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Group

13th Edition of International Conference on

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

21-22
OCT 2022

VIRTUAL EVENT

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BOOK OF ABSTRACTS

13TH EDITION OF INTERNATIONAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

21-22 OCT

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ABOUT MAGNUS GROUP

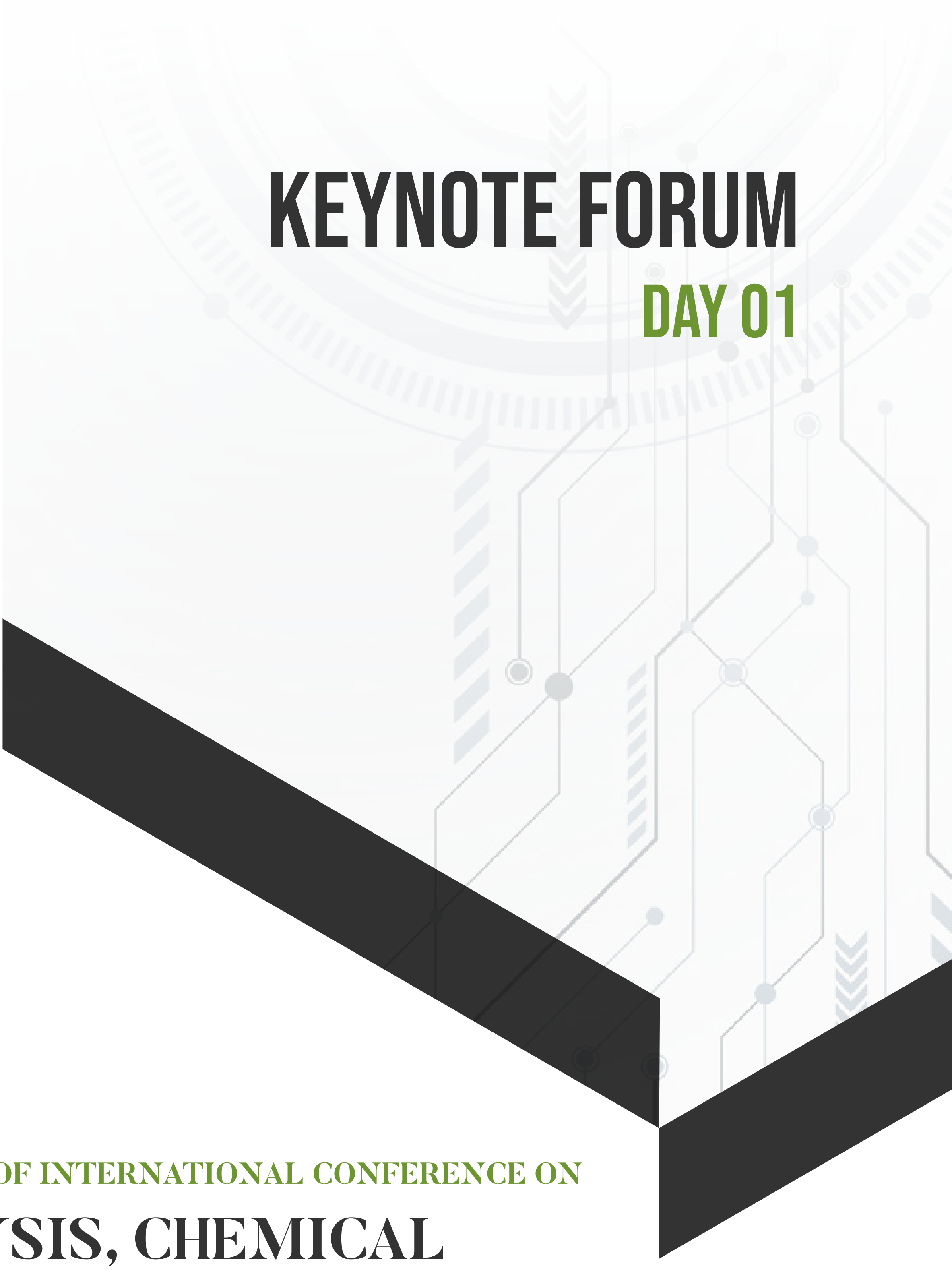
Magnus Group (MG) is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and 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 CATALYSIS 2022

Magnus Group is pleased to invite you to participate in the Online Event- ‘**13th Edition of International Conference on Catalysis, Chemical Engineering and Technology**’ during October 21-22, 2022 organized around the theme *Assembling Trivial Keys in Catalysis and Chemical Engineering*. This Catalysis 2022 is the International platform which brings together the collection of investigators who are at the forefront in the field of Catalysis and Chemical Engineering. The scientific program will include oral presentations of sub-disciplines, keynote sessions led by eminent scientists and poster sessions presented interactively by junior scientists and graduate students. It is the ultimate meeting place for all the experts worldwide for new interdisciplinary scientific collaborations and networking. With its scientific sessions, you are provided assurance to explore the latest technologies and breakthroughs that are specific to your area of work. No doubt the event has a broad scope of topics and continued in parallel sessions relative to the specific area of research.

We are confident that our conference will provide you with an incredible chance to explore new horizons in your field and we hope to see you at our upcoming Catalysis-2023 conference during October 26-28, 2023 at Boston, Massachusetts, USA.



KEYNOTE FORUM

DAY 01

13TH EDITION OF INTERNATIONAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

21-22 OCT

Stanislaw Dzwigaj

Sorbonne Universite, Laboratoire de Reactivite de Surface

Application of metal single-site zeolite catalysts in enviromental catalysis

The metal ions well dispersed at zeolite framework are considered to be active sites of catalytic processes. Therefore, the incorporation of these metals into zeolites as isolated tetrahedral sites appears to be the important task. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions results in the reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite. During my keynote talk the design of single-site zeolite catalysts with transition metal will be described and characterized by different physical techniques both at the macroscopic (XRD, BET, TPR, TEM) and molecular level (FT-IR, NMR, DR UV-Vis, XPS, EPR, XAFS). The application of metal single-site zeolite catalysts in environmental catalysis will be discussed. This two-step postsynthesis method applied in this work allowed obtaining metal single-site zeolite catalysts active in different catalytic processes such as oxidative dehydrogenation of propane into propene, selective catalytic reduction of NO_x to N_2, production of 1,3-butadiene or hydrogen from renewable sources, including ethanol obtained from biomass. Their catalytic activity strongly depended on the speciation and amount of metal incorporated into zeolite structure as well as their acidity.

Audience Take Away:

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

Biography:

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

Eleonora Aneggi

Department of Agricultural, Food, Enviromental and Animal Sciences,
University of Udine, Udine, Italy

Heterogeneous-Fenton process for enhanced liquid waste treatment

Innovations in water technology are fundamental to finding solutions to the nowadays challenges: climate change, resource shortages, emerging contaminant, urbanization and sustainable development. Nowadays the use of conventional wastewater processes is becoming increasingly challenging mainly due to the presence of biorecalcitrant organic matter. Liquid waste can be produced by all sectors of society including wastewater from industrial processes and they can be divided into subgroups depending on their nature and toxicological risk. Therefore, an emerging technology is needed to deal with these highly concentrated and toxic non-biodegradable pollutants. Advanced oxidation processes (AOP) such as Fenton, Fenton-like and hybrid processes have been successfully employed for the treatment of different types of wastewaters. These processes typically rely on the generation of highly reactive hydroxyl radicals, which in turn attack the organics and degrade them. The conventional Fenton process generates large volumes of sludge that needs to be disposed, creating a serious environmental and economic problem. The heterogeneous Fenton process is the most viable solution for the treatment of wastewaters because it produces lower amount of sludge, the catalysts are recyclable and these features make this process feasible in terms of scalability and economics. However, there is a growing need for the development of new active catalysts to be employed in Fenton-like process, with extended life, improved activity and selectivity. Here we focused on two different liquid waste, a pharmaceutical pollutant (model solution of ibuprofen) because of its environmental impact on the receiving waterbodies and a landfill leachate which contains refractory organic compounds, characterized as persistent.

The conventional biological treatment plants are unable to completely remove these recalcitrant compounds and advanced oxidation processes are require.Copper-based heterogeneous catalysts have developed for the treatment of liquid wastes using a Fenton like process, as a potential pre-treatment before wastewater treatment line. Copper supported on zirconia (Cu/Zr) exhibited a promising activity with an almost complete degradation of ibuprofen (98%) and 60% of mineralization, while working with the leachate a 67% of abatement of pollutants is obtained. A special attention has been devoted to the toxicity of the treated liquid waste. These catalysts do not produce toxic metabolites which is important when considering the degradation of water pollutants and harmful liquid wastes discharged to Integrated Water Cycle.

In addition, steel scale waste (SSW), a by-products of steel production containing oxides in large quantity has been tested as a heterogeneous Fenton-like catalyst for the treatment of landfill leachate The idea of exploiting a waste (steel waste) to be used it in the treatment of liquid waste is related to the perspective of more sustainable processes within a circular economy. At mild conditions SSW successfully removed about 75% of the recalcitrant organic loading from landfill leachate, resulting a promising material for the treatment of heavily polluted wastewater streams. These findings appear extremely important into a circular economy perspective, because steel scale waste is produced in huge quantities and could be effectively used as a catalyst in a highly polluted liquid waste treatment process.Summarizing this study highlights the potential of two different catalysts (a home-made and an industrial waste) for the removal of organic compounds from liquid waste via heterogeneous Fenton-like process.

Audience Take Away:

- Recent insight on heterogeneous Fenton process
- Development and characterization of novel catalysts
- Evaluation of the degree of oxidation (mineralization or partial degradation of organic compounds in liquid waste)
- Optimization of reaction variables

Biography:

Dr. Eleonora Aneggi is a temporary researcher at the University of Udine. She graduated in Chemistry in 2001 at University of Trieste and in 2007 she obtained her PhD at the University of Udine. Her main scientific interests are catalytic processes, mainly related to environmental. Her research activity involves the development of advanced catalytic materials for atmospheric and water pollutants. She worked on various national and international projects. She has been the winner of numerous national and international awards.She is author or co-author of 58 scientific publications in top international journals. (Scopus H-index=23, n. of citations 2505).

Tokeer Ahmad

Nanochemistry Laboratory, Department of Chemistry, Jamia Millia Islamia, New Delhi, India

Designing multifunctional nanostructures for H_2 energy applications

Multifunctional nanostructures find the possibility for their applications in water splitting processes for hydrogen generation as a renewable source of green energy. Photocatalytic generation of hydrogen in water splitting process by using as-prepared nanoparticles has also been studied under the visible light irradiations which showed a significant H_2 evolution reaction rate. Fe_3O_4 nanocubes were prepared in one pot process for the electrochemical water splitting and supercapacitor applications. As-synthesized Fe_3O_4 nanocubes with high specific surface area of 268 m^2g^{-1}, are ferromagnetic at room temperature and affects the electro-catalytic activity of the electrode materials. Similarly, the catalytic activity of ultrafine RuO_2 was examined against the Horseradish peroxidase enzyme (HRP) and applied as sensor for the detection of H_2O_2 in the solution. Besides that, the stimulating bifunctional electro-catalytic performance of RuO_2 nanoparticles was studied under different atmospheric conditions for electrochemical hydrogen energy. The studies of Yttrium Ferrite nanoparticles by citrate precursor route reveal the formation of monophasic orthorhombic $YFeO_3$ nanoparticles with fairly uniform distribution of nearly spherical particles, high specific surface area of ~338 m^2/g and visible band gap of 2.5 eV. Photocatalytic generation of hydrogen by using $YFeO_3$ nanoparticles has also been studied under the visible light irradiations which showed a significant H_2 evolution reaction rate up to 131.6 µmol $h^{-1}g^{-1}$. Some more studies on renewable energy will also be discussed.

Biography :

Prof. Tokeer Ahmad did his masters (chemistry) from IIT Roorkee and Ph.D. from IIT Delhi. Presently, he is full Professor at Jamia Millia Islamia, New Delhi. Prof. Tokeer Ahmad has supervised 9 PhD's, 74 postgraduates, 9 research projects, published 120 research papers and two books with research citation of 4225, h-index of 38 and i10-index of 80. Prof. Ahmad is active reviewer of 110 journals, delivered 98 Invited talks and presented 120 conference papers. Prof. Ahmad has received DST-DFG award, ISCAS Medal, Inspired Teacher's President Award, Distinguished Scientist Award and elected as Member of National Academy of Sciences India. Prof. Ahmad has been figured in World Top 2% Scientists by Stanford University, USA and has been recently conferred the prestigious Maulana Abul Kalam Azad Excellence Award of Education for the outstanding contribution in the field of education.

Haibo Ge

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

Distal functionalization via transition metal catalysis

The ubiquitous presence of sp^3 C–H bonds in natural feedstock makes them inexpensive, easily accessible, and attractive synthons for the preparation of common and/or complex molecular frameworks in biologically active natural products, pharmaceutics, agrochemicals, and materials. However, the inertness of these bonds due to the high bond dissociation energies and low polarity difference between the carbon and hydrogen atoms makes them challenging reaction partners. Moreover, the desired site-selectivity is often an issue in reactions with multiple analogous sp^3 C–H bonds. To overcome these problems, transition metal-catalyzed C–H functionalization has been developed with the assistance of various well-designed directing groups which can coordinate to a metal center to deliver it on a targeted C–H bond through an appropriate spatial arrangement, enabling C–H activation via the formation of a cyclometalated species. However, the requirement of often additional steps for the construction of the directing groups and their subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. A promising solution would be the utilization of a transient ligand which can bind to the substrate and coordinate to the metal center in a reversible fashion. In this way, the directing group is installed, sp^3 C–H functionalization occurs, and the directing group is then removed *in situ* without affecting the substrate function after the catalysis is finished. Overall, the whole process occurs in a single reaction pot. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C–H functionalization reaction.

Audience Take Away:

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

Biography:

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

Anne M. Gaffney

University of South Carolina, Columbia, South Carolina, USA

Plastic Trash to Monomers and Intermediates – PTMI

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

Biography:

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

SPEAKERS

DAY 01

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Bio-methane generation from anaerobic digestion of agricultural waste: Feasibility and fertilizer recovery: Effect of supplemented nutrients and intermediate temperature

Md Nurul Islam Siddique*, Zaied bin Khalid
Faculty of Ocean Engineering technology & Informatics, University Malaysia Terengganu (UMT),Kuala Nerus, Terengganu, Malaysia

The simultaneous digestion of many substrates could explain the growth in demand for organisms drawn in by anaerobic digestion. This study looked into the effect of supplements on the co-digestion of growth substrates. An extra improvement plan that expects a critical occupancy in anaerobic digestion was applied in three phases, 37 °C, 40 °C, and 50 °C. At 37 °C, biogas output increased to 1.38 times that of the control as a result of the adjustments. Furthermore, the excellent use of this newly discovered mid-temperature, 40 °C without additions, significantly impacted an innovative mindset (56 percent of VS end and 8.4 L-biogas). mL-CH4/g-VS was 1.24 times that of the system without any additional improvement during anaerobic co-digestion at 50 °C, and biogas output exceeded 11.3 L with supplements. The findings show that the modified course of action increases co-digestion at each temperature. On the advanced scale, the most commonly used temperature was 37 °C, which had the greatest impact on the use of improvements during the anaerobic process. Sludge was recovered from the digester at a rate of 0.09 m3 sludge/m3 substrate, while water was recovered at a rate of 0.86 m3 sludge/m3 substrate. The sludge that has been processed can be used as compost, and the water can be used to water plants. 3.77 years was discovered to be the time it took to repay the investment. As a result, it's possible that the current research may be acknowledged as a potential green option for waste management around the world in the near future.

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.

Kinetics of catalytic hydrogenation of propene – Investigations based on graph theory

Mirosław Szukiewicz*[1], Adrian Szałek[1], Elzbieta Chmiel-Szukiewicz[2]
[1]Department of Chemical and Process Engineering, Rzeszow University of Technology, al. Powstancow Warszawy Rzeszow, Poland
[2]Department of Department of Organic Chemistry, Rzeszow University of Technology, al. Powstancow Warszawy Rzeszow, Poland

The kinetics of heterogeneous catalytic reactions is the topic of theoretical and practical importance. Theoretical aspects are concerned with determination of the process run, stages, limitations etc., while in practical applications kinetic experiments were applied to assist reactor design and scaling up of various processes. Both directions overlap and in many articles are discussed simultaneously. The most often applied method is to find a single step having the strongest influence on the process rate. This step is selected from a sequence of elementary steps. In the literature, there are present a lot of works that present successful application of the concept, however in many instances failed attempts are reported - the kinetic equations are of not sufficient precision, as for the gas phase hydrogenation of propene process. In this work, we present a procedure based on graph theory and completed with statistical analysis that helps to obtain a high precision kinetic equation for the mentioned process. The method substantially differs from rate determining step approach. On the basis of the catalytic cycle proposed, the general form of the kinetic equation is derived without any additional assumptions. It allows considering all possible interactions between the reagents and the species. The most promising variant, that is a linear catalytic mechanism, was developed and tested. Statistical analysis allows simplifying the equation to obtain the form that includes only statistically significant variables. For the considered process, the kinetic equation obtained characterizes of the large precision confirmed by values of statistical indicators and the criterion. The residual sum of squares is more than 15% less than for the best equation founded in literature. The form of kinetic equation is not previously reported in literature and rather cannot be derived on the basis of classical approaches.

Audience Take Away:

- The most often reported in literature works are based on a choice of the step that has the strongest influence on the process rate, what is potential source of errors. Presented here, kinetic Investigations are based on graph theory, and it allows considering all possible interactions between reagents and species in a kinetic equation, so have not mentioned above limitations. The equation developed is of larger precision than any of presented in large numbers in the literature
- The results of work help to develop in practice the kinetic equation concerning gas-phase heterogeneous process
- The precise kinetics gives a deep insight into a process, and it is necessary for designing and scaling up processes

Biography:

Prof. 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 engineering.

Catalytic performance of modified delaminated zeolite ITQ-2 in selective catalytic reduction of nitrogen oxides with ammonia

Agnieszka Szymaszek-Wawryca*[1], Urbano Diaz[2], Bogdan Samojeden[1], Monika Motak[1]
[1]AGH University of Science and Technology, Faculty of Energy and Fuels,Krakow, Poland
[2]Instituto de Tecnologia Quimica, Universidad Politecnica de Valencia (UPV-CSIC), Valencia, Spain

The emission of nitrogen oxides (NO_X) from stationary and mobile sources is among very significant environmentalissues. According to the Best Available Techniques, currently the most efficient method to reduce NO_X production is selective catalytic reduction with ammonia (NH_3-SCR). This technology aims to transform NO_X into nitrogen and watervapor on the surface of the catalyst. The commercial SCR systems typically use vanadium-based catalysts, for example V_2O_5-TiO_2 promoted with MoO_3 or WO_3. However, weak activity below 300 °C and the narrow temperature window of 300-400 °C, combined with sulfur dioxide oxidation above 300 °C and easy deactivation by alkali compounds, limits further application of these catalysts on the industrial scale. Therefore, the goal of our work wasto design an alternative catalyst free from the disadvantages mentioned above.

Zeolites modified with transition metals are generally considered as the leading alternative catalysts for V_2O_5-TiO_2.It results from their high activity in broad temperature window, high stability, and resistance to poisons present in the flue gas, such as SO_2. Despite the interests in zeolites as the precursors of new NH_3-SCR catalysts, only few studiesconsidered application of ITQ-2 in this reaction. ITQ-2 is a delaminated zeolite, belonging to the MWW family. It is obtained from 2D precursor, MCM-22 (P) by swelling and subsequent delamination. ITQ-2 exhibits so-called house of cards structure and very high specific surface area of ca. 700 $m^2 \cdot g^{-1}$. Well-defined pore structure and the abundance of acidic sites makes ITQ-2 an excellent candidate for new catalyst of NH_3-SCR.

The catalytic activity of metal-zeolites is determined by the speciation of the active phase. To date, research on the incorporation of metals into zeolitic frameworks has mainly focused on the methods such as ion-exchange or impregnation. However, in the case of ion-exchange usually multiple repetitions of the procedure are required to obtain the desired amount of the active phase. Impregnation results in pore-blocking upon aggregation of metal oxidesin the channels. In contrast, one-pot synthesis of zeolites reduces the preparation procedure to only one step and yieldswell-dispersed metal species. To our knowledge, no one has examined catalytic performance of one-pot synthesized Fe-ITQ-2 in NH_3-SCR.

According to the above-mentioned, our work describes the design of the new NH_3-SCR catalyst, Fe-ITQ-2, preparedby one-pot synthesis. We analyzed the dependence of catalytic performance on Si/Fe molar ratio in the samples. We compared the obtained results to the activity of the reference, Fe-ion-exchanged ITQ-2. The physicochemical propertiesof the catalysts were analyzed using ICP-OES, X-ray diffraction, UV-Vis and FT-IR spectroscopy, low-temperature sorption of N_2, SEM microscopy, and NH_3-TPD.

Our work has demonstrated that one-pot synthesis results enables preparation of highly active catalyst in low- temperature range of the reaction. The effect can be ascribed to the presence of isolated Fe^{3+} cations, incorporated intothe zeolitic framework and highly acidic character of Fe-ITQ-2. Our study provides the foundation for a new way of preparing catalysts of NH_3-SCR supported on MWW zeolite.

Acknowledgement:
The authors wish to acknowledge the National Science Center of Poland (Preludium 19 project, no. 2020/37/N/ST5/00186) for the foundation of the research.

Audience Take Away:

- The presentation will refer to the application of the representative of MWW zeolites, ITQ-2 in an environmentally important technology, selective catalytic reduction of nitrogen oxides with ammonia
- Information given during presentation will be an added value for all participants, who are interested in the development of novel catalysts for the decrease of nitrogen oxides emission through selective catalytic reduction with ammonia (NH_3-SCR)
- The researchers interested in the field of catalysts and modified zeolites could possibly expand the presented studies, for example by preparing similar materials with different chemical composition
- The research undoubtedly provides a practical solution of the problem of extensive emission of nitrogen oxidesfrom stationary sources, since the prepared catalysts exhibit satisfactory reduction of NO in low-temperature range and relatively low concentration of nitrous oxide (N_2O) in the flue gas during the reaction
- The method used for the modification of ITQ-2 with iron has not been reported yet. Therefore, it can assist in the design of novel catalysts of advantageous features, provided by well-dispersed active sites

Biography:

Agnieszka Szymaszek-Wawryca graduated as MSc at the AGH University of Science and Technology, Poland in 2018.She started her PhD in the research group of Prof. Monika Motak. Her field of studies is modification and application of aluminosilicates in selective catalytic reduction of nitrogen oxides with ammonia. She interned in Instituto de Tecnologia Quimica in Valencia (2020, 2021), University of Paris (2019), and she was an ambassador of one of the biggest Polish chemical companies. She is Principal Investigator of Preludium 19 project funded by the National Science Centre of Poland and scholarship holder of AGH Chancellor (2020-2022).

Experimental analysis of delivering various liquid fuels to Molten Carbonate Fuel Cell (MCFC)

Olaf Dybinski*, Jaroslaw Milewski
\Warsaw University of Technology, The Faculty of Power and Aeronautical Engineering, Institute of Heat Engineering Nowowiejska Warsaw, Poland

During presentation, results of experiments of fuelling Molten Carbonate Fuel Cell with low molecular liquid fuels (methanol, ethanol, propanol isomers, butanol and glycerol) will be presented. As MCFC temperature during operation reaches 650°C and anode is made of nickel, which is a typical catalyst in steam reforming reactors for hydrocarbons, this creates perfect conditions for steam reforming of proposed fuels to take place. In standard conditions, MCFC requires hydrogen as fuel – but hydrogen is a difficult fuel to transport, distribute and store. One of solutions to avoid problems with pure hydrogen is to use liquid fuels (ex. alcohols) as hydrogen carriers. Those fuels can be easily transported and stored in already existing technologies (containers, tanks, pipes etc.) in liquid state at standard conditions. Also most of them are a product of natural phenomena that can be found in everyday life, such as alcohol fermentation, where most of the analysed compounds are created as a product of reaction performed by yeast.

The results of experiments that will be presented contains data on electric power that could be achieved when fuelling MCFC with various fuels at various water:Fuel compositions in comparison to pure hydrogen used as fuel. Stoicchiometric steam:Carbon compositions of the fuels have been analysed in ratios 2:1, 3:1, and 4:1 for each of 6 used fuels: methanol, ethanol, propan-1-ol, propan-2-ol, butan-2-ol and glycerol fuel. Results were compared with fuel cell powered by pure hydrogen, showing little decrease in performance, but still delivering positive heat balance. Strengths and weaknesses of proposed solutions have been presented. Results of experiments prove that liquid fuels can be used for fuelling molten carbonate fuel cells, thanks to composition of fuel electrode (porous nickel anode) and temperature of operation of fuel cell, which act as a catalyst for the process. In the anode channel and mainly on the anode surface, steam reforming process of hydrocarbons occurs, resulting in creation of hydrogen elements, which take place in the electrochemical process of fuel cell operation right after creation. This allows fuel cell to consume hydrogen generated by steam reforming and power fuel cell directly. In this examination only internal steam reforming was analysed (without external steam reformer). Results of this study shows that problems concerning hydrogen fuel can be easily avoided by utilising liquid fuels, with little decrease of fuel cell performance.

Audience Take Away:

- Audience will learn what electric power can be received from the molten carbonate fuel cell when fuelling with other fuels than pure hydrogen
- Audience will see how does steam to carbon ratio impact the performance of the fuel cell fed with various hydrocarbon fuels
- Knowing typical optimal conditions of temperature, catalyst applied and steam: Carbon ratio in the steam reformers used for reforming hydrocarbons, it can be compared to efficiency of internal steam reforming of alcohols in case of internal reforming taking place in molten carbonate fuel cell
- Audience will learn what impact does liquid fuel have on anode chamber (anode, current collector), especially concerning higher rate alcohols and carbon deposition effect

Biography:

Olaf Dybinski is a PhD candidate at Warsaw University of Technology (WUT), covering fields of hydrogen production, utilization and storage, fuel cells applications and modelling and also energy efficiency of systems in buildings and industry. He graduated WUT in 2015 earning MS engineering degree. In 2016 joined prof. Jaroslaw Milewski team in Fuel Cells Department in Institute of Heat Engineering of WUT, performing experiments and mathematical modelling over molten carbonate fuel cells utilizing alternate fuels requiring internal and external steam reforming for performance. Since 2019 working as an research and educational assistant at Warsaw University of Technology.

Some studies on the adsorptive removal of phenol from wastewater

Ashanendu Mandal
Doctorate in Chemical Engineering, University of Calcutta, Kolkata, India

Phenol being a severe environmental pollutant needs to be removed from wastewater before its surface discharge. Adsorptive removal of phenol is gaining popularity due to its low cost and many researchers are still focusing on the application of new adsorbents. This research aims for phenol removal by four bio-adsorbents viz. guava tree bark, rice husk, neem leaves and activated carbon from coconut coir and four industrial waste adsorbents viz. rice husk ash, red mud, clarified sludge from basic oxygen furnace and activated alumina. The surface characterization of the adsorbents were carried out by SEM, XRD, FTIR and BET analyzers. The phenol removal percentage was investigated 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 removal percentage was obtained as high as 97.50%. The kinetic study showed that the pseudo-second order was best fitted for all adsorbents except red mud. The kinetic testing showed that 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 sludgerespectively.Thethermodynamics showed that the spontaneity, randomness and endothermic/exothermic nature of the adsorption process were different but conclusive. The ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient established that the experimental and predictive data were within the allowable range. The scale-up designs and the safe disposal of used adsorbents were also studied for their commercial applications. The research concludes that the adsorbents used in this study are effective for phenol removal and also for circular economy in many countries.

Biography:

Ashanendu Mandal has graduated as B. Sc in Chemistry and then B. Tech in Chemical Engineering from University of Calcutta. He has got his M. Tech Degree in Chemical Engineering from IIT, Kharagpur. He has acquired MBA degree in Finance from IGNOU, New Delhi and has undertaken an Advanced Management Program from IIM Calcutta. He has also acquired the Degree of Ph. D. (Tech) in Chemical Engineering from University of Calcutta. Dr. Mandal has worked in ONGC for more than 34 years and his experience includes commissioning, modifications, safety, operations, artificial lifts, pressure maintenance, EOR and planning in offshore and onshore oilfields. He has also vast experience in marketing of upstream and downstream petroleum products. Dr. Mandal has published technical papers in Chemical Weekly and research papers in international journals. He has visited more than 25 countries for attending training programs and for participating in international conferences as invited speaker or panelist. Dr. Mandal is a lifetime member of Indian Chemical Society and Indian Science Congress.

Photocatalytic degradation of antibiotic pharmaceutical pollutant by a magnetic material, Aluminium Ferrite (ALFEO$_3$)

Bhuvanasundari*[1], Tiju Thomas[2]
[1,2]Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, India

Sulfamethoxazole (SMX) is one of the widely used antibiotics in human and animal medical treatments. Traces of unexploited SMX are found in surface and ground waters, which cause the emergence of antibiotic resistance bacteria and antibiotic resistance genes. Due to low biodegradability of SMX, it is reasonable to develop catalytic degradation methods for its removal for SMX from the wastewater. Photocatalytic wastewater treatment is one among the Advanced Oxidation Process (AOP) which remove/degrade targeted pollutants from wastewater. Here, a magnetic photocatalyst, Aluminium ferrite (AlFeO$_3$) is used to test the degradation of SMX using visible light.

Aluminium ferrite is a prepared by the co-precipitation method. The structural property of AlFeO$_3$ before and after the photocatalytic degradation are characterized. The wide optical absorption (250 nm – 600 nm) of the catalyst enables the photocatalytic degradation using UV and Visible light. The magnetic property of AlFeO$_3$ enables the retrieval of the catalyst after the degradation process and allows catalyst reusability. The photocatalytic experiment is carried out using Xenon lamp with model SMX pollutant. The degradation of the pollutant and the degraded by-products are analyzed using Liquid Chromatography – Mass Spectroscopy(LC-MS) technique. The results indicated that the catalyst can completely degrade SMX and the degradationpathway is proposed in this work. Thus Aluminium ferrite is a potential candidate for sunlight driven targetedpollutant removal in wastewater treatment.

Audience Take Away:

- Advantage of perovskite metal oxide materials for photocatalytic application
- Learn about AlFeO$_3$ synthesis and the feasibility of large-scale production
- Properties and photocatalytic efficiency of prepared AlFeO$_3$ material
- The degradation mechanism of Sulfamethoxazole by AlFeO$_3$

Biography:

Ms. Bhuvanasundari is a Ph.D. student at IIT Madras, India. She graduated M.Sc. with a specializationin Material Science from Anna University, India. She joined the Applied Nanostructures Engineering and Nanochemistry (ANEN) research group of Dr. Tiju Thomas. Her area research includes materials engineeringfor photocatalysis, photocatalytic materials for wastewater treatment.

Doping mechanism in carbon, nitrogen and sulfur tridoped TiO_2

S. Girish Kumar
Department of Chemistry, School of Engineering and Technology, CMR University, Bagaluru campus, Bengaluru-Karnataka, India.

The non-metal co-doped titania finds promising for the design and development of solar light harvesting photocatalyst. In particular, tridoping of C-N-S into TiO_2 has been very attractive because of its unique features like simultaneous and relatively low energy substitution of carbon, nitrogen and sulfur from the cheaply available precursors (thiourea, L-cystine and L-cysteine), stabilization of the anatase crystal structure, red shift in the band gap response towards the solar spectrum. The other advantage is the the absence of any impure phase formation even at elevated annealing temperature and therefore, high doping density can be achieved conveniently.

Despite these unique merits, intense research on C–N–S-TiO_2 could not be found in the literature owing to the complexity in the doping process. In this presentation, doping mode of each dopant in the C-N-S-TiO_2 with respect to the reaction conditions and contradictions about the doping states of each dopant in the codoped system will be discussed. The concepts like modifications of defect structures, dopant distribution, doping mode and mutual interferences among will be dealt. It would be emphasized that the codoping process is quite complicated as several doping modes can be observed for each dopant, which are coupled to the preparation conditions.

Audience Take Away:

- As the research interests on non-metal doped titania is widespread, the presentation appeals to the wider audience working on the semiconductor photocatalysis. It would definitely provide a deeper understanding on the relationship between the precursor chemistry and the doping process
- Draw meaningful conclusion on the optimization of the preparation conditions including the annealing temperature, time, and ambience and also on the precursor's concentration
- The lowering of annealing temperature provides a way to fabricate the materials in the larger scale
- The choice of the precursors may be conveniently selected which will help to reduce the economy involved in the preparation method
- A photocatalyst with larger red shift in the band gap can be obtained by altering the reaction conditions
- The strategy can be expanded to other widespread oxide photocatalysts

Biography:

Girish is active in the interdisciplinary area of scientific research associated with materials chemistry and physics. He has published 44 research articles which have received more than 6300 citations. He is serving as Associate Editor for 'Chemical Papers-SPRINGER' and 'Applied Surface Science Advances- ELSEVIER' along with potential member in the Reviewer Panel Committee, RSC Advances. He has reviewed more than 1600 manuscripts from 175 journals. He has been recognized as 'Top 2% world scientist' by the survey conducted by 'Stanford University, USA (2019 and 2021) and 'Top 1% reviewer' by the Publons (2018 and 2019).

Reduction of toxic dyes using recyclable core shell nanoparticles catalyst

Khalida Naseem
Department of Basic and Applied Chemistry, Faculty of Science and Technology, University of Central Punjab, Lahore, Pakistan

Industrial effluents consist of various toxic dyes and nitro-aromatic compounds that are harmful to environment and cause water pollution at large level. Therefore, removal/degradation of these toxic pollutants from the wastewater sources is need of time. Here, silver nanoparticles fabricated polystyrene-poly(N-isopropyl meth acrylamide-acrylic acid) core shell particles were prepared via precipitation polymerization method and used as catalyst to degrade toxic dyes such as Congo red (CR), Rhoda mine B (RhB) and Methylene blue (Mb) in the presence of sodium borohydride ($NaBH_4$) as reducing agent. Controlled reactions were also performed to prove high activity of core shell nano-catalyst. Pseudo first order kinetic model was applied to investigate the degradation reactions of toxic dyes. It was concluded that prepared composite nano-catalyst increased the rate of reduction reactions and made the reaction kinetically feasible. Nano-catalyst maintained it activity even in case of simultaneous degradation of toxic dyes.Dyes reduction reactions were evaluated on the basis of Langmuir Hinshelwood (L-H) mechanism. Pollutants degradation was also performed under different reaction conditions such as catalyst dose, $NaBH_4$ and amount of toxic dye. Percentage activity of hybrid catalyst was maintained up to fourth reusability cycle for reduction of toxic dyes.

Audience Take Away:

- They learn the methodology to prepared polymers microgels with different morphologies
- They will learn to fabricated different metal nanoparticles in polymer micorgels to prolong their life span
- They will learn to use their composite particles as catalyst for the treatment of wastewater

Biography:

Dr. Khalida Naseem obtained her PhD degree in Chemistry from School of Chemistry, University of the Punjab, Lahore. She served as a Lecturer in Kinnaird College for Women, Lahore from August 2016 to June 2017. She served as Research Assistant at the University of the Punjab from October 2017 to October 2019. She is currently serving as Assistant Professor in Faculty of Sciences, University of Central Punjab, Lahore. She has published 45 articles in international journals of good repute with an accumulative impact factor of 217.342. She presented her research work as poster/oral presenter at National and International level. Her area of research is the synthesis of smart polymers, microgels, hybrid polymer microgels, metal nanoparticles fabrication and their use in the field of catalysis, adsorption and water treatment. Dr. Khalida Naseem is a member of the Chemical Society of Pakistan and American Institute of Chemical engineers (AIChE).

Grapefruit debittering by simultaneous naringin hydrolysis and limonin adsorption using immobilized naringinase

Paulina Urrutia*, Mariela Munoz, Jessica Holtheuer, Lorena Wilson
School of Biochemistry Engineering, Pontificia Universidad Catolica de Valparaiso, Valparaiso, Chile

Naringin and limonin are the two main bitter compounds of citrus products such as grapefruit juice. To reduce or remove bitterness in citrus juices below the threshold level for consumer acceptability, several physicochemical and biochemical strategies have been developed; however, up to now the problem has not been completely solved. The aim of this investigation was to evaluate a single strategy that incorporates the advantages of physical and biochemical approaches for citrus juice debittering. The proposed strategy was based on the design of an immobilized biocatalyst of naringinase able to simultaneously hydrolyze naringin and adsorb limonin, reducing their concentration in grapefruit juice below their thresholds. Naringinase was covalently immobilized in the heterofunctional supports butyl-glyoxyl agarose (BGA) and octyl-glyoxyl agarose (OGA) through glyoxyl groups of carriers, while the alkyl chains of the supports were utilized for limonin adsorption. The immobilized biocatalysts were characterized in terms of optimal pH and temperature and were compared with soluble enzyme. Debittering of grapefruit juice was evaluated using soluble enzyme, enzyme-free supports, and immobilized catalysts. Enzyme immobilized in BGA reduced naringin and limonin concentrations in 54 and 100%, respectively; while the use of catalyst immobilized in OGA allowed a reduction in 74 and 76%, respectively, obtaining a final concentration of both bitter component under their detection threshold. The use of OGA biocatalyst presented better results than when soluble enzyme or enzyme-free support was utilized. Biocatalyst was successfully applied in juice debittering along five repeated batch of 24 h each, and the final residual activity of biocatalyst was over 60%. These results show the potential of this strategy for citrus juice debittering and could offer a technical and economic advantage in relation to the processes currently utilized. Acknowledgement: This research was funded by Chilean Fondecyt Grant.

Audience Take Away:

- The new advances in support functionalization allows us to use the carrier not only for the improvement of enzyme performance but also to adsorbed undesired molecules
- The improvement of debittering process by a single strategy that incorporates the advantages of physical and biochemical approaches, being possible to compare three strategies: free enzyme; enzyme-free support; immobilized enzyme
- A single strategy that effectively combines both principles could offer the technical and economic advantage of reducing the number of operations required for citrus juice debittering

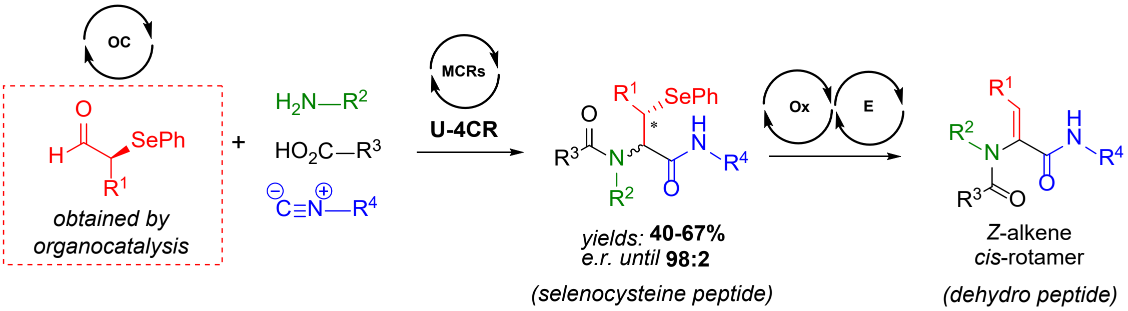
Biography:

Dr. Urrutia studied Biochemical Engineering at the Pontificia Universidad Catolica de Valparaiso (PUCV), Chile and graduated in 2007. She worked as Engineer for one year and then join the Biocatalysis group of PUCV receiving her PhD degree in 2013. After one year of postdoctoral fellowship supervised by Dr. Wilson in the same institution, she obtained the position of Researcher at the research center CREAS, Chile. This year she obtained the position of Associated Professor at the PUCV. She has published 14 research articles in WoS journals and participated in two book chapters.

Combining organocatalysis and multicomponent reactions: A sequential synthesis of sec-containing peptides and dehydropeptides

Alexander F. de la Torre*[1], Odette Concepcion,[1] Daniel G. Rivera,[2] Marcio W. Paixao[3]
[1]Department of Organic Chemistry, Faculty of Chemical Science, University of Concepcion, Concepcion, Bio Bio, Chile
[2]Center for Natural Products Study, Faculty of Chemistry, University of Havana, Zapata y G, La Habana, Cuba
[3]Center of Excellence for Research in Sustainable Chemistry (CERSusChem), Department of Chemistry, Federal University of Sao Carlos – UFSCar, Rodovia Washington Luis, - Sao Carlos - Sao Paulo - Brazil

The efficient design, scalable synthesis of biologically relevant compounds with high structural similarity to natural products remains a challenge to chemical synthesis areas. Metal transition catalysts have been extensively employed for the synthesis of bioactive compounds. However, the combination of metal-free asymmetric methodologies like Organocatalysis with Isocyanide-based Multicomponent reactions (IMCRs) is a new trend to produce natural and natural-like compounds. The asymmetric aminocatalytic functionalization of aldehydes - via enamine mechanism - followed by IMCRs, provides a convergent and stereoselective way to obtain in one-pot manner different scaffolds (e.g.,hydroquinolines, cyclopentenes, peptoids and depsipeptides). These compounds can be accessed with high economy atoms, good yields, excellent stereo and regioselectivity, and a high degree of scaffold diversity. The current work is directly related to the merging of Organocatalytic and IMCRs reactions to obtain novel natural-like enantioenriched selenocysteine *N*-alkylated peptides and also dehydropeptides under mild conditions. The synthetic protocol to the access of selenocysteine *N*-alkylated peptides comprises the organocatalytic asymmetric insertion of phenylselenium into aliphatic aldehyde moiety followed by the classic Ugi four-component reaction (Ugi-4CR) under mild conditions. After further optimization, selenocysteine compounds were obtained with up to 98:2 *e.r.,* in good yield, as determined by chiral ultra-performance convergence chromatography (UPC^2) analysis. We next study the oxidative-elimination of the phenylselenocysteine group to access some dehydropeptides containing ΔAbu and ΔPhe with high regioselectivity (Scheme 1). We demonstrated by 1D and 2D NMR spectroscopic analysis that Z alkene and cis-rotamer preferably formed for all synthesized compounds.



Scheme 1. Synthesis of selenocysteine and dehydro *N*-alkylated peptides obtained by merging organocatalysis and Ugi-4CR.

Biography:

Dr. Alexander F. de la Torre received his B.Sc. and M.Sc. degrees in Chemistry from the University of Havana (Cuba). He then joined the research group of Prof. Marcio W. Paixão at the Center of Excellence for Research in Sustainable Chemistry, Federal University of São Carlos (Brazil). He received his Ph.D. degree in 2015 at the same institution. After a postdoctoral CNPq fellowship at the same institution, he moved to Chile and obtained a postdoctoral FONDECYT fellowship and the position of Assistant Professor at the University of Concepcion (Chile). He has published more than 25 research articles in SCI(E) journals.

Enzyme-sulphide coupling for light-induced water splitting and CO_2 reduction

J. C. Conesa*[1], M. Osgouei[1], S. Zacarias[2], I. A. C. Pereira[2], S. Shleev[3],M. Pita[1], A. L. De Lacey[1]
[1]Instituto de Catalisis y Petroleoquimica, CSIC, Madrid, Spain
[2]ITQB, Universidade Nova de Lisboa, Oeiras, Portugal
[3]Biomedical Science, Faculty of Health and Society, Malmo University, Malmo. Sweden

Many sulphide semiconductors are photocatalytically active in significant ranges of the visible spectrum; our group has shown this, specifically, for In_2S_3 and SnS_2 (R. Lucena *et al.*, Catal. Commun. 2012, 20, 1; *ibid.* Appl. Catal. A: General, 2012, 415-416, 111). Furthermore, by including V in these sulphides we have shown how their photocatalytic activities can be further extended to even the NIR range (P. Wahnon *et al.*, Phys. Chem. Chem. Phys. 2011, 13, 20401; R. Lucena *et al.,* J. Mater. Chem. A 2014, 2, 8236). Here we will show how coupling these sulphides with enzymes of hydrogenase or laccase types allow photoevolving H_2 or O_2.

First, we could show that combining In_2S_3 with a hydrogenase it was possible to generate photocatalytically H_2 in presence of a sacrificial agent (C. Tapia *et al.*, ACS Catalysis 2016, 6, 5691). Then, we showed that combining In_2S_3 with a laccase it was possible to generate O_2 photoelectrochemically (C. Tapia *et al.*, ACS Catalysis 2017, 17, 4881), this being the first time that such enzyme-sulphide combination allowed photoevolution of O_2. A similar photoelectochemical generation of O_2 could be shown by combining SnS_2 with a laccase enzyme (C. Jarne *et al.*, ChemElectroChem 2019, 9, 2755).Some of us carried out recently work which coupled an electrode with a formate dehydrogenase enzyme, including was active species, so that it was possible to reduce electrocatalytically CO_2 to formate (J. Álvarez-Malmagro *et al.*, ACS Appl. Mater. Interfaces 2021, 13, 11891). Ongoing work will be shown here in which combining this latter enzyme with In_2S_3 nanoparticles allows to perform the same task photocatalytically.

Audience Take Away:

- How these sulphides can use all the wavelenghts in which they are active
- How, when substituted by V, they can be extended to longer wavelengths
- How they can be combined with hydrogenase or laccase enzymes to generate H_2 or O_2
- How In_2S_3 can be combined with a formate dehydrogenase enzyme to generate formate photocatalytically

Biography:

J.C. Conesa entered the ICP staff in 1979. He was ICP Director in 2014-2018, and is now Ad Honorem Professor in ICP. He was first in Spain using synchrotron radiation to study heterogeneous catalysis; also first in CSIC using quantum calculations to understand them. Active in XPS and FTIR (including *operando*), EPR and UV-Vis-NIR spectroscopies. He worked on CeO_2-supported metals/oxides for H_2 production, keeping always interest in photocatalysis. He belongs to the Steering Committee of AMPEA, a JP of the European EERA for sustainable energy. His >200 articles and book chapters received about 10000 citations, producing a Hirsch index h=57.

KEYNOTE FORUM

DAY 02

13TH EDITION OF INTERNATIONAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

21-22 OCT

Nikolaos C. Kokkinos

Department of Chemistry, School of Science, International Hellenic University, Kavala, Greece

A holistic approach for scaling-up novel catalytic processes

Many novel precursor catalysts, catalytic systems and even catalytic processes are being developed and studied in research laboratories without being able to reach chemical industry. Laboratories and institutes usually consume resources for further studying novel catalytic processes and not for scaling them up into industrial catalytic processes. On the other hand, chemical industry as well as oil and gas industry keen on turnkey solutions. The main scope of this study is a holistic approach of novel catalytic processes starting from the early stage of research and development until its overall financial audit. Hence, a novel application of heterogenized homogeneous catalysis applied on the neuralgic sector of energy was thoroughly examined taking into advantage its pioneering benefit that is the efficient and convenient recovering of the catalyst.

Although energy sector has confronted with many difficulties in recent years, such as the extreme price variability in short periods, the instability of global supply and demand, and the increasing internal competition with numerous alternative forms of energy; a turn on in the use of new immersive technologies will offer to the industry high levels of productivity at low cost, while at the same time remaining profitable and competitive. The proposed methodology based on a sixfold process. Firstly, the research and development on the laboratory took place. Then, the chemical catalytic process was modelled and simulated. The next step is a verification, validation and testing of the model with the proper feedback from the laboratory experiments. Immersive technologies were used in order to create a virtual reality environment of the real field. Afterwards, the whole catalytic process was simulated in a virtual control room environment for supervisory, control and data acquisition of the chemical process. Finally, a dynamic overall financial audit of the industrial catalytic process implemented in real time. Consequently, a ready-to-use environment for the chemical industry was designed and developed.

Audience Take Away:

- Heterogenizing homogeneous catalysts and taking advantage of their pioneering benefits
- Modeling and simulating of novel chemical process with complicated substances for an effective scale-up study
- Verifying, validating and testing of the chemical process model
- Applying immersive technologies in industrial catalysis
- Financially auditing of industrial catalytic processes in real time

Biography:

Dr Nikolaos C. Kokkinos is Associate Professor at the Department of Chemistry 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 the 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) of Hephaestus Advanced Laboratory at IHU. 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.

EKT. Sivakumar

Visiting Professor, Department of Ceramic Technology, Anna University, Chennai, Tamilnadu, India

Photocatalytic performance of nitrogen doped reduced Graphene Oxide-WO_3 composite

In this study, we have been synthesized porous hybrid N-doped graphene oxide (NGO)-WO_3 composite for photo degradation efficiency tested with methyl orange (MO) decomposition under visible-light irradiation. The NGO- WO_3 composite were synthesized by a by microwave-assisted hydrothermal method. The synthesized NGO- WO_3 composite were characterized by X-ray diffractometer (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), UV-Vis spectrophotometers. The particle sizes were obtained to be 34 nm for NGO-WO_3 composite was determined by XRD spectra and further confirmed by TEM analysis. Adding WO_3 into NGO further results improve surface morphology and shift in the energy band gap from 3.40 eV to 2.26 eV was observed for the pure WO_3 and NGO-WO_3 composite. The photo catalytic activity of the NGO-WO_3 composite tested with MO decomposition under visible-light irradiation. Visible light irradiation are contributed for degradation of 70% of MO dye within 120 min for NGO-WO_3 composite compared with 40% degradation efficiency by pure WO_3. The main reason for a remarkable increasing in the degradation efficiency of the composite which considered WO_3 is associated with NGO on reduction in size of the particles, decreases electron hole pair recombination and increasing efficiency of charge carrier separation and extended the visible light adsorption range. Furthermore, the possible reaction mechanism for the dye degradation of NGO-WO_3 composite was also discussed. Hydrothermal method was economically feasible, improved optical properties of WO_3, we can consider these material very effective photo catalysis for various organic dyes.

Audience Take Away:

- Aware of Nano photocatalysts have been intensively examined because of their increased surface area which sturdily influences their physiochemical properties.
- To examine the photocatalytic nanoparticles for potential application for the degradation of organic and biological wastes.
- This research work aims to reveal the recent works on the photocatalytic degradation of organic pollutants in the presence of nano photocatalyst.

Biography:

Dr. E.K.T. Sivakumar, Visiting Professor Department of Ceramic Technology, Anna University, Chennai, is a /Scientist / Philanthropist/ Educationalist/ and an academician-cum-researcher with an immense passion for serving Motherland and its people.He has authored more than 24 books in English and Tamil. He has participated in various national and international seminars, workshops, and scientific conferences and presented papers on a range of scientific topics. He received Scientist of the year 2008 by NESA NEWDELHI. He is a recipient of many such awards. SSCE's Eminent Scientist Award 2020 is another feather to his cap and also a motivation to serve society even more.

POSTERS

DAY 02

13TH EDITION OF INTERNATIONAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

21-22 OCT

1D/0D Heterojunction nanohybrids extremely excitons transfer for superior photocatalytic hydrogen evolution and NO_2 gas detection at ambient temperature

V. Navakoteswara Rao*, J M Yang
Nano-convergence Technology Division, National Nanofab Center, at Korean institute of science and technology (KAIST), Daehak-to, Yuseong-gu, Daejeon Republic of Korea

Photocatalytic hydrogen generation and room temperature gas sensors are promising to minimize environmental pollution and carbon-based gas emissions [1]. In this work, TiO_2 nanoparticles grown onto CdS nanorods were designed via two-stage facile synthesis to obtain 1D/0D unique heterostructures. Subsequently, titanate nanoparticles loading onto CdS surfaces, with an optimized titanate concentration (20 mM) showed noteworthy superior photocatalytic hydrogen generation (21.4 mmol/ h/ g_{cat}) under 1.5G air mass solar light irradiation. The recyclability of the optimized nanohybrids for six cycles, each cycle has 4 h, indicating that the prepared hetero-structured photocatalyst is an excellent stable material for a prolonged lifetime energy application. In addition, the optimized active CRT-2 was used for an effective room temperature NO_2 gas detection. The CRT-2 sensor showed a higher response (69.16 %) towards NO_2 gas (100 ppm) at room temperature (RT) with the lowest detection limit of ~118 ppb when compared to its pristine counterparts. The CRT-2 sensor showed a short response/recovery time, good cycling stability, and excellent selectivity to NO_2 gas at RT. The NO_2 gas sensing performance of CRT-2 sensor was further boosted using the UV light (365 nm) activation energy. As expected, under the UV light, the sensor exhibited a remarkable gas sensing response with a fast response/recovery and a significant selectivity towards NO_2 gas. Furthermore, a long-term stability test under dark and UV light towards 100 ppm of NO_2 gas was performed at RT and the results showed a significant response continuously for up to 6 weeks without any major loss in the sensor response, signifying that the developed sensor is more reliable for stable gas sensing applications. Thus, excellent photocatalytic and gas sensing performances of CRT-2 material can be ascribed to its high surface area, morphology, synergistic effect, enhanced charge generation, and separation. The constructive 1D/0D CdS@TiO_2 heterojunction material is highly efficient for multi-applications such as energy generation, environmental monitoring, and safety at RT (See in Figure).

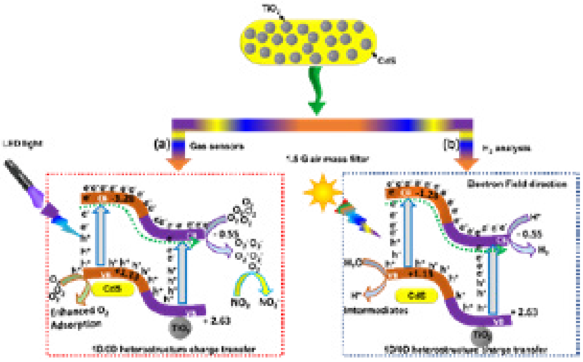


Figure Plausible reaction mechanism for the photocatalytic H_2 gas production over CdS/TiO_2 nanohybrid via water splitting under direct sunlight irradiation and NO_2 gas sensors.

Keywords: Photocatalyst, heterostructures, hydrogen, sensors, stability, and environmental pollution.

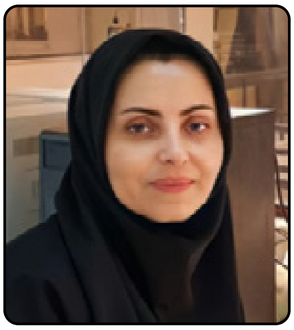
Acknowledgments This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science, and Technology (MEST) [Project Number 6 2020R1F1A1075480] and the Brain Pool program of MSIT [Project Number 2021H1D3A2A02081839]

Audience Take Away:

- By presentation, the audience will learn how to synthesize monodispersed Nano spheres followed by facile methods (Review any current data and analytics, look to previous successes among your audience, and Create buyer personas, comments, and engagements
- Experiment with content and updates to your products and services.)
- Yes, it is research peoples have very useful for expanding their research, especially energy application
- Creative problem-solving is an approach that identifies unique solutions to issues through a process of problem identification and resolution planning. It goes beyond conventional approaches to find solutions to workflow problems, product innovation, or brand positioning. Developing the skill of creative problem-solving requires constant improvement to encourage an environment of consistent innovation. Creative problem-solving is considered a soft skill, or personal strength. In an interview, you may be asked to give examples of times you've demonstrated this ability. Employers ask this question to understand your thought process, learn how you address challenging situations and clarify how you can bring value to their organization
- Our designing morphology is a new ideal strategy for enhancing the suppression of photo corrosion, as well as superior photocatalytic overall water splitting as well as toxic gas detection application

Biography:

Dr. V. Navakoteswara Rao was awarded a Bachelor of Science (Maths, Physics, and Chemistry) in April 2011 from Sri Venkateshwara Arts College, Tirupati affiliated with Sri Venkateshwara University, Tirupati. He has obtained a Master of Science in the Department of Chemistry in April 2014 from Sri Venkateshwara University, Tirupati. Further, He has received a Bachelor of Education in Physical Science and Mathematics Methodology in November 2015 from Sri Krishna Devaraya University. He qualified Council of Scientific Industrial Research (CSIR-UGCNET) All India Rank 43rd rank in chemical sciences 2014 and Graduate Aptitude Test in Engineering (GATE-2018) with a GATE score is 340. He was selected and MNRE: YVU-CECRI Project worked as a Junior Research Fellow as well as enrolled Ph.D. on Hierarchical Composite Nanostructure Photocatalyst For Water Splitting Under Solar Light Irradiation under the supervision of Prof. M.V. Shankar in Nanocatalysis and Solar Fuels Research laboratory during March 2016 to April 2018 as a Junior Research Fellow. Later he was upgraded from Junior Research Fellow to Senior Research Fellow (May 2018 to March 2019). To continue doctoral research V. Navakoteswara Rao was awarded Senior Research Fellowship by the Council of Scientific Industrial Research (CSIR-SRF) Pusa; New Delhi, India. In order to, he has selected prestigious followership which is the Brain pool program-2021 working as a senior scientist at the Korea Advanced Institute of Science & Technology (KAIST), Daejeon, Republic of Korea. He has authored 40 publications, 1 book (Monograph), 2 book chapters, and presented papers in 27 international and national conferences he won two best poster presentation awards in National/International conferences and a cumulative Impact factor is 315.5 with H-Index 19, I-10 Index-25, and Cite score is 1255 (Various journals Had been cited).



Influence of extra-framework aluminum on the lifetime of faujasite y zeolite under isooctane cracking

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[3]Behdash Chemical Company, Qazvin, Iran

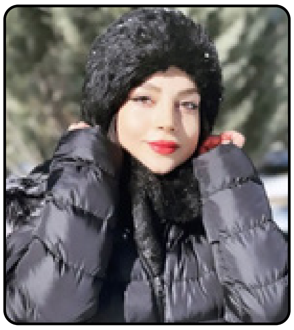
Zeolite Y with Faujasite structure includes high surface area, high thermal/hydrothermal stability, and large pore volume. Tunable acidity is responsible for its application as an acid catalyst in several crucial industrial chemical processes. The micro-porous structure of zeolite Y limits the accessibility of the large feedstock molecules to pore active sites. Moreover, such mass transfer limitations may cause a fast catalyst deactivation and undesired secondary reactions. To improve the mass transfer limitations, catalytic effectiveness in chemical reactions, and decrease the coke formation several approaches were proposed. synthesis of extra-large pore zeolites, synthesis of zeolite with mesopores. And generated interconnected mesoporous structures with intrinsic micropores have been suggested. Post-synthesis treatment was found to be the most practical method for obtaining hierarchical zeolites by desilication and dealumination methods including steam treatment, leaching methods with acidic or basic media. And chemical templates. It is generally known that the post modification processes especially steaming, generates extra-framework Al (EFAL) species with lewis acidity, which contributes to increased cracking activity. These EF cations play a significant role in determining the catalytic properties of zeolites. The work, described here, introduces lewis acidity by using different concentrations of the aluminum precursor into HY zeolite followed by calcination. The resulting catalysts were characterized by means of XRD, XRF, and nitrogen-physisorption. Catalytic testing was investigated over the HY catalysts for cracking of iso-octan. X-ray diffraction and nitrogen physisorption suggest that the zeolitic framework is retained after these treatments. With an increase in the total extra-framework aluminum in the modified zeolites, there was a considerable increase in the number of Lewis acid sites, which is a synergic effect on the coking rate and rapid deactivation of zeolite, thus the catalytic lifetime decreased after ion exchange.

Audience Take Away:

- Faujasite Y zeolite is an applicable catalyst for petrochemical industries that notices the characterization of it results in optimal use with higher efficiency. On the other hand, generated products over these improved catalysts have a significant influence on reducing energy consumption and environmental pollution
- After treatment of zeolites as catalytic cracking, produced Extra-framework Al should be extracted from the catalyst. If there are EFAl species in the zeolite cages, the catalytic property is affected. Leaching methods are used for the elimination of this species. But, these species, as lewis acid sites, have different roles in different applications. we investigated the influence of EFAl in the lifetime of catalysts that are used for the cracking of alkanes. you can study this kind of lewis acid in the efficiency of other catalysts

Biography:

Azam Samiei studied Chemistry at the International University of Imam Khomeini, Iran, and graduated an MS in 2003. She then joined the research group of Alopan Company for anodizing of Aluminium. In 2005 she joined to R&D group of Behdash Chemical Co. that started the production of Zeolite 4A and researched other kinds of zeolites such as 3A,13X, and NaY. In 2018 she joined to R&D group of FCC catalysts in Behdash Chemical co. for management of the analytical methods for Fcc catalysts.



A novel approach to calibration methodology of WD_XRF applied in elemental analysis of zeolite compounds and FCC samples with high accuracy and precision_

Mahta_Badienezhad_*[1,2], Shabnam Sohrabnezhad[2], Azam Samiei[1,3] , Sajjad Habibzadeh[1,4]
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[2]Department of Chemistry, Faculty of Science, University of GuilanRasht, Iran
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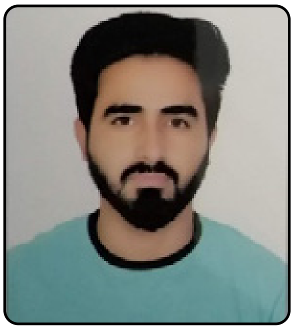
X-ray Fluorescence spectrometry (XRF) is offered in terms of quantitative, fast, and reliable analysis in a wide range of mineral compounds. The intensity of the fluorescence X-ray radiation emitted from the analyte is used for the quantitative analysis of elements in the sample. However, there is no simple proportion between the intensity of X-ray fluorescence and concentration of each element, due to the interaction between the emission of secondary fluorescent radiation and the sample matrix, especially when the matrix contains heavy elements. While matrix effects cannot be reduced or omitted during sample pretreatment, perfect matching between standards and samples, and adjusting of the calibration based on standard reference materials (CRMs) with a matrix quite similar to the test sample are required for better estimates. The present paper describes an innovative XRF calibration method using validated samples and an inert binder, to make some matrix-matched standard samples. The uncertainty-weighted least-square linear regression (UWLR) model was applied for the authentic quantitative multi-elemental analysis. Moreover, the effect of the parameters such as particle size, spectral line interferences, and moisture content of the samples on the accuracy of XRF was assessed. This evaluated method was adapted to determine five major elements, including Al, K, Na, Si, and La in the most common type of synthetic zeolites and Fluid catalytic cracking (FCC) samples like A, Y, and ZMS-5. Variations represented that the limits of detection were 0.20%, 0.12%, 0.31%, 0.18%, and 0.10%, respectively which computed from statistical analyses of duplicate sample aliquots, with RSD <2% for most elements mentioned above, and RSD < 5% for Na. Analytical accuracies were verified by Inductively Coupled Plasma Spectroscopy (ICP) measurements and classical analysis with reliable ASTM test methods.

WD-XRF analysis, Calibration method, Zeolite sample, UWLR model, Fluid catalytic cracking,

- With large-scale mineral concentrating operations, the trustworthy analysis will play a major part in the development of automatic control systems. X-ray Fluorescence spectrometry (XRF) is applied for simultaneous multi-elemental analysis in a wide variety of mineral compounds without dissolution, digestion, and destruction of the samples and usually requires only a minimum of sample preparation. Previous studies indicated that WD-XRF quantitative analysis is carried out by the calibration curve method and is strongly common for measuring raw mineral compounds. This technique requires its methods to be calibrated using Standard Reference Materials (SRMs), Certified Reference Materials (CRMs), and Geochemical Reference Materials (GRMs). While, This work is devoted to the novel calibration method of WD_XRF for improving the accuracy of quantitative determinations of elements, based on the in-house standards of different types of zeolite samples.
- Since the calibration strategy in X-ray fluorescence spectroscopy is depending on the sample preparation, and in pressed pellets particle size, water content, and matrix effects are the main interference factors for multi-element analysis, it can be applied the CRM samples. The advantage of the methodology adopted in this article is to have valid calibration coefficients able to ensure good results of accuracy for wide compositional spectrum. Furthermore, it is not to be underestimated the fact that the empirical coefficients, which account for the matrix effects, are obtained on in-house standards, consisting of chemicals and mixtures of them. We have developed UWLR model for the calibration methodology for the first time using in-house zeolite samples. The advantage of this method is its ability to compete with CRM samples.

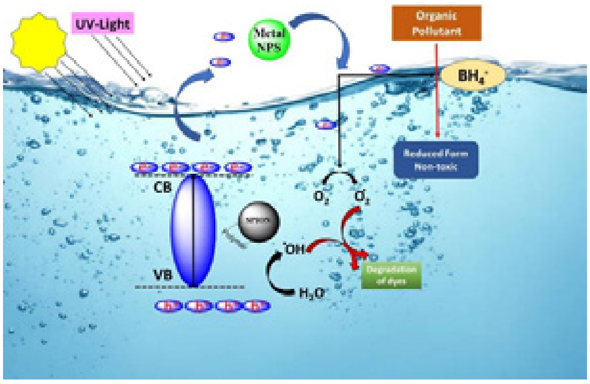
Biography:
Mahta Badinezhad is the Ph.D candidate in Analytical Chemistry at the Guilan University. She received her *master's degree* at Imam Khomeini International University, where she worked in the DDS and published two manuscript in this field. The she joined the research group of Behdash Chemical Co. in 2020. She has been active in various organic and inorganic fields and very skilled in working with different instruments including XRF, XRD, BET, PSA, GC-MS, GC-HS, HPLC.



Fabrication of magnetically recyclable nano photocatalyst decorated with transition metal nanoparticles for the reduction of organic contaminants and photodegradation of Azo dyes

Iftkhar Ahmad*, Saiqa Ikram
Bio/Polymer Research Laboratory, Department of Chemistry, Jamia Millia Islamia University, New Delhi , India

Photocatalytic reduction of nitroaromatic compounds and azo dyes present in wastewater by nanostructured materials is a promising process for the treatment of contaminated water. Nanocomposites decorated with metallic nanoparticles in their matrix are an important class of heterogeneous catalysts with high catalytic activity. Functionalized polymers are low cost materials that offer excellent support for catalysts to render stability to metallic nanoparticles. Recently, the catalytic reductive discoloration of dyes assisted by $NaBH_4$ has received great attention due to its simplicity and very quick operating protocol. In this type of process, nanoparticles of noble metals (e.g., Ag, Au, Ru, and Pt) supported on polymer matrixes can be applied as efficient catalytic materials. However, the high cost and scarcity of noble metals and derived catalysts impede their wide application in wastewater treatment procedures. As a result, the replacement of catalysts containing noble metals by cheaper analogs based on transition metals (e.g.,Cu, Ni, Zn etc.) has emerged as a goal for further research. The hybrid nanocatalyst can easily be recovered and reused successfully for the five consecutive reaction runs with the same catalytic performance. Because of its high photocatalytic efficiency, cost-effectiveness, good magnetic separation performance, non-toxicity, and strong thermal and chemical stabilities, the synthesized magnetic nano-photocatalyst has potential application in wastewater treatment.

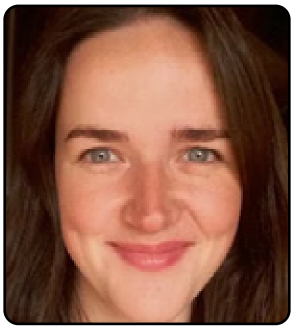


Audience Take Away:

- Most the photocatalyst are not 100 % recovered after photocatalytic reaction. Hence we develop magnetic nanophotocatalyst which can be easily recovered using an external magnet and also shows high catalytic efficacy
- In industries we can replace expensive catalyst by our synthesized catalyst which is economical,ecofriendly and shows high chemical and thermal stability

Biography:

Iftkhar Ahmad was born in Kishtwar Jammu and Kashmir, India. He has done his masters in physical chemistry from Jamia Millia Islamia. He is currently a Ph.D. scholar in the department of chemistry Jamia Millia Islamia New Delhi, India.He is working on the topic, Development of transition metal incorporated magnetically recyclable nanophotocatalyst for the removal of organic pollutants .



New derivatives of lasalocid acid as efficient ion carriers

Monika Papsdorf*[1] and Radosław Pankiewicz[2]
[1,2]Adam Mickiewicz University, Faculty of Chemistry, Poznan, Poland

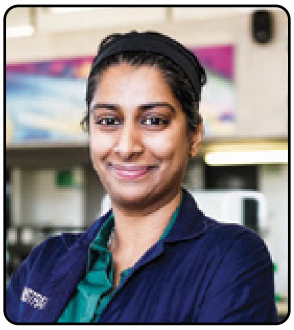
Ionophore antibiotics are a large group of naturally-occurring compounds produced by different species of Streptomyces. There are common used in the animal husbrandy industry and veterinary as e.g. feed additives and medicine. Lasalocid acid is classified as the most often utilized natural antibiotics used in the poultry and cattle holdings. Those feed additives are used to prevention and treatment of coccidiosis. Ionophore comprises in their molecular structure both the lipophilic, as well as the hydrophilic counterparts, they are able to transport metal cations across lipid membranes. They disrupt the natural ion transport systems in cells and exhibit a variety of biological antibacterial, antiparasitic, antiinflammatory or antiacancer properties. Even slight structural modifications of the antibiotic may result in changes within the complex from the structural point of view, which follows the ability of the ionophore to bind metal ions and transport them through the cell lipid layers. In case of the biologically active compounds this might confer to their antimicrobial properties.

Audience Take Away:

- What are ionophore antibiotics
- How to modifications and study of natural ionophore antibiotics
- Become acquainted with the new chemical compounds with potential applications in analytics, food industry, veterinary medicine and medicine

Biography:

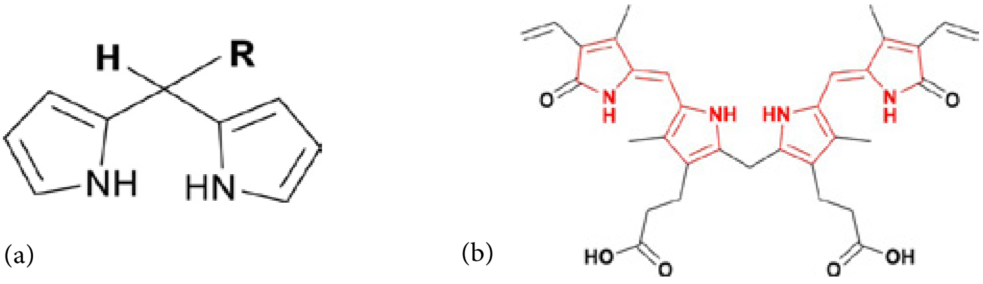
MSc. Eng. Monika Papsdorf studied Chemistry at Adam Mickiewicz University, Poland and graduated as MSc in 2017. She started her PhD in the research group of Prof. Radosław Pankiewicz. Her field of studies is modification and physicochemical research of natural ionophore antibiotics. She interned in Technical University in Dresden.



Dipyrromethanes: Structural analogues for probing the chemistry of bilirubin pigments

Mathura S*, Joseph, C. J., Gqoba, A., Nkomo, R., Madakane, N. G
University of the Witwatersrand, Johannesburg, South Africa

2,2'-Dipyrromethanes (dipyrranes) are a class of ligand that is partially conjugated and comprising two pyrrole rings fused at the meso carbon atom (Fig1a). These ligand systems serve as precursors for the synthesis of porphyrins and related macrocyclic structures. Formed by the condensation of an aldehyde with excess pyrrole under controlled conditions, dipyrranes are exceedingly popular as sensors, probes and catalysts. This is primarily due to their predictable transition metal coordination chemistry and favourable fluorescent properties. Our interest in dipyrranes (and their transition metal complexes) is their structural similarity to bilirubin, thus serving as a suitable analogue for probing the coordination chemistry of bilirubin pigments (Fig 1b). This preliminary work reports on the successful synthesis and spectroscopic characterization of selected *meso*-substituted dipyrranes: 5-phenyl dipyrromethane; 5-(4-hydroxyphenyl) dipyrromethane and 5-(4-nitrophenyl) dipyrromethane. Ligands were synthesized using methods adapted from Lindsey et al., and characterized by spectroscopy (NMR, UV-Vis, LCMS, IR), melting point analysis and crystallography.



(a) (b)

Figure 1: (a) general structure of dipyrromethane ligands (dipyrranes) indicating structural similarity to bilirubin pigments; (b)general structure of bilirubin pigments

Acknowledgements: This work is based on the research supported wholly or in part by the National Research Foundation of South Africa(Grant number: MATH021)

Audience Take Away:

- This work will contextualize dipyrromethanes and their significance in porphyrin synthesis (can be used as examples for teaching undergraduate coordination chemistry, chelation and transition metal chemistry)
- This work will discuss the significance of dipyrromethanes as structural analogues for bilirubin pigments(thus expanding on possible probes for bilirubin solution chemistry studies and diagnostics)

Biography:

Dr Sadhna Mathura is an academic at the University of the Witwatersrand in Johannesburg, South Africa. She obtained her Doctorate in Bioinorganic Chemistry from the same institution for her significant contribution to the understanding of vitamin B_{12} and cobalt chemistry. Her work was recognised through several doctoral scholarships and doctoral publications. She provided quality Chemistry training to 3 postgraduate students, and well over a 100 undergraduate students, many of whom have gone on to further their Chemistry career. She is a member of the chemistry professional bodies: IUPAC, ACS, RSC, FASC and SACI.

SPEAKERS

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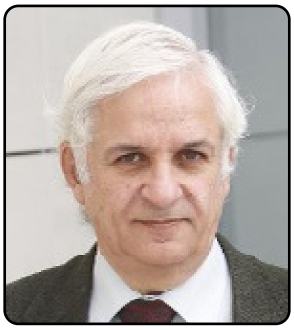
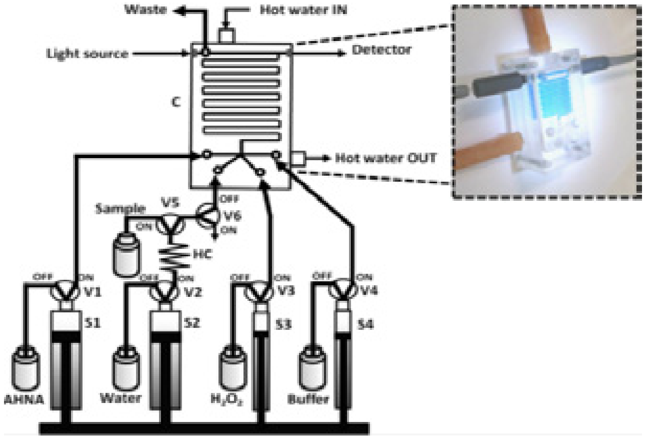


Automated In-chip catalytic spectrophotometric methods

VIctor Cerda*[1], Sergio Ferreira[2], Piyawan Phansi[3]
[1]Sciware Systems, SL, Bunyola, Spain
[2]Dep. Chemistry, Universidade Federal da Bahia, Brazil
[3]Dep. Chemistry, Fac. Science & Techn., Thepsatri Rajabhat Univ., Thailand

The development of automatic analyzers based on flow techniques, like FIA, MSFIA, SIA, MPFS, etc., involves the use and continuous innovation of fluidic devices. The new trends go toward miniaturization of sophisticated fluidic platforms, like chips, requiring continuous advances in this field. The availability of a mechanic and electronic workshop together with the know-how to build new 3D fluidic devices provides the tools for the creation of innovative instrumentation and stimulates the creativity of analytical chemists. In this contribution we will present how to build and use of new flow-based fluidic devices, together with the tools required, such as computerized controlled lathes, milling machines, laser engraver machines, low-temperature co-fired ceramics technology and 3D printers, highlighting their strong and weak points. In addition, some flow based methods exploiting innovative fluidic platforms applied in catalytic spectrophotometric methods are presented as a way of example of the possible devices that these tools can provide and their potential applications.



Audience Take Away:

- This presentation will help how to build compact flow systems for kinetic-catalytic methods
- The presented chips may be used by other faculties to expand their research or teaching
- It will improve the accuracy of a design, and provide new information to assist in a design of compact systems

Biography:

Victor Cerda, graduated and PhD in Chemistry by the University of Barcelona. Became Full Professor of Analytical Chemistry in 1982 at the University of the Balearic Islands. He has conducted 41 Ph.D. Thesis, written 14 books, and collaborated with 14 chapters in other scientific books. He has published 620 papers and presented 847 contributions in national and international symposia. Has been organizer of more than 15 international symposia. Has been the Head of the Department of Analytical Chemistry and the first Head of the Department of Chemistry of the UIB. Has been Vice-President of the Spanish Society of Analytical Chemistry.

Synthesis of catalytically active filter materials via plasma-mediated method for application in electro-fenton process for degradation of pharmaceuticals

Fee J. Kaeufer[1,2*], Rebekka Maess[2], Angela Kruth[1], Heike Kahlert[2]
[1] Leibniz Institute for Plasma Science and Technology, Greifswald, Germany
[2]University of Greifswald, Greifswald, Germany

To this day conventional wastewater treatment plants are not able to eliminate all organic pollutants. That is why thedevelopment of new technologies is necessary. An option that has shown promising results is the application of differentadvanced oxidation processes (AOP). They all produce highly reactive species like free hydroxyl radicals. Those are non-specific and can degrade almost all organic compounds into carbon dioxide, water and inorganic ions. One AOP, which has proven high reaction yields, is the Fenton reaction. In this study, a heterogeneous electro-Fenton approach is investigated. The catalytic iron-based material was producedvia a plasma-mediated sputtering method. Different settings were applied during the sputtering process to optimize the deposited catalyst. The so produced iron oxide layers were coated onto carbon felt. Coated felts were then used as filtersby applying them in a three-electrode set-up as working electrodes.

The process was applied to different pharmaceuticals as model pollutants and run in a flow through system. It was demonstrated that the active catalytic material is suitable for initiating a Fenton reaction and therefore causing a degradation of pharmaceuticals with remarkable performance. Additionally, it was found that the produced radicals donot only cause reactions at the electrode's surface but that reactions continue outside the flow through system as shownby recorded reaction kinetics. A pharmaceutical degradation of over 90% was achieved as well as the degradation of by-products.The catalytic material was characterised via several different methods to determine morphology, structure and chemicalcomposition. This way a relation between the characteristics of the material and its activity was studied. As such, our results show that precise control of synthesis parameters enable fine-tuning of the catalytically active material towardshigh pollutant degradation performance.

Audience Take Away:

- Insights into plasma-mediated technology to produce catalytically active material
- About advanced oxidation procedures and their application in wastewater treatment
- Electro-Fenton processes and their advantages
- Degradation kinetics of pharmaceuticals

Biography:

Fee J. Kaeufer studied Environmental Sciences at the University of Bielefeld where she received her bachelor's degree in 2015. She continued her studies at the University of Greifswald with a focus on Environmental Chemistry and Analytical Chemistry. After her graduation, she worked in a laboratory conducting analysis of environmental samples before returning to scientific work in 2020 when she started her Phd as a collaboration between the Leibniz Institute for Plasma Science and Technology and the University of Greifswald. In her Phd project she is studying thedevelopment of a novel electro Fenton filter to degrade pharmaceuticals in wastewater.

Monitoring the relationship between specific surface area and total pore volume with silica amount using novel method and SI/AL ratio in Fluid Catalytic Cracking (FCC) through XRF, XRD and N_2-Porosimetry Analysis

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[2]Department of Chemistry, Faculty of Science, University of Guilan, Rasht, Iran
[3]Department of Chemistry, Faculty of Science, Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran
[4]Department of Chemical Engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran

Currently, The effects of acid activation, surface area and pore structure of Fluid catalytic cracking (FCC) have shown enormous potential in the oil refinery industry. FCC catalysts are continuously being modified and new systems developed to meet changing demands, e.g. the ability to convert crude oil into a more valuable product, such as gasoline and olefin by acts of zeolite as a solid acid catalyst and comprises of inter-linked tetrahedral with Si and Al joined by oxygen bridges. Results of the present work demonstrate that on the grounds of the properties and expected behavior of FCC, combined XRF, XRD, and N_2-porosimetry analysis enabled the monitoring and comprehension of specific surface area and total pore volume on the amount of silica (SiO_4) and alumina (AlO_4). *X-ray fluorescence* spectrometry (*XRF)* showed a high silicate content level after leaching which was obtained by the novel and cost effective calibration method, X-ray diffraction spectrometry (XRD) indicates the highest Si/Al ratio value in the final product, and samples had a combination of types I & II adsorption/desorption isotherms achieved by N_2-porosimetry analysis. Si/Al ratio of 2–5, specific surface area around 230–300 m^2/g, and total pore volume within 0.19-0.25 m^2/g indicates the formation of porous zeolite crystal in its sodalite cage and presence of intermediate mesostructured Zeolite Y catalyst. The relative precision (measured as the relative standard error) in XRF is better than ±3% and the limits of detection were 0.2%, 0.12%, 0.31%, 0.18%, and 0.1% for Al, K, Na, Si, REE (Rare Earth Elements), respectively. All analyses have technically applied the ASTM test methods to achieve results with high accuracy and precision.

Fluid catalytic cracking, Zeolite, *X-ray fluorescence* spectrometry, N_2-porosimetry analysis.

- The Fluid Catalytic Cracking (FCC) technology is one of the pillars of the modern petroleum industry which converts the crude oil fractions into many commodity fuels and platform chemicals, such as gasoline. Although the FCC field is quite mature, the research scope is still enormous due to changing FCC feedstock, gradual shifts in market demands and evolved unit operations.
- The Fluid Catalytic Cracking (FCC) is a secondary refining process used primarily for conversion of the high-boiling, high-molecular weight fractions of petroleum to more valuable fuels. Fuel production from the FCC process accounts for about 35–50% of the total gasoline produced worldwide in the petroleum industry. The FCC unit represents the heart of the refinery, and the latest design that is still much used in the refineries around the world consists of two main vessels: a riser (reactor) and a regenerator that are interconnected to permit transferring the spent catalyst from the reactor to the regenerator and the regenerated catalyst back to the reactor in a cyclic manner. One of the significant achievements that have contributed to the ever-growing popularity of the FCC has been the introduction of Zeolite catalysts. Zeolites are hydrated alumina silicate materials made from inter-linked tetrahedral of alumina (AlO_4) and silica (SiO_4). Characterization of the FCC is done by various methods such as XRF, XRD, BET analysis. The important point is that, XRF analysis of present work was done using the novel method of calibration without any CRMs and SRMs with

the least impact of the matrix-effect. Due to this method, costs are greatly reduced and it is suitable for different industries with various products.

Biography:

Mahta Badinezhad is the Ph.D candidate in Analytical Chemistry at the Guilan University. She received her *master's degree* at Imam Khomeini International University, where she worked in the DDS and published two manuscript in this field. The she joined the research group of Behdash Chemical Co. in 2020. She has been active in various organic and inorganic fields and very skilled in working with different instruments including XRF, XRD, BET, PSA, GC-MS, GC-HS, HPLC.

Catalytic biotransformations by peroxidases

Meera Yadav
Department of Chemistry, North Eastern Regional Institute of Science and Technology, Nirjuli, Itanagar, Arunachal Pradesh, India

Heme enzymes known as peroxidases (E.C.1.11.1.7) use hydrogen peroxide as an electron acceptor to catalyse a variety of oxidative processes. There are two significant environmental challenges that are driving the current interest in catalytic bioconversions.

(i) Using H_2O_2 as an environmentally benign oxidant to replace or substitute heavy metal salts and other reagents used in conventional oxidations.

(ii) The main problem is the growing interest in producing chemicals in chemical processes with high chemo selectivity, regioselectivity, and stereo selectivity in order to produce superior byproducts. Peroxidases, a type of redox enzyme, are crucial in achieving these two objectives. The fruit juice-derived enzyme had a high peroxidase activity of around 9.0 IU. To explore the catalytic potential of the peroxidase enzyme, the rate of reaction catalysed by the enzyme was determined using guaiacol as the substrate and in the presence of various oxidising agents. It was discovered that V_2O_5 was a better oxidising agent than H_2O_2 in this experiment. By releasing Br_2 and I_2, the enzyme encourages the halogenation process. When Ca^{2+}, Mg^{2+}, and Cd^{2+} are present, enzyme activity is increased; when Zn^{2+} and Ni^{2+} are present, enzyme activity is decreased. These metal ions' nature of inhibition has also been studied.

Keywords: Redox enzyme; Peroxidases; Biotransformations; Halogenation; Bioremediation

Biography:

Dr. Meera Yadav completed her Master's and Ph.D in Chemistry from DDU Gorakhpur University, Gorakhpur, Uttar Pradesh, India. She was awarded CSIR-SRF (2000-2003), twice as DST- Woman scientist A (2005-2008) & (2013-2016) and UGC- Dr. D. S Kothari Postdoctoral Fellow (2009-2012) at Department of Chemistry, Gorakhpur University, Gorakhpur. Her research area includes, purification, characterization and applications of Metalloenzymes- Lignin peroxidase, Mn-peroxidase, Laccase and Chloroperoxidase, isolation of fungal strains producing ligninolytic enzymes, their structural-functional studies using X-ray crystallography, spectroscopic and fast reaction kinetic techniques. Use of enzymes in synthetic inorganic and organic chemistry. She has served two years as guest lecturer in Madan Mohan Malviya Technical University (MMMTU), Gorakhpur. Currently she is working as an Assistant professor in the Department of Chemistry, North Eastern Regional Institute of Science and Technology (NERIST), Nirjuli, Itanagar, Arunachal Pradesh, India. She has attended and participated in more than 30 national and international seminars and conferences. She has guided one Ph.D and five students are being involved in various research activities in her laboratory. Eight students have submitted their M.Sc dissertation under her guidance till now. She has published more than 40 research papers in reputed national and international peer reviewed journals and reputed standard books. She has also reviewed many research papers. She is life member of American Chemical Society, Indian Council of Chemists and Indian Society of Chemists and Biologists.

Mechanical characterization of PEEKH-HA composite as an orthopedic implant

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[1]Mechanical Engineering Department, North Eastern Regional Institute of Science and Technology, Nirjuli,
Arunachal Pradesh, India
[2] Mechanical Engineering Department, Sikkim Manipal Institute of Technology, Sikkim Manipal University, Majitar, India
[3]Metallurgical and Materials Engineering Department, Indian Institute of Technology, Kharagpur, India

Nowadays research in the biopolymers are prominent area for research in medical fields. The metallic implants are used in many numbers for the orthopedic surgeries. But some unavoidable issues are arising after surgeries like stress-shielding, osteogenesis imperfection, etc. To overcome such issues re-surgery is only one painful option available for the patient. Sometimes this option is not feasible for the weak and old patients. Which results in increased the life risk in such situation. Hence a biopolymer may be the best solutions to eliminate such problems. Polyether ether ketone (PEEK) and Hydroxyapatite (HA) are having biocompatible characteristic with different Mechanical properties. Hence in this paper three different compositions of PEEK-HA are considered and the composites were prepared using compression moulding technique. To compare the mechanical properties for different compositions of PEEK-HA, the porosity and tensile strength were calculated. Unlike the other techniques, the fracture toughness was evaluated through J- integral method to ensure the matching of the cracking phenomenon with the human bone. Tribological properties e.g. wear resistance and plasticity index for all compositions of PEEK and HA were executed in both static and dynamic mode. The result reveals that, PEEK5HA can be used for the possible bone replacement.

Audience Take Away:

- How the polymer implant can be used as an orthopedic implant?
- What is the present problem with the polymer implant material?
- What are the advantages of polymer implant material?
- How the fracture toughness will help full for a polymer implant material?

Biography :

Dr. Sujoy Kumar Dey Studied in Haldia Institute of Technology in India and graduated in 2009. After that join in Masters in Engineering at Indian Institute of Engineering Science and Technology, Shibpur and received degree in 2011. Then he joined North Eastern Regional Institute of Science and Technology, India after some years of industrial experience and received PhD degree in 2022. In his journey he is working in Sikkim Manipal Institute of Technology since 2012 as an Assistant Professor. He has published more than 2 research articles in Scopus and one SCIE journals.

Ethylene dimerization: Development of anti-fouling agents

Sibo Lin[1*], Motaz Khawaji[2], Dana A. Wong,[1] Mohamed Elanany[2], Wei Xu[2]
[1]Aramco Services Company: Aramco Research Center – Boston, Catalysis Technology Group, Cambridge, MA, USA
[2] Saudi Aramco: Aramco Research Center – KAUST, Chemicals R&D Lab, Thuwal, Saudi Ara

Titanium- and aluminum-catalyzed ethylene dimerization to 1-butene (AlphaButol process) has been practiced industrially for decades, yet inevitable reactor fouling with polyethylene byproduct remains a fundamental challenge. Spectroscopic data has shown that a complex mixture of Ti(III) and Ti(IV) species are formed, depending on the Al/Ti ratio and presence of ligands such as tetrahydrofuran. This concomitant mixture of species has frustrated mechanistic analysis and rational prevention of reactor fouling. Herein, we utilize computational molecular modelling (extended tight binding theory and density functional theory as implemented in XTBDFT) to examine the mechanism of 1-butene and polyethylene formation with computational molecular modelling, and we develop novel anti-fouling agents that effectively reduce polyethylene formation while retaining 1-butene productivity. This technology has been patented and licensed across the industry.

Audience Take Away:

- Industrial vs. academic research priorities
- Application of molecular modeling to improving catalysis
- Importance of conformational searching for mechanistic molecular modelling

Biography :

Sibo Lin obtained his B.S. Chemistry degree from Indiana University in 2008, followed by his Ph.D. Inorganic Chemistry degree from Caltech in 2014. He spent 4 years as a postdoctoral fellow at MIT, and then moved across the street to start his industrial career at Aramco's Boston Downstream Research Center (2018 – present), where he serves as a project lead, developing catalysts for olefin oligomerization and membranes for sour gas separations.

CuNiMoP composite electrocatalyst for glycerol electro oxidation

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Electrocatalyst composite consisting of copper (Cu), nickel (Ni), molybdenum (Mo) phosphorus (P) was synthesized and evaluated for the electro-oxidation of glycerol. An autocatalytic chemical reaction technique in an aqueous media containing the component ions of the composite was used to synthesize the catalyst on an activated substrate. The electrocatalyst was characterized using scanning electron microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), X-ray Diffraction (XRD) and various electrochemical techniques, including Cyclic voltammetry (CV), Linear Sweep Voltammetry (LSV), Chronoamperometry and Electrochemical Impedance Spectroscopy (EIS). A combination of voltammetry and high-pressure liquid chromatography product analysis was used to evaluate the activity of the electrocatalyst towards glycerol oxidation. Use of a mixture of reducing agents, specific ratios of metalions in solution, pH, oxygen content of the autocatalytic solution and temperature conditions were identified for co- deposition of all four catalyst components. CV results showed that the composite catalyst as prepared was active forglycerol oxidation in alkaline media and the activity was comparable to that of Pt under similar conditions and betterthan mono- or bi-metallic combinations of the components.

Tafel analysis of the LSV results indicated exchange current densities ranging from 0.18 – 0.6 mA cm^{-2} for different deposition times and Tafel slopes of 120 – 130 mV/decade. Constant potential oxidation of glycerol between 0.5 - 1.3V (vs. Ag/AgCl) on CuNiMoP/C catalyst showed that as prepared catalyst selectively favored the production of formic acid at the lower potentials. At intermediate potential of 0.9 V, glyceraldehyde/dihydroxyacetone (DHA) are favored while at 1.1 V tartronic acid and mesoxalic acid are the major products. At potentials higher than 1.1 V, competing parasitic reactions reduced the glycerol conversion and product yield. Glycerol conversion of 62% was achieved at 1.1 V compared to 3 – 38% with Pt catalystunder similar conditions. Rates of reaction, measured in terms of current density, were found to be low for potentialslower than 0.7 V. Constant potential oxidations at 0.7 V for three different 24-hour cycles showed catalyst deactivationfrom leaching of Cu. These results have potential importance in direct alkaline glycerol fuel cell applications.

Audience Take Away:

- Audience will learn and be able to use technique to synthesize multi-elemental (non-precious metal)electro catalyst on most substrates including non-conductive substrates
- Learn about electro catalyst that has comparable activity to Pt that can be used in direct glycerol fuel cell
- Results provide information to assist in the design of direct glycerol fuel cell
- Provides information on the product selectivity for glycerol oxidation

Biography:

Dr. E. Eric Kalu is a Professor of Chemical and Biomedical Engineering atFAMU-FSU College of Engineering. He received B.Sc (Hons) First Class degree in Chemical Engineering fromUniversity of Lagos in 1984. He then joined Prof. C. W. Oloman at UBC, Vancouver where he obtained his MASc degree. He then joined Professor R. E. White's electrochemical group at Texas A&M University where he obtained his Ph.D. in 1991. After three years of industrial experience and a postdoctoral training at University of South Carolina, Columbia, he joined the joint-college of Florida A&M University and Florida State University in 1995 as anAssistant Professor where he rose to full Professor. He has published more than 100 research articles in electrochemical, chemical engineering and materials chemistry journals.

Microkinetic modeling of ammonia oxidation over Pt(211): The role of the surface coverage

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The effect of surface coverage (θ) on single NO^*, N^* and O^* and double NO^*–(N^*–Pt), NO^*–(O^*–Pt), N^*– (O^*–Pt) and O^*–(N^*–Pt) co-adsorbed systems on Pt(211) stepped surface has been studied by using periodicdensity functional theory (DFT). The effect of the surface coverage on the activation energies of elementary reactions for the ammonia oxidation network was also investigated at θ values of 1/12 and 1/6 mL, respectively. It was found that binding energy for single and double adsorption decreases almost linearly as θ increases. This effect is stronger for double co-adsorbed systems than for single adsorption cases. A threshold coverage (θ^T) of 0.08 mL for which the linear dependency of binding energies with θ will tail off was estimated. Activation energies also decrease as θ increases, with the lateral interactions between the reactants being the major contributor to the overall energy barrier. Finally, the results of this study permit theinclusion of the surface coverage effects not only on the enthalpies of reaction but also on the activation energies for products formation during ammonia oxidation modeling, ensuring the thermodynamic consistency.

Audience Take Away:

- People working in chemical kinetics, catalytic activity and heterogeneous catalysis will learn how to use periodic molecular modeling to get insight into the reaction mechanism taking place at the catalyticsurface.
- This research provides all the parameters needed to include the surface coverage effect in the micro kinetic modeling of ammonia oxidation on platinum Pt(211) which appears to be a more activesurface for product formation than the most thermodynamic stable facet Pt(111).
- Finally, with the results of this research, the microkinetic modeling of ammonia oxidation on platinumusing chemical kinetics simulators such as Chemkin or Fluent can be carried out in a thermodynamically consistent way, avoiding fitting and other approximations that can result in inaccurate modeling of the catalytic process

Biography:

Dr. Juan David Gonzalez studied Chemistry at Antioquia University and graduated in 2008 with honors. He then joinsProf. Fanor Mondragon's research group at the Chemistry Institute of the same university to do a Master of Science in Chemistry. In 2013 he won the prestigious Australian Award and Australian Leadership Award to do his Ph.D. in Chemical Engineering at The University of Sydney. He received his Ph.D. in 2017. In 2018 he returned to his home country Colombia and obtained a position as an associate professor at Remington University.

Removal of chloride ions from copper solution, using electrodialysis techniques, to recover uranium through ion-exchange

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[2]University of Santiago de Chile, Chile

This study shows the technical feasibility to recover uranium from copper Pregnant Leaching Solutions (PLS) using ion-exchange, after a removal of chloride ions using the electrodialysis (ED) technique. The original copper PLS solutions came from the National Copper Corporation (CODELCO), from their hydrometallurgical operations, which contained high concentrations of chloride ions. These solutions contained average concentrations of 22 g/L chloride ions, pH 1.5 – 1.8 and 20 mg/L uranium. The high chloride contents made the uranium recovery technically unfeasible, because of the high volumes of chemical reagents needed to operate. To eliminate the chloride ions selectively, a modified electrodialysis (ED) process was developed. The ED process was made of a three–compartment cell. This system removed selectively the chloride ions, and replaced them with sulphuric ions, without modifying the composition of the copper PLS solution, to allow a continuous operation of the copper production plant. The ED process decreased the chloride content from 22 g/L to 6 g/L. Finally, static and dynamic load tests were performed for both the original PLS and the treated PLS, using 3 different anion exchange resins: Dowex-1, Lewatit A365 and Lewatit MP62-WS. The loading capacity of the ion-exchange resins was increased 4 times approximately.

Audience Take Away:

- This work shows a process to selectively remove chloride and uranium ions from a copper pregnant leaching solution, to improve the safety of the operation, by avoiding the accumulation of radioactive materials through the hydrometallurgical operation
- The audience will be able to see an application of electrodialysis different than the conventional processes, applied to problems of the uranium industry
- The results obtained in this project will allow to expand the possible applications of electrodialysis, to solve problems in various areas of the chemical industry

Biography:

He obtained both my professional title of metallurgical engineer and my master's degree in Extractive metallurgy in 2014. In 2020, finished PhD studies at Universidad de Santiago de Chile, in the Engineering Sciences doctoral program, with mention in Process Engineering. Currently, He is a researcher at the Chilean Nuclear Energy Commission (CCHEN). He work can be separated in two different areas: The development of new methodologies for the purification of valuable elements through metallurgical and chemical processes, focused towards the production of radiopharmaceuticals for nuclear medicine: uranium, molybdenum and rare earths; and chemical purification of materials for energy sustainability.

Participants List

UPCOMING CONFERENCES

14th Edition of Global Conference on
Catalysis, Chemical Engineering and Technology
March 13-15, 2023 | Singapore| Hybrid Event
https://catalysis.magnusconferences.com/

15th Edition of International Conference on
Catalysis, Chemical Engineering and Technology
May 22-23, 2023 | Tokyo, Japan | Hybrid Event
https://catalysis-conferences.com/

16th Edition of Global Conference on
Catalysis, Chemical Engineering and Technology
September 14-16, 2023 | Valencia, Spain | Hybrid Event
https://catalysis-conferences.magnusgroup.org/

17th Edition of International Conference on
Catalysis, Chemical Engineering and Technology
October 26-28, 2023 | Boston, Massachusetts, USA | Hybrid Event
https://catalysiscongress.com/

Questions? Contact

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