions, covering a wide range of substrates, with thorough examination of the scope and the limitations of the reactions settings and with practical applications of each reaction system.

Audience Take Away

- The advantages and disadvantages of different systems for direct acylation of amines with inactivated esters.
- The full scope and limitations of the proposed reaction settings.
- A novel way for the synthesis of phosphoamidates.

Biography:

Dr. Slavchev has a bachelor's degree in applied chemistry and a master's degree in medicinal chemistry from Sofia University, Bulgaria. He obtained his Ph.D. in organic chemistry from Universite Paris Descartes, France in 2019. Since then he has been working on a permanent position as assistant professor in the Institute of Organic Chemistry with Center of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria. His main spheres of interest are the design of new synthetic processes and working with biologically active substances.

G. A. Sycheva
Russian Academy of Sciences,Russia

Spontaneous and catalyzed Crystal Nucleation in Glass of the $Li_2O–SiO_2$ System

The results of studying the kinetics of spontaneous (homogeneous) and catalyzed (heterogeneous) crystal nucleation in silicate glass is presented for glasses in the $Li_2O–SiO_2$ system. Nucleation is catalyzed via the photosensitive mechanism by adding poorly soluble impurities, shifting the glass composition towards the higher content of one of the components (autocatalysis), and by passing steam through the glass melt. The fundamental characteristics of crystal nucleation are obtained. The composition ranges with the maximum and minimum steady state crystal nucleation rates are identified. There has been keen interest in the fundamental problems of crystal nucleation and growth in glass due to the development of new glass ceramic materials. The fabrication of these materials is based on the controlled crystallization of glass with tailored compositions, which would be impossible without knowing the general regularities of crystal nucleation and growth in glass. A quantitative description of the experiment is a major challenge when studying the homogeneous and heterogeneous crystal nucleation and amorphization and crystallization processes in glass. In this study, we investigated homogeneous crystal nucleation and the main methods for catalyzing the crystal nucleation for glass in the $Li_2O–SiO_2$ system.\

Audience Take Away

My research helps to speed up the search for the region of compositions in which the crystal nucleation rate becomes maximum and helps to construct temperature dependences of the nucleation rates. If the researcher needs a material with a minimum nucleation rate, then he should use compositions outside the temperature dependence of the nucleation rate. If the researcher needs to obtain a completely crystallized product, then he must choose compositions within the maximum temperature dependence of the crystal nucleation rate. Knowledge of the temperature dependences of the rate of nucleation and growth of crystals is important for practical application. Using the results of my research can speed up the path from scientific research to practical implementation.

Biography:

Dr. Sycheva studied the technology of glass and silicate materials at the Leningrad Institute of Technology, and received a master's degree in 1972. She joined the Laboratory of Physical Research of Glass at the Institute of Silicate Chemistry, Leningrad, USSR. She defended her PhD thesis in 1987 at the same institute. G. A. Sycheva devoted her entire scientific life to the study of the origin of crystals in glasses. Since 2015 she held the position of head of the Laboratory of the Structure and Properties of Glass (LSSS). She has published more than 100 scientific papers in scientific journals.

Ellen Cristine Giese
Center for Mineral Technology, Brazil

Lamp phosphor powder bio-hydrometallurgical based recycling: It is possible an E waste circular bioeconomy?

The metallurgical industry has been looking for hydrometallurgical-based processes as an option in recent years because of some related inherent advantages, such as the ability to handle waste electrical and electronic equipment (WEEE or e-waste) with feasible waste management and lower energy consumption. E-waste contains economically significant levels of precious, critical metals and rare-earth elements (REE), apart from base metals and other toxic compounds. Recycling and recovery of critical elements from E-waste using a cost-effective technology are now one of the top priorities in metallurgy due to the rapid depletion of their natural resources. This paper focuses on the perceptions of recovery of REE from waste fluorescent powder regarding a possible transition toward a bio-based economy. An overview of the worldwide production of E-waste and REE is also demonstrated to reinforce the arguments for the importance of E-waste as secondary sources of some critical metals. Based on the use of biosorption, we argue that the replacement of conventional steps used in E-waste recycling to recover metals of strategic and economic importance by bio-based technological processes can be possible. The bio-recycling of E-waste follows a typical sequence of industrial processes strongly used in classic hydrometallurgy with the addition of bio-hydrometallurgical processes such as bioleaching and biosorption. We use the case study of REE biosorption as a new technology based on biological principles to exemplify the potential of urban biomining. This perspective of transition between conventional hydrometallurgy for recovering metallic values for biohydrometallurgy helps to define which issues related to urban mining can influence the mineral bioeconomy, which helps to describe some future directions for sustainable recycling to achieve the United Nations' Sustainable Development Goals (SDGs).

Audience Take Away

- The spent FL are already recycled at least partially, and adding processing steps to make better use of their phosphoric components can add significant economic value to the process.
- It is necessary to reconcile the different costs and benefits of pollution avoided through collection and recycling, in addition to evaluating the different stages and processes required for industrial recycling, be it phosphor powder or other types of E-waste. In the FL case, despite the current dominance of the LED market, it is necessary to put an end to the environmental liability formed by the thousands of FL discarded in the world.
- The low ambition scenario for phosphor powder from spent FL recycling is an estimate of the status quo. Achieving higher REE recovery rates depends on several factors, beginning with a collection. Legislation on the management of E-waste and the intensification of measures to reduce dependence on REE imports will be essential to obtain autonomy over the raw CRM essential for economic and technological development in the coming years. This implies measures to diversify the supply of primary and secondary sources through sustainable and efficient processes, which must be based on clean and green technologies, especially bio-based technologies.
- As if that challenge were not enough, the COVID-19 crisis revealed the speed and breadth with which global supply chains can be stopped. The major world political powers have in recent months established an ambitious plan to recover from the pandemic, to increase strategic autonomy, which will end up promoting the transition to an ecological economy where the bioeconomy will play a fundamental role in meeting most industrial demands through the implementation of bioprocesses.

Biography:

Dr. Ellen is researcher at the Center for Mineral Technology (CETEM) at Extractive Metallurgy and Bioprocesses group since 2013, where coordinates projects in Biohydrometallurgy and Extractive Mettalurgy. Bachelor's of Science (Chemistry) (2002), specialization in Applied Biochemistry (2004) and master's in Biotechnology (2005) at Universidade Estadual de Londrina (Brazil). Doctorate in Food Science and Engineering (2008) at Universidade Estadual Paulista Júlio de Mesquita Filho (UNESP, Brazil). Post-doctoral terms in Biotechnology projects at Universidad de Castilla-La Mancha (Spain, 2008-09), Lakehead University (Canada, 2009-10) and Universidade de São Paulo (USP) (Brazil, 2011-12). She has published more than 60 research articles in SCI(E) journals.

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Synthesis and formation of the Pd - MnOx / cordierite structure catalyst for CO oxidation

Monolithic blocks remain the preferred carrier for the preparation of catalysts used in gas cleaning processes. From the analysis of the published data, it can be concluded that the development of automotive catalysts depends on the solution of the following problems:

- search of a composition for the preparation of effective non-platinum and mixed catalysts for cleaning of exhaust gases from CO, CH4, NOx;
- simplification of technological methods for applying a secondary coating on the surface of aluminosilicate and metal blocks with its subsequent fixation.

It is believed that oxides of cobalt, copper and manganese are the most promising for the use in automotive catalysts for cleaning of exhaust gases. Manganese-palladium catalyst applied on the surface of alumosilicate-cordierite [(Mg, Fe)2Al4Si5O18] honeycomb blocks is presented. Manganese and palladium oxides are applied to the surface of the alumosilicate block by means of a one-time diffusion saturation with solutions of manganese nitrate and palladium chloride. The developed method allous to obtain samples of catalysts containing manganese and palladium oxides that are uniform in composition and morphology. In this case, palladium covers the surface occupied by manganese oxide, without penetrating into the depth of the pores clogged with MnOx particles. The method for preparing of the Mn-Pd catalyst includes processing the samples with an ammonia water solution. The obtained samples are more active in the CO oxidation reaction than the samples formed by other methods (hydrogen or formate). The dispersity of manganese oxide particles is about 100 nm, and the size of palladium particles is 29-34 . Treatment of the catalyst with ammonia water causes in the formation of a palladium ammonia complex, which decomposes to yield palladium black. It can be concluded that the treatment with ammonia water leads to the completion of the formation of the active surface of the catalyst and a decrease of the temperature of complete oxidation of CO. The work is carried out by supporting of Shota Rustaveli Scientific National Fund of Georgia (Grant N 18-750).

Audience Take Away

- The method of treating palladium-containing catalysts with ammonia water allous to achieve the completion of the formation of the active surface and reduce the temperature of complete oxidation of CO.
- It may be suggested that the selected conditions of one-time diffusion saturation simplifies the technology of applying active components to the surface of alumosilicate blocks.
- Manganese oxides can play the role of a secondary carrier and an active component.

Biography:

Dr. Vitaly Bakhtadze graduated from the Georgian Polytechnic Institute with a degree in technology of inorganic substances. 1964 - 1974 a post-graduate student and then a researcher at the catalysis laboratory of the Institute of Inorganic Chemistry and Electrochemistry of the Georgian Academy of Sciences. From 1974 to the present day, head of the catalysis laboratory. He published over 50 scientific articles.

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