



CAT 2019

5TH EDITION OF
GLOBAL CONFERENCE ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

SEPTEMBER 16-18, 2019

LONDON, UK

Theme:
Novel Explorative Approaches trending in
Catalysis, Chemical Engineering and Technology

Park Inn by Radisson Hotel & Conference Centre
Bath Road, Heathrow, Middlesex
UB7 0DU, London, UK

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5th Edition of Global Conference on
CATALYSIS, CHEMICAL
ENGINEERING & TECHNOLOGY

Theme:

*Novel Explorative Approaches trending in Catalysis,
Chemical Engineering and Technology*

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LONDON, UK

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CAT 2019



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CAT 2019



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Pacific Northwest National
Laboratory, USA



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CAT 2019



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and Technology, USA



Reza Shahbazian Yassar
University of Illinois, USA



Rongsheng Cai
Swansea University, UK



Saikat Chakraborty
Indian Institute of Technology
Kharagpur, India



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Tsinghua University, China



Yuqi Wang
Northwest University, China



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University of Chinese
Academy of Sciences, China

Thank You

All...

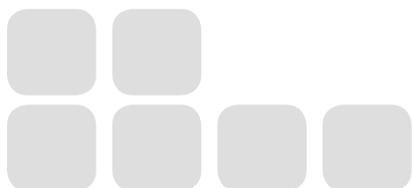
Welcome

Message



Dear congress visitors,

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



Stanislaw Dzwigaj
Sorbonne University-CNRS
France

Welcome

Message



Dear colleagues!

I am honored to greet you on the opening of the Catalysis 2019 conference. Catalysis currently occupies a leading place in various fields of chemical technology and environmental protection. The possibilities of catalysis are constantly expanding and they are aimed at obtaining energy carriers, fuels and valuable monomers, playing an important role in sustainable development of society. In recent years, much attention is paid to the development of new approaches to obtaining highly active and selective catalytic systems, as well as to using of new raw materials for important products producing. Globally, chemical nanotechnologies are fully related to the development of efficient new generation catalysts what is linked to understanding of mechanisms of active centers evolution, which ensure high activity of important catalytic reactions. I express the hope that the conference will allow us to hold a fruitful discussion and exchange our views on important aspects of catalysis.



M. Tsodikov

A.V.Topchiev Institute of Petrochemical Synthesis RAS
Russia

Welcome

Message



Dear visitors of CAT 2019, it is a pleasure for me to write some welcome notes. Especially I want to draw your attention to the increasing innovation potential of combining chemical science with process technology and engineering.

Some people regard both (organic and catalytic) chemistry as well as process technology /chemical engineering as almost mature sciences. I find it interesting that at the interface of these sciences , innovation takes place at a high speed.

As a case in point : The capability to 3-D print reactors in various metals using technologies at competitive costs , is now established. This enables to unlock the full potential of e.g. highly exothermic and/or very high (or low) temperature and/or hazardous chemistries. This has especially impact on pharmaceutical and other fine- and specialty chemicals fields. We come in an era where 'the reactor design will follow the chemistry' instead of the other way around (' batch reactor').



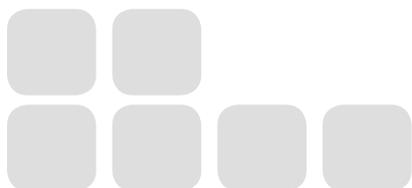
Dr Rinus Broxterman
Innosyn B V, Geleen,
The Netherlands

Welcome

Message



Dear scholars, it is my great honor and pleasure to welcome you to the CAT-2019 conference that promises to provide innumerable opportunities to network, share ideas and collaborate. Many important chemical reactions require inputs of energy to proceed. Catalysts, however, can promote these transformation by lowering the energy required to complete the reaction. It is hard to imagine the world today without the impact of catalysis on the fundamental aspects required for life, namely energy, food and water. To make a catalyst more efficient, a molecular level understanding of the catalyst material, the reaction kinetics, intermediates, active centers and pathways are important. Modern diagnosis tools, in particular operando spectroscopies and imaging techniques that are capable of capturing reaction processes at critical length and time scales, have been or are being successfully developed to advance the field of catalysis science that we will be able to learn from this conference.



Dr. Jian Zhi Hu
Pacific Northwest National Laboratory,
USA

Welcome

Message



Dear Colleagues,

The European Union, through the SET-Plan, suggested that in the future energy system, H₂ should be produced from renewable feedstock using renewable energy in order to be considered “zero CO₂”, so resulting in a practically closed carbon cycle with no impact (in terms of anthropogenic emissions) to the environment. In this way, a process intensification is mandatory. The approach to process intensification regards process-intensifying equipment, characterized by designs that optimize mass, heat, and momentum transfer (e.g. monolithic catalysts) and process-intensifying methods, involving the application of alternative energy sources, so leading to compact, safe, energy-efficient, and environment-friendly sustainable processes. In particular, the use of structured catalysts with high thermal conductivity, could overcome the heat transfer limitations that occur in both endothermic and exothermic reactions. CAT2019 provides the platform for excellent scientific exchange in the key issues of catalysis and process intensification.



Eugenio Meloni

Industrial Engineering Department, University of Salerno
Italy

Welcome

Message



Dear conference attendees, it is a pleasure to welcome you to the 5th Global Conference on Catalysis, Chemical Engineering & Technology. In this conference, you can catch up on various cutting-edge developments in Catalysis and Chemical Engineering, which will help society to face some of the most important World's challenges. This is also a great opportunity for people from academia and industry to meet and share the knowledge of their recent advances in these fields, as well as the perfect scenario for networking and creation of new collaborations.



A handwritten signature in blue ink, appearing to read 'J. A. Diaz Lopez'.

Dr. Jose Antonio Diaz Lopez
Universidad Politecnica de Madrid,
Spain

Welcome

Message



Dear congress visitors, it is pleasure and honor to write a few welcome notes. Environmental catalysis plays a major worldwide role in improving our atmosphere and reducing pollution. Through the next decade, catalysis will continue to provide attractive means to remove undesirable pollutants. Environmental catalysis is used to improve our environment as well as new and emerging catalytic solutions. Many major types of pollutants will be discussed with a focus on commercially applied processes using catalysis as a solution. Number of specific catalysis opportunities will be discussed as new perspective approaches to make clear our environment. The exchange of experience of researchers in different areas of environmental catalysis will help in the future to prevent further environmental pollution.



A handwritten signature in black ink, appearing to read 'Kukueva V', on a light gray background.

Kukueva V
Cherkassy State Technological University,
Ukraine

keynote speakers



Stanislaw Dzwigaj
Sorbonne Universites
France



Reza Shahbazian Yassar
University of Illinois
USA



Froidevaux Renéto
University of Lille
France



Claude de Bellefon
University of Lyon
France



Jose Antonio Diaz Lopez
Universidad Politecnica de Madrid
Spain



Q. B. Broxterman
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Eugenio Meloni
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Jian Zhi Hu
Pacific Northwest National
Laboratory, USA



John Zhu
The University of Queensland
Australia



M.V.Tsodikov
A.V.Topchiev Institute of
Petrochemical Synthesis RAS
Russia





About

MAGNUS GROUP

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

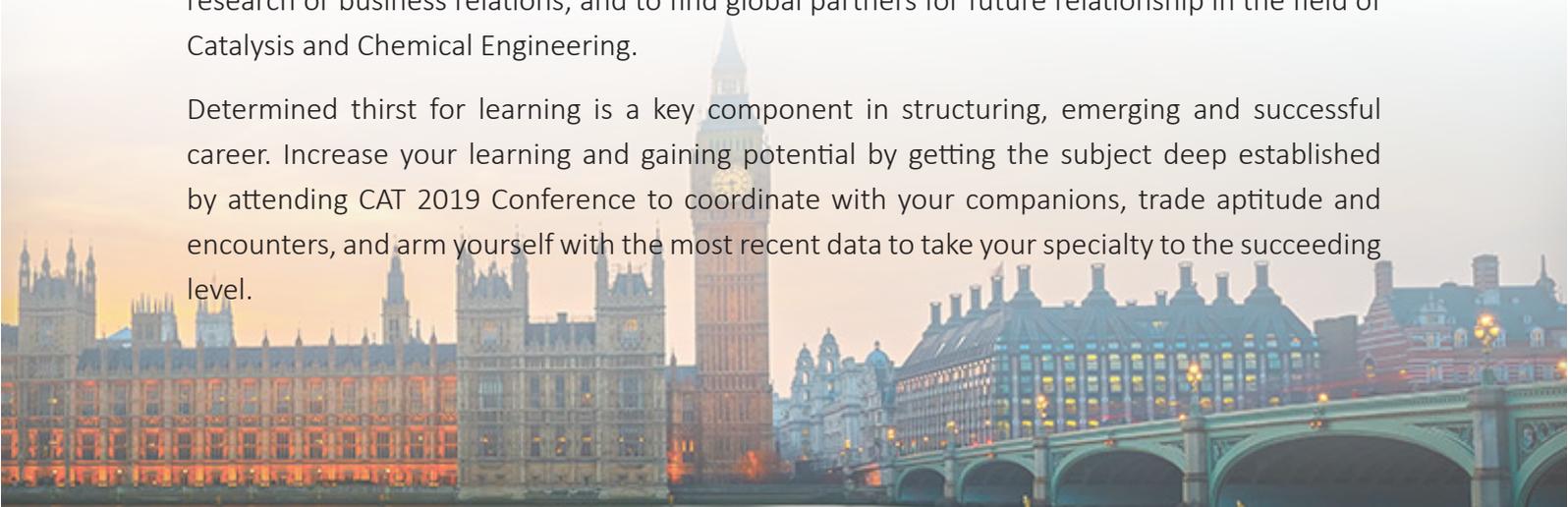
Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions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

About CAT 2019

On behalf of the Organizing Committee and Advisory Board, we take immense pleasure in inviting you to London, UK for the 5th Edition of Global Conference on Catalysis, Chemical Engineering & Technology during September 16-18, 2019.

CAT 2019 will be a platform to discuss a broad range of topics related to Catalysis and Chemical Engineering for the academicians, scholars, investigators, Chemical Engineering Researchers, industrialists and associated experts in the field of Catalysis and Chemical Engineering from all over the globe for sharing familiarity, exchanging ideas, collaborate and to showcase their research results about all features of their work and application experiences, to establish research or business relations, and to find global partners for future relationship in the field of Catalysis and Chemical Engineering.

Determined thirst for learning is a key component in structuring, emerging and successful career. Increase your learning and gaining potential by getting the subject deep established by attending CAT 2019 Conference to coordinate with your companions, trade aptitude and encounters, and arm yourself with the most recent data to take your specialty to the succeeding level.



ABOUT PUBLISHING PARTNER



catalysts

an Open Access Journal by MDPI

Catalysts (ISSN 2073-4344; Impact Factor: 3.465) is an open access journal of catalysts and catalyzed reactions published monthly online by MDPI, providing a rigorous and rapid peer-review. Manuscripts are peer-reviewed and a first decision provided to authors approximately 13.4 days after submission; acceptance to publication is undertaken in 5.5 days (median values for papers published in this journal in the second half of 2018)

/Catalysts/ has been indexed by the Science Citation Index Expanded (Web of Science), Scopus and other databases (<http://www.mdpi.com/journal/catalysts/indexing>) and has 100,000+ page visitors each month. According to web of science's data, the impact factor for /Catalysts/ 2017 is 3.465. The 5-year impact factor is to 3.873. Catalysts now ranks in Q2 of the "Chemical, Physical" category. According to Scopus data, CiteScore for /Catalysts/ 2017 is 3.23, which ranks in Q1 of the "Chemistry, Physical and Theoretical Chemistry" category, and Q2 of the "Chemical Engineering, Catalysis" category.

Publication Information:

CAT 2019 participants will receive a benefit of 25% waiver on article processing charges.

ABOUT PUBLISHING PARTNER



Emission Control Science and Technology is a forum for publication of the latest research on control of emissions from mobile and stationary sources.

- The only forum devoted solely to Emission Control Science and Technology.
- Competing publications are either in a different area [catalysis or environmental science] or are not peer-reviewed.
- Balanced mixture of rapid communications, research papers, and review articles.
- Broad appeal: market includes industry, government, and academia.

Papers are also welcome on various aspects of development and technology. The investigation may be experimental, theoretical, or computational.

- Examples of topics that may appear in the journal include:
 - Emission control in mobile (road, land, sea, air) and stationary (e.g. power generation, industrial processes) applications.
 - Materials for and formulations of novel substrates and catalysts, such as those used in Diesel Oxidation Catalyst (DOC), Three Way Catalysts (TWC), Diesel Particulate Filters (DPF), Selective Catalytic Reduction (SCR), Lean NO_x Trap (LNT), combined catalysts (e.g. DPF+SCR or DPF+LNT in one substrate), slip catalysts, or reformer catalysts.
 - Performance of emission control system components such as sensors, injectors for fuel and reducing species, exhaust inserts and mixers, etc.
 - Effects of operational parameters (e.g. flow, temperature, species concentration) and design approaches (sizing, layout, insulation, etc) on regulated and unregulated emissions and emission control system efficiency and performance.
 - Basic and applied research on specific components (e.g. nanoparticles, N₂O and other non-regulated pollutants) of emissions and their mitigation.
 - System considerations such as engine-out to tailpipe efficiency, optimization, PGM management, and formation of secondary species.
 - Engines, combustion, fuels, or lubricants as they would affect emission reduction technologies or post combustion processes.
 - Testing, durability and compliance such as cycles, certification, aging, NVH, in-field (on-vehicle) performance and analysis, and in-use compliance.
 - Analysis of current and future emission regulations (including those in the developing world).
 - Biological and environmental effects of emission control technologies.

Publication Information:

Conference Proceedings will be published in Emission Control Science and Technology for free as a Special Issue. All submissions will be subject to customary peer review of Emission Control Science and Technology before they are considered for publication.

DAY 1

KEYNOTE FORUM

5TH EDITION OF GLOBAL CONFERENCE ON

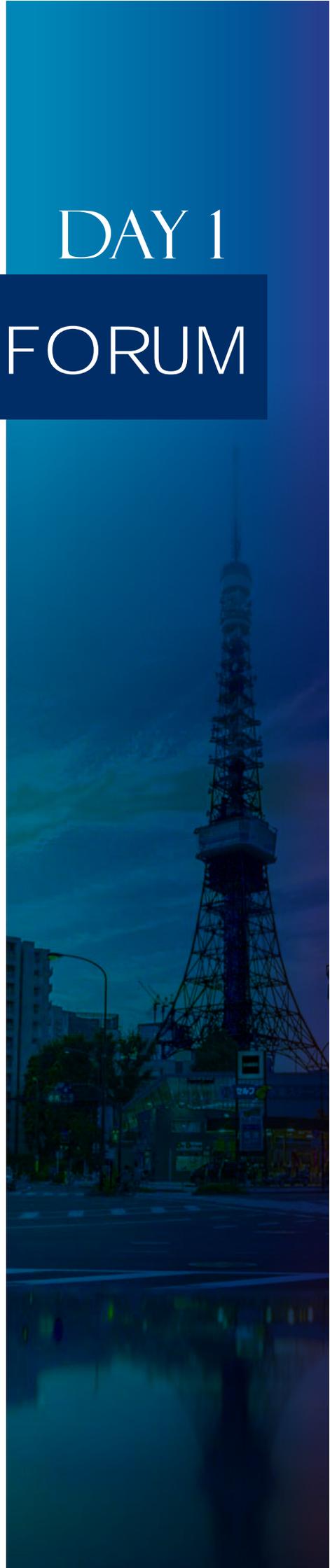
CATALYSIS,
CHEMICAL
ENGINEERING &
TECHNOLOGY

SEPTEMBER

16-18, 2019

LONDON, UK

CAT-2019





Biography

Professor Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris) he obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements he received the title of professor. His published work includes more than 160 papers published in reputable international journals.

Design of metal single-site zeolite catalysts for application in industrial and environmental catalysis

Stanislaw Dzwigaj

Sorbonne Université-CNRS, Laboratoire de Réactivité de Surface, Paris, France

The metal ions well dispersed at zeolite framework are considered to be active sites of catalytic processes. However, the incorporation of these metals into the zeolite materials as well dispersed metal species appears to be the important challenge. 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 Plenary Talk the design of new single-site zeolite catalysts with transition metal species will be described and characterized by different physical techniques both at the macroscopic level (chemical analysis, XRD, BET, thermal methods (TPR, TPO, TPD), TEM) and molecular level (FT-IR, NMR, diffuse reflectance UV-Vis, XPS, EPR, XAFS). The application of single-site zeolite catalysts in different catalytic processes important in industrial and environmental catalysis such as oxidative dehydrogenation of propane into propene, epoxidation of propylene into oxide propylene, selective catalytic reduction of NO_x to N₂, production of 1,3-butadiene from renewable sources, including ethanol obtained from biomass will be discussed. This two-step postsynthesis method applied in this work allowed obtaining single sites zeolite catalysts with mononuclear metal species active in above mentioned processes. Their catalytic activity strongly depends 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

Reza Shahbazian-Yassar is a professor of Mechanical and Materials Engineering at the University of Illinois at Chicago. He received his PhD in Materials Science from Washington State University in Pullman, WA, and served 7 years at Michigan Tech as chair associate professor of nanotechnology. He has published more than 160 papers in journals such as Science, Nature Nanotechnology, Nature Communications, Advanced Energy Materials, Nano Letters, and many more. He was the President for Midwest Microscopy Society, a member of Steering Committee for ASME NanoEngineering for Energy Committee, and the former chair of the Advanced Characterization, Testing, and Simulation (ACTS) Committee at The Materials Society (TMS). He is also on Editorial Board for Metallurgical and Materials Transactions A (MMTA).

In-Situ TEM studies of chemically-complex alloy catalysts

Reza Shahbazian-Yassar

University of Illinois, USA

The field of catalytic science has emerged toward new nanoparticulate materials with novel chemical compositions. This presentation will encompass the PI's efforts on in-situ transmission electron microscopy of novel nanoparticle alloys with applications in catalysts. For these studies, we utilized aberration-corrected TEMs with capabilities to resolve the atomic positions at <1 Å resolutions and chemistry at <0.4 eVs. To perform in-situ TEM, we studied the nucleation and growth of nanoparticles on liquid solutions in real time using fluidic specimen holders. Interestingly, we observed that the atomic structure of 2D materials significantly affect the crystal structure of in-situ grown Au nanoparticles. We have shown the core-shell Au-Pt nanoparticles have novel structural properties when templated on two-dimensional (2D) materials. We studied the structural and chemical transformations within these materials under elevated temperatures and gas environment. In addition, the atomic resolution studies of chemically-complex alloys provide new opportunity to correlate the structure and chemistry of catalysts with their performance.



Biography

He received his PhD degree in 2001 at the University of Lille. Now he is professor in Enzyme Engineering and Biotechnology at the same institution in the Charles Viollette Institute. He started his career in bioactive peptide production by enzymatic way and the development of reactors. From 2014, he works on the development of "hybrid catalysis" concept, resulting in the combination of bio- and chemo-catalysis. He is leader of a team in Biotechnology/Biotransformation which is a constituent team of Viollette Institute. He has been coordinator of national projects on hybrid catalysis development (2015-2018 GENESYS; Program Research 2016-2018 with IFMAS). He is partner of BIOHEC project (European project Life+, 2016-2020) for biodiesel production from cooked oils. He is part of the user Committee of REALCAT platform. 6PhD already supervised, 4PhD ongoing, 4 postdoctoral already followed. He has published more than 35 publications in peer review journals, 2 book chapters, 1 patent.

From sequential chemo-enzymatic approach to integrated hybrid catalysis: Concept and examples

Renato Froidevaux

Univ. Lille, INRA, ISA, Univ. Artois, Univ. Littoral Côte d'Opale, EA 7394 - ICV - Institut Charles Viollette, F-59000 Lille, France

Efficient and eco-responsible valorization routes for renewable carbon source are highly desirable, and every field of catalysis should be mobilized as the key to success for a selective valorization of such a polyfunctional substrate. Biocatalytic processes are already or about to be industrialized and heterogeneous or homogeneous catalysis, alone or in combination, have shown high efficiency for biomass valorization, but lack of selectivity still causes problems in the products separation steps. In the very last years, a new paradigm of catalysis has emerged to answer the challenges of selectivity and productivity by combining biocatalysis and chemocatalysis. Indeed, in a conventional approach, biotechnologies and chemocatalysis are sequentially processed. However, recently, successful one-pot transformations have been realized, simultaneously taking advantage of both technologies, under the concept of the so-called 'hybrid catalysis'.

In this context, we propose two new conceptual pathways involving hybrid catalysis to overcome limitations resulting from the enzymatic glucose isomerase thermodynamic equilibrium between glucose and fructose, which is a key step when subsequently targeting HMF as a product. These concepts are based on a complexation/transport strategy and a hybrid isomerization, respectively. Both combinations are relatively simple to achieve and the first results validate the proof of concepts in both cases: (1) The limitations resulting from the enzymatic glucose isomerase thermodynamic equilibrium between glucose and fructose has been actually overcome with a glucose conversion of 70%, while it is limited to 46%, without fructose transport; (2) Concerning the valorisation via sorbitol, we demonstrated the chemical compatibility between sorbitol dehydrogenase and an organometallic complex used for the cofactor regeneration and ca. 2 cofactor regenerations by the chemocatalyst can be observed. However, the pH zones of the enzyme and the organometallic complex seems to be conflicting to enable reaching high yields. A modification of one of both catalysts could extend the pH zone toward the zone of the other catalyst.

Audience Take Away:

Our approaches can be applied to other reactions of interest in the context of biomass valorization, and even, in other fields of chemistry and biotechnology. One-pot bio- and chemocatalytic processes have an important role to play in future technologies, especially with a large potential for converting biomass to value-added chemical products, using a minimal number of steps in a selective and productive fashion, thus playing an important role in building a more sustainable chemical industry.



Biography

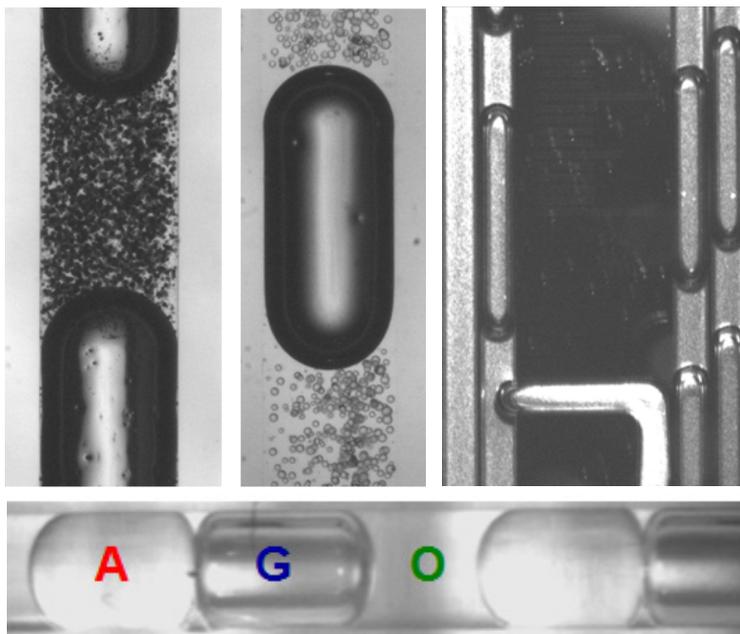
After a PhD at the University of Strasbourg and two fellowships (NSF at PennState USA, AvH at TU Munich) to work on organometallic chemistry, Claude de Bellefon received a research fellow position at CNRS Strasbourg. He then moved to industry as associate researcher at Rhône-Poulenc (Lyon) to develop catalytic hydrogenations. In 1995, he founded the Catalytic Process Engineering team at CPE Lyon, the School of Chemistry and Chemical Engineering, University of Lyon. He is a Research Director at CNRS and the Scientific Director of CPE Lyon. His main research interests are multiphase reactors, homogeneous heterogeneous catalysis, micro-structured reactors, flow-chemistry, and process intensification.

Catalysis in segmented flow from lab scale to production

Claude de Bellefon

Catalytic Processes Lab, CPE Lyon, CNRS UMR5285, University of Lyon, Lyon, France

Flow chemistry is a rapidly developing technology that enables batch-to-continuous synthesis from the lab scale to industrial production. Monophasic flow, including liquid flow through a fixed bed of solid (cartridge), is the dominating contacting motion since most of the chemistry is monophasic, or performed with a solid which in general is the catalyst. However, segmented flow – also called Taylor flow – is largely used when two fluid phases – one phase being a liquid, the other being either a gas or a liquid – are used. Segmented flow develops as a train of bubbles (droplets) in a continuous liquid phase when the size of the bubbles (droplets) is close or larger than the diameter of the reactor. Thus, segmented flow could typically be observed in small tubes or capillaries found in many flow chemistry equipment's such as those commercialized by Syrris, Vapourtech, Kobelco to name a few. The very specific fluid motions of Taylor flow lead to very efficient properties such as mixing and mass and heat transfer. Furthermore, more than two fluid phases could be contacted and solids could also be transported at quite high loadings. Such versatility opens the field to many applications in catalysis and material synthesis. During the lecture, beside the basic hydrodynamic properties of segmented flow, many possible utilisation of segmented flow for performing catalysis and material synthesis will be presented in particular solutions to use solids and gas-liquid or liquid-liquid mixtures. Examples were solid catalysts are transported as slurry for hydrogenation reactions, or examples were segmented flow is combined with the properties of Open Cell Foams (OCF) as catalyst supports for the very exothermic hydrogenation of terpenes will be presented. Very exothermic and fast O₂ oxidations of organics are also performed in segmented flow with scale-up example to several kg. Last, the synthesis of metallic nanoparticles of Ru and RuCu without ligands and with very interesting size and size distribution could also be performed in hydrogen-ionic liquids segmented flow. Finally, segmented flow could also be used to operate several cascades catalysis using the droplets as milli-reactors.



Examples of segmented flow (a) H₂-water- 50 g/L Ni/SiO₂ (b) G/L/beads (c) O₂-cyclohexane at 30 bar, 200°C (d) Aqueous-gas(H₂)-Organic (hexane) G/L/L flow.

Audience Take Away:

- Develop flow processes rather than batch and learn about advantages and drawbacks of segmented flow-catalysis.
- The lecture will help the audience in their job with many examples with diverse catalysis, homogeneous or heterogeneous, and also producing nanoparticles using segmented flow.
- Continuous production at the lab scale can help solving research scale-up issues to produce gram quantity of new materials / active principle. Also, it can be implemented for teaching practicum.
- Continuous production is a tool to improve production, in quantity and quality (selectivity). Practical solutions and commercial reactors will be commented, including mass and heat transfer issues.

SPEAKERS

5TH EDITION OF GLOBAL CONFERENCE ON

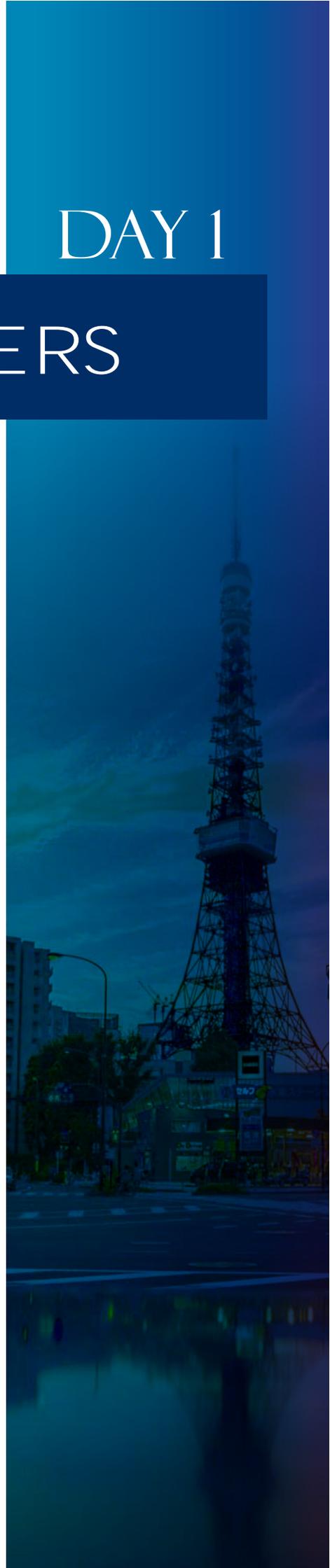
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Hydrogen from clean biogas: A proof of concept of integrated process

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The steam reforming (SR) of natural gas plays a key role in the production of syngas ($\text{CO} + \text{H}_2$) or H_2 , widely used to produce chemicals, fuels or energy. However, the depletion of fossil fuels and the increasing environmental constraints, have in the last decades prompted the attention towards renewable fuels. The main candidate to replace the natural gas (NG) is the biogas obtained by anaerobic fermentation of organic wastes or not edible biomass that, after removal of most pollutant compounds, is a mixture of CH_4 and CO_2 (clean biogas or CB) in variable amounts (35-50 vol.%). Currently CB is used to produce energy in cogeneration plants or biomethane (by CO_2 SWAP) to be introduced in the NG distribution grid. The Dry Reforming (DR) may potentially convert both CH_4 and CO_2 , although the many drawbacks (high reaction temperature and catalyst deactivation) limit its commercialization. Steam Reforming (SR) is an attractive option, although the CO_2 fraction is barely converted in presence of high steam contents, decreasing the overall productivity. A promising upgrading is represented by the combined S/DR process, in which by controlling the amount of steam fed it is possible to limit catalyst deactivation and obtain syngas directly suitable for downstream applications as hydrocarbon or methanol synthesis. The syngas may be further upgraded through the Water Gas Shift (WGS) reaction, that allows to tune the H_2/CO ratio or to improve the H_2 production, developing an integrated process. Aim of this work was to proof this idea by developing new Ni-based catalysts and Cu-based catalysts, prepared by controlled calcination of hydrotalcite-type (HT) precursors, to be investigated in S/DR of CB or WGS of the obtained syngas. The catalysts were deeply characterized before and after the tests to collect useful information to improve the performances by tuning catalyst composition and properties.

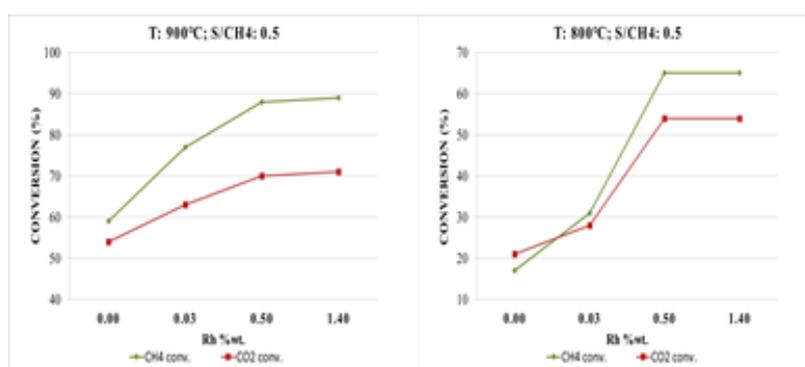


Fig. 1. CH_4 and CO_2 conversion as a function of the Rh content and reaction conditions

A Ni-Mg-Al (Ni 10 wt.%) was used as benchmark evidencing a low activity together with a fast deactivation due to carbon formation and/or NiO reoxidation. The addition of very small amounts of Rh gave rise to a significant increase of activity and stability with time-on-stream, regardless of the reaction conditions adopted (Fig. 1). The H_2/CO molar ratio of the outlet stream was between 1.2-2.7 as a function of the temperature and amount of steam fed. Adding a further WGS step at high (HTS) or, better, medium (MTS) temperature it was possible to increase the H_2 -content in the outlet stream, lowering the CO content in the outlet stream to < 1.2 vol.%. The data collected support the conceptual idea of a process, integrating S/DR and WGS steps, with a configuration leading to advantages in the energy balance of the process and decreasing the capital and operational expenditures (CAPEX and OPEX).

Audience Take Away:

- Clean biogas as valuable alternative to Natural Gas produce syngas or H_2
- Advantages of the combined Steam/Dry Reforming process
- An integrated process to improve the hydrogen productivity
- To tune the H_2/CO ratio as a function of the downstream applications

- Hydrotalcite-type phases as useful precursors of multicomponent catalysts.

Biography

In 1972, Prof Vaccari graduated in Industrial Chemistry with honors at ALMA MATER STUDIORUM – University of Bologna, where he was Assistant Professor, Associated Professor, from 2002 Full Professor of Industrial Chemistry and from 2006 to 2018 Head of the Department. Awards: 1993 Italian Federation of Chemical Industries; 1996 Italian Catalysis Group; 2004 Professor HC of the Universidad del Litoral (Arg); 2010 Gold medal “P. Pino” of the Italian Industrial Division; 2011 Chemical Engineering Club; 2018 Silver Plate “G. Fauser” of the of Italian Catalysis Group. He is author of 270 papers, 270 Congress Communications and 20 Patents (16 EU or WO), with H-index = 43 and 11,120 citations. Active in the R&D of new catalytic processes of economic and environmental relevance, he has been Task and/or Team Leader of 7 EU Projects, Coordinator of 2 National Projects, and Team Leader of many National and International Projects in collaboration with Research Institutions or Companies. He is member of the Editorial board of Applied Clay Science and was Guest-Editor of 4 Special Issues of Applied Clay Science, 4 of Catalysis Today and of the book “Natural Conversion V”, Studies in Surface Science and Catalysis, Vol. 119.

Room temperature reduction of carbon dioxide using localized surface plasmon energy

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World's increasing energy demand can be easily met by the fossil fuel reserves for next several decades without an impact on environments if the carbon dioxide (CO₂) emission can be reduced or mitigated. Photocatalytic conversion of CO₂ to useful chemicals is an attractive option but not practical yet due to low conversion rate and high cost of precious metal catalyst used. Here, we show that localized surface plasmon (LSP) resonance energies of aluminum (Al) plasmonic nanoparticles, excited by high energy electrons, can be used to reduce CO₂ by carbon at room temperature according to the reverse Boudouard reaction: CO₂+C → 2CO. Al nanoparticles, with diameters ranging from 30 nm to 300 nm, were loaded on either amorphous carbon film or polycrystalline graphite support and introduced in an environmental transmission electron microscope (ETEM), equipped with a monochromated electron source (80 meV energy resolution) and operated at 80 kV, to excite Al LSP resonance modes, and characterize the CO₂ reduction rate based on the measured carbon etching rate. In CO₂ environment of ≈ 50 Pa, the carbon etching was observed near Al nanoparticles at a rate that is ≈ 10 times faster than in the regions away from the particles when irradiated by the same electron beam flux. Electron energy-loss spectroscopy was used to measure the thickness reduction of graphite around the Al particles to obtain the net carbon etching rate due to the energy provided by LSP resonance. Carbon etching rates were also obtained as function of the number of Al nanoparticles, CO₂ pressure, and LSP resonance amplitude. A complete analysis of mechanism and scalability details will be presented. Potentially the reduction can be achieved using sunlight to excite LSP resonances on Al particles and that will make this cost-effective process scalable at industrial level requiring only sunlight and earth-abundant Al and C for CO₂ reduction.

Audience Take Away:

- We show LSP resonance energies of plasmonic nanoparticles may replace thermal energy to achieve room temperature reactions.
- Fast (high energy) electron can be used to simultaneously excite all available LSP resonance modes on a plasmonic particle.
- Al is earth abundant and cheap plasmonic metal with LSP resonance energies spanning from visible to deep UV range and is ideally suited to achieve room temperature reactions.

Biography

Dr. Renu Sharma received a B.S. and B.Ed. in Physics and Chemistry from Panjab University, India; M.S. and Ph.D. in Solid State Chemistry from the University of Stockholm, Sweden. Renu came from Arizona State University to National Institute of Standards and Technology in 2009, and is currently a Project Leader in the Nanoscale Imaging Group. Renu has been a pioneer in the development of environmental scanning transmission electron microscopy (E(S)TEM), combining atomic-scale dynamic imaging with chemical analysis to probe gas-solid reactions. She is Fellow of Microscopy Society of America, has given over 90 invited presentations, published 5 book chapters and over 200 research articles.

Catalytic hydrogen release from Amine-Boranes

Veeranna Yempally, Salvador Moncho, Edward Brothers, Ashfaq Bengali*

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The reaction of a bidentate pyrrole based rhenium tetracarbonyl complex (**1a**) with dimethylamine borane at room temperature results in rapid dehydrogenation. Hydrogen generation was detected at temperatures as low as 238K and NMR spectroscopy provided evidence for the initial formation of a Re-H-B bound adduct at these temperatures. The rate of the dehydrocoupling reaction was significantly influenced by the electron density on the metal center and the identity of the alkyl group (CH₃ or CF₃) on the ketone carbon of the pyrrole ligand. Thus, increasing the electron density on the metal center by substituting the acid CO ligand with donor groups resulted in significantly decreased reactivity while replacement of the electron donating CH₃ group on the ketone carbon with CF₃ yielded a ten-fold reduction in reaction rate. DFT calculations supported the experimental findings and suggested that the overall reaction occurs in three main steps to include, de-chelation of the organic carbonyl group from the metal center and coordination of the amine-borane to the resulting vacant site, activation of the B-H and N-H bonds, and finally metal mediated heterolytic coupling of H⁺ and H⁻ to yield H₂. The bifunctional nature of **1a** incorporating both an acidic Re center and basic oxygen center, coupled with the hemi-lability of the organic carbonyl group, are key motifs of this catalyst that result in efficient thermal dehydrogenation of dimethylamine borane.

Audience Take Away:

- Utility of organometallic complexes in catalyzing organic transformations.
- The feasibility of using amine-boranes as hydrogen storage materials
- Identification of key molecular characteristics that result in an efficient metal based catalyst

Biography

Dr. Ashfaq Bengali is currently professor of chemistry at Texas A&M University at Qatar. He received his Ph.D from the University of Minnesota and completed his postdoctoral training at the University of California-Berkeley and Los Alamos National Laboratory. His expertise is in the application of time resolved infrared spectroscopy to study the photo-induced chemistry of transition metal based organometallic complexes. He has published over 60 papers in high-impact peer reviewed journals of chemistry.

Production of hydrogen by catalytic partial dehydrogenation of a commercial fuel for HT-PEM fuel cell applications

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Hordes³

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Integration of fuel cell systems in electrified transportation calls for the development of efficient processes for high purity hydrogen supply. Partial dehydrogenation of liquid fuels has recently emerged as a transition technology for hydrogen delivery purposes. The reaction is carried out on a complex mixture of hydrocarbons and the principle is to extract from fossil fuels a small fraction of the available hydrogen, which is used by the fuel cell, while the dehydrogenated hydrocarbon mixture retains suitable properties for its use as a fuel in a combustion engine. The challenges lie in improvement of hydrogen productivity without detriment to the purity of the hydrogen generated, which requires development, optimisation and scale-up of advanced catalysts, as well as process optimisation. The choice of the catalyst is crucial for the partial dehydrogenation process; it must produce H₂ without compromising the original fuel properties. An ideal catalyst must be sulfur tolerant, generate sufficient hydrogen of high purity, be selective to dehydrogenation and avoid cracking reactions responsible for coke deposition and catalyst deactivation

The partial dehydrogenation (PdH) of a commercial gasoline (SP95E10) was carried out in a continuous flow reactor at 370°C and 8 bar. The catalyst used was 1 wt% Pt-1 wt%Sn-0,5 wt% In supported on alumina prepared by a sol-gel technique, and the active phase was added by incipient wetness impregnation. This catalytic material showed a very good activity and high selectivity, leading to a gas production of 2300 NL/h-kgcat with 99% hydrogen purity and very low amounts of CO and methane.

The hydrogen produced was fed to a HT-PEM fuel cell operated at 160 °C. At a current density of 200 mA/cm² the performance of the fuel cell with the hydrogen produced by partial dehydrogenation was close to that obtained with pure hydrogen. The complete recovery of performance to that with pure hydrogen indicates the absence of any irreversible catalyst poisoning effect when using the PdH hydrogen, and no voltage loss over a 13 h period of measurement.

Audience Take Away:

- Catalytic partial dehydrogenation of hydrocarbons can provide enough hydrogen of high purity, free of CO and CO₂, to feed a fuel cell.
- The partial dehydrogenated hydrocarbon maintains its original fuel properties with the requisite specifications to be used as jet fuel.
- The partial dehydrogenation of hydrocarbons is a transition technology toward more electrified ways of transports.
- Hydrogen production is possible at distribution sites (storage and distribution) and on-board vehicles for supply of electrical energy to auxiliary systems.

Biography

Rafael Garcia Garrido studied Chemical Engineering at the University of Málaga, Spain and graduated in 2015. After that, he started a Master degree in Chemical Engineering at the University of Málaga. During his second year of Master he joined the research group of Prof. Yeung in the department of chemical and biological Engineering, Hong Kong University of Science and Technology. He received his Master degree in 2017 in the University of Málaga. He joined the research group of Prof. Jones as a phd student in the Institut Charles Gerhardt, Montpellier, France.

Design for Recycling: Catalyst and support materials in energy storage systems

Annukka Santasalo-Aarnio

Assistant Professor, Department of Mechanical Engineering, School of Engineering Aalto University, Finland

In order to provide the human kind energy but simultaneously mitigating the climate change the share of renewable energy production must be increased. To balance the intermittence renewable energy production, various different energy storage systems have been proposed such as lithium ion batteries and electrolyzers. Additionally, also fuel cells that would convert the chemically stored energy back to electricity with high efficiency would come to the market. All of these before mentioned applications include scarce and/or very expensive metal materials. As their volume increase significantly, there is a concern where these critical elements required as their catalyst will be obtained and therefore, their recovery from the end of life devices is at high importance.

Currently, the catalysis research has been focusing on a design-for-performance approach where variety of exotic, high cost metal elements has favored. In addition, the research trend has been towards nanomaterials, alloys, hybrid materials and ultra-thin coatings to decrease the amount of these raw materials in each application. However, at the same time, their recovery becomes impossible and less economically feasible. This is contradictory with the aim for design-for-recycling where the selected raw materials are design in a way to facilitate their recovery at the end of life products. This speech addresses these phenomena, and how research community should address them while planning the new material solutions to the energy storage devices.

Biography

Prof. Santasalo-Aarnio completed her doctorate in physical chemistry with the catalyst and support material development for fuel cells at the Aalto University School of Chemistry 2012. After this she continued her work with a post doc project on solar energy storage for H₂ with bench-scale SO₂ depolarized electrolyser. She obtained a university lecturer position for material science and engineering 2015 where she has been involved in recycling of energy devices such as lithium-ion batteries and fuel cells. With the strong collaboration with Helmholtz institute, she has developed new insight in how to take into account recyclability in the planning phase of energy storage solutions. She was appointed as assistant professor of energy conversion and storage at the school of engineering in September 2018 where she will continue the work on renewable energy interaction to energy policy.

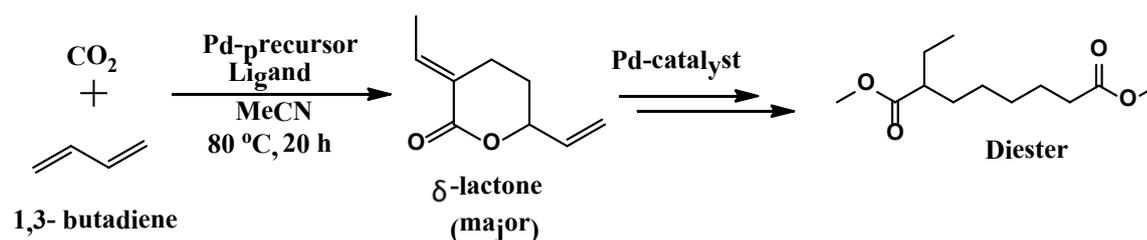
Catalytic CO₂ valorisation to building block molecules

Soyeb Pathan,¹ Francesco Ferretti,² Muhammad Sharif,² Ralf Jackstell,² Muhammad Anwar,¹ Sreekanth Reddy Pogula,¹ Sarim Dastgir,¹ Matthias Beller²

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²Leibniz-Institut für Katalyse e.V. an der Universität Rostock, A.-Einstein-Str. 29a, 18059, Rostock, Germany.

Valorisation of CO₂, an abundant C-1 feedstock, to platform chemicals could contribute to support the goals of energy transition, and reduce environmental impact and carbon footprint. Although significant advances have been made in the area of CO₂ transformation to valuable organic compounds, however the more challenging as well as complicated selective syntheses have recently become a subject of increasing attention. However, due to inherent thermodynamic stability of CO₂, the development of suitable catalytic systems for the desired transformations is vital for its activation.



Scheme 1. CO₂ valorisation to diesters via δ-lactone pathway

In consideration of the above aspects, palladium and chelating phosphine ligands based- catalytic systems were developed for CO₂ valorisation (Scheme 1). The influence of various phosphine ligands were studied in the presence of Pd(acac)₂ to develop superior catalytic system compared to the known systems, for synthesis of δ-lactone from 1,3-butadiene and CO₂ in high selectivity and yield. Further, in order to valorize δ-lactone to other monomers, catalytic system was developed for the alkoxy-carbonylation of δ-lactone to produce novel unsaturated diesters. Moreover, these unsaturated diesters were selectively hydrogenated to saturated or mono-saturated diesters, or 2-ethyloctane-1,8-diol which provide new opportunities for synthesis of novel building blocks for functional materials and renewable polymers. Preliminary results towards heterogeneous catalyst material development will also be presented.

Acknowledgement:

Financial support from Qatar National Research Fund, A member of Qatar foundation, Qatar (Grant Numbers NPRP9-212-1-042, & NPRP8-235-1-055), is gratefully acknowledged. The Core Lab of QEERI and analytical department of LIKAT are also acknowledged for the analytical support.

Designing photocatalyst nanostructure for enhanced photon-to-conversion efficiency and hydrogen production

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As well as direct energy conversion in solar cells, sunlight can be used as the energy source for water depollution or hydrogen production. These two are inexorably linked as both use photocatalysis as their energy conversion mechanism. Photocatalytic depollution of water has attracted great attention and many studies have been published in the last decade; however, improving photocatalytic efficiency, as well as making the process industrially viable remains challenges. Additionally, the conversion of water to hydrogen fuel using photocatalysis is one of the most promising strategies for industrial-scale production.

Titanium dioxide is by far the most popular photocatalyst; it is cheap, inert and reasonably active. However, TiO_2 has a large band gap (3.2 eV for anatase and 3.0 eV for rutile) can only be excited by UV light, which lower the solar energy conversion efficiency and limit its use in the visible range (small absorbance factor). Therefore, engineering the architecture of the plasmonic photocatalyst in core-shell or 3D photonic crystals leads to the enhancement of light harvesting properties and improved photon-to-energy conversion for hydrogen production. In core-shell nanostructure, the photocatalyst behave as a photonic “NanoLens” mimicking the focusing of light observed for the lens-like epidermal cells. Thus, the core-shell nanostructure acts as a convex nanolens to reinforce the electromagnetic field at the nanostructure surface. Designed in photonic film with chiral nematic structure the mesoporous structure with a 3D architecture, titanium dioxide showed improved efficiency of the conversion of light to energy.

The material was characterized by means of different techniques, such as BET, WAXS, polarized optical microscopy, UV-Visible spectroscopy, TEM and Time Resolved Microwave Conductivity (TRMC). TRMC results show an improvement of the charge carrier density produced under illumination at the photocatalyst surface. This strategy enables to avoid the use of higher amount of Nobel metal to reach higher efficiency of photocatalytic production of hydrogen

Audience Take Away:

- New photocatalyst conception: synthesis and design
- Dynamic of photogenerated charge carriers assessment
- Photocatalytic hydrogen production

Biography

Dr. Ghazzal studied inorganic Chemistry at the “université Claude Benard de Lyon”, France. He received his PhD in 2008 at the “université Paul Verlaine de Metz”, France. After one year as an assistant professor, he went as a postdoctoral fellowship at the Institute of Condensed Matter and Nanosciences - université catholique de Louvain”, Belgium. He moved as a researcher in the “université de Namur” and, then at the “université de Mons” working as a senior researcher in the Laboratory of Surface and Interfacial Physics, Belgium. In France, he obtained a permanent position of an Assistant Professor at the “Laboratoire de chimie physique-université Paris-Sud/université paris-Saclay”. She has published more than 20 research articles in peer-reviewed journals and 2 patents.

Chemistry of graphene: Adsorption of CO at pristine, doped and defected supported graphene

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Due to its electrical properties graphene (G) has been successfully used as a sensing element for the detection of different gases reaching very high sensitivities (ppm or better), which are ascribed to the doping induced by adsorption. The sensitivity depends critically on the chemical nature of the gas and is lower for CO than for other poisoning species. The nature of the active sites is, however, still unclear. The value of the heat of adsorption determines the sensitivity and the range of temperatures at which the sensor can operate. In order to clarify these issues we investigated experimentally adsorption of CO on G supported on polycrystalline Cu and on Ni(111) by HREELS and XPS.

No signature of adsorbed CO was found after exposure both at RT and at 100 K for G/Cu, while chemisorbed CO was observed after just a few L at 100 K for G supported on Ni(111). This result indicates that the nature of the substrate plays an essential role in the adsorption process. The heat of adsorption is estimated to be ~0.58 eV/molecule at low coverage, so that equilibrium coverage of ~0.1 ML is expected at RT under a CO partial pressure of only 10 mbar. We identify top-bridge graphene as the most reactive co5.

Doping G/Ni(111) by N₂⁺ ion bombardment allows for the formation of a second, more strongly bound moiety, characterized by a CO stretch frequency of 236 meV and by an initial heat of adsorption (0.85 eV/molecule). The presence of N (in pyridinic or substitutional sites) enhances therefore significantly the chemical reactivity of G/Ni(111) towards CO.

We also investigated the role of isolated defects, which were created by low energy Ne⁺ ions bombardment on single layer graphene supported on different substrates (polycrystalline Cu and Ni(111)). We find that no CO adsorption occurs for defected Graphene (G^{*})/Cu, while vibrational signatures of the presence of CO are observed for G^{*}/Ni(111). Two moieties, desorbing just above 350 K, are present under vacuum conditions after exposure at RT. The frequency and the relative intensity of the observed vibrational features indicate that CO chemisorbs at the G/Ni(111) interface close to the vacancies rather than at the defected G layer. The red-shift of the C1s binding energy suggests that in such regions detachment of the G layer from the substrate occurs.

Unfortunately defects of G/Ni(111) are not a good candidate as active sensing site since amending of vacancies occurs, as demonstrated by the reduction of the adsorbed coverage in subsequent CO doses followed by annealing at 380 K. We suggest that a Boudouard reaction involving two intercalated CO molecules take place under graphene cover, producing CO₂, which desorbs, and C, which repairs the vacancy

Audience Take Away:

Surface Science experimental investigation of the chemical reactivity of graphene

- Role of the substrate in determining the reactivity of the Carbon layer
- Role of defects in repairing the damage in graphene layer
- Estimate the sensitivity of a possible detector

Biography

Dr. L. Vattuone graduated in Physics in 1990 and received his PhD in 1994 at the University of Genova, Italy, under the supervision of prof. Mario Rocca. In 1995 he joined the Department of Chemistry of the University of Cambridge as a post-doctoral Research Associate (supervisor Prof. Sir David A. King). From 1996 to 1999 he was a post-doc in the University of Genova and in INFN. In 1999 he was appointed as Staff Researcher at the University of Genova and in 2012 he became Associate Professor of Condensed Matter Physics. He co-authored more than 110 papers (see <http://orcid.org/0000-0003-3718-6470>)

Diesel fuel adulteration issues in Nigeria

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The non-standard refining and sale of adulterated diesel fuel is a major challenge facing the people of the Niger Delta Region of Nigeria. This problem is associated with engine performance issues, environmental pollution and loss of substantial revenue to the government. Adulteration detection in diesel fuels is very complex because the adulterants are compounds that are already present in the fuels. For this study, six different samples of non-standard refined diesel fuel were collected from local refineries in the creeks of the Niger Delta and a sample from government retail outlet. The samples were analysed for their physicochemical properties such as density, cetane index, distillation properties of the fuel, flash point, pour point, Kinematic viscosity, calorific value and water content. An Agilent 7890B coupled to an Agilent 5977B Mass Selective Detector was used to determine the concentration of Volatile Organic Compounds (benzene, toluene, m-Xylene, p-Xylene and o-Xylene) in each sample whilst a LECO CHN628 was used to determine the elemental analysis of the samples. The results indicate a large fluctuation in physicochemical properties. The flash point of all non-standard refined samples was below 30°C, while the commercial diesel from government retail outlet had a flash point of 65.5°C. All locally refined samples had very high pour points and a very high concentration of volatile organic compounds (VOC) compared to commercial diesel fuel from the government retail outlet. All test were carried out according to ASTM designations D975-19a, ASTM D6304-A, ASTM D5950, ASTM D4057-18, IP 123, IP 365, IP380 and IP 71.

Audience Take Away:

- Non-standard refined diesel samples from Nigeria, will have issues with classification, storage and transportation as a result of their very low flash points
- The high water content in lead to microbial growth during storage
- The high content of free water in some samples can react with other chemicals in the fuel to cause corrosion
- GC/MS analysis showed very high concentration of volatile organic compounds (Benzene, Toluene, m-Xylene, p-Xylene and o-Xylene) that are dangerous to the environment

Biography

Oyinkepreye Lucky Bebetidoh studied Marine Engineering at the Rivers State University, Nigeria where he graduated with a BSc in 1997. He worked in the private sector as a marine engineer from 1998 through to 2008. In August 2008 he joined the Niger Delta University, Nigeria as a Principal Engineer in the Estate Department. In 2012 he proceeded to Coventry University in the United Kingdom where he obtained his MSc in 2013. On his return back home he converted to the Academic cadre, where he became a Lecturer in the Department of Marine Engineering. He is presently studying for his PhD in Marine Technology at Newcastle University, Newcastle upon Tyne, United Kingdom.

Effect of the electronic state of Cu, Ag, and Au on diesel soot abatement

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¹Instituto de Ciencias, Benemérita Universidad Autónoma de Puebla, Puebla, México

²Instituto de Física, Benemérita Universidad Autónoma de Puebla, Puebla, México

³Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla

Noble metals such as Au, Ag and Cu supported over semiconducting ZnO are well-known heterogeneous oxidation catalysts. All of them have been utilized for the oxidation of diesel soot with varied success. However, Au-supported ZnO is seen to be superior among them. Here we present a comparative study of all these three catalysts for diesel soot oxidation, to explain why Au/ZnO is the best among them, demonstrating the contribution of electronic states of metals in composite catalysts. The electronic states of Cu, Ag, and Au determined by X-ray photoelectron spectroscopy (XPS) on 1wt%Cu/ZnO, 1wt%Ag/ZnO, and 1wt%Au/ZnO catalysts were correlated with their diesel soot oxidation activities. Although all three catalysts present reasonable diesel soot oxidation activities at relatively low temperature, while 1%Cu/ZnO and 1%Ag/ZnO oxidize only about 60% of the deposited diesel soot around 250°C, 1%Au/ZnO oxidizes 100% of the deposited diesel soot, at temperature as low as 230°C. The activity of the catalysts is attributed to the formation of stable $M^0-M^{\delta+}$ bifunctional catalytic sites at the metal-ZnO interface, which enhances the contact efficiency of solid diesel soot on $M^{\delta+}$ and generates superoxide species on M^0 moieties. The stability of the bifunctional $M^0-M^{\delta+}$ sites is controlled by the electronic interactions between the metal (M) and n-type semiconductor ZnO at their interface. Very high activity of 1%Au/ZnO is attributed to the presence of Au^{3+} at the catalyst surface which generates a stronger coulombic force with diesel soot electrons. We demonstrate a direct relation between the diesel soot oxidation activity of these three metals and their electronic states at the catalyst surface.

Audience Take Away:

- In this investigation, we demonstrated that the simple preparation method, high activity, and high stability of the Au nanoparticles in diesel soot oxidation presented in this study might lead to its utilization as the part of commercial catalytic converter for diesel engines, despite the price of gold is currently a bit higher than the price of Pd, Pt or Rh, which are commonly used as active species for diesel emission abatement.
- We propose a model, in which, the difference in the metal electronic states is governed through the differences in electronic interactions of the metallic nanoparticles with ZnO at their interfaces
- Researches may use the proposed model to explain the behavior of other metal-semiconductor heterogeneous oxidation catalysts.

Biography

Dr. Grisel Corro studied Chemistry at the Benemerita Universidad Autonoma de Puebla, Mexico in 1980. She received her Docteur d'Etat degree in 1983 at the Université de Poitiers, France. She obtained the position of Professor at the Benemerita Universidad Autonoma de Puebla. She has published 79 research articles in Sciences Journals.

Auto-thermal reforming of biogas to syngas: Thermodynamic optimization for low CO₂ emissions

Xuejing Chen^{1*}, Yuchen Gao, Yanran Guo, Jianguo Jiang

¹School of Environment, Tsinghua University, Beijing, China

The innovative utilization of renewable energy sources, such as biogas, with relatively low carbon emission have drawn increasing attention. Biogas is a mixture of mainly methane and carbon dioxide that is produced by the anaerobic digestion of residual biomass. Biogas reforming can convert two greenhouse gases to valuable syngas, which is beneficial to environment protection. However, the multiple components in biogas remain a big problem in the selection of biogas reforming technology and parameters. The effects of components besides CH₄ and CO₂, such as O₂, have not been sufficiently studied on biogas reforming. The process of combining dry and partial oxidative reforming of methane, also known as auto-thermal reforming of methane, have been reported to be effective in compensating energy consumption of dry reforming and adjusting the H₂/CO ratio of syngas.

This paper, we focus on the thermodynamic optimization of biogas auto-reforming process with various operations conditions (gas components, temperature, and pressure). A minimum Gibbs free energy method and economic-technical analysis method based on Aspen-Plus was applied to modeling the biogas auto-thermal reforming process, with the optimization of biogas conversions, selectivity, energy consumption, and CO₂ emissions. Results show that carbon deposition can be reduced by increasing O₂ contents and reaction temperature. The auto-reforming of biogas stand for a good option for biogas utilization with minimum CO₂ foot print.

Audience Take Away:

- This research represents a good option for catalytic utilization of biogas.
- An energy-efficient biogas auto-thermal reforming process was simulated under various temperatures and gas components.
- Carbon deposition can be reduced by optimization O₂ content and temperature.
- The auto-reforming of biogas stand for a good option for biogas utilization with minimum CO₂ foot print.

Biography

Dr. Xuejing Chen studied Environmental Engineering at School of Environment, Tsinghua University and received her PhD in 2017. After that she joined Institute of Process Engineering, Chinese Academy of Sciences as a research fellow. Now Dr. Chen is a postdoctoral researcher supervised by Dr. Jianguo Jiang at Tsinghua University. She has published more than 20 research papers in SCI journals.

Rapid, ionic-liquid mediated catalytic conversion of lignocellulosic Sunn hemp fibres to biofuel precursors

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²PK Sinha Center for Bioenergy and Renewables, Indian Institute of Technology Kharagpur, 721302, West Bengal, India

Lignocelluloses from non-food crops are considered to be the most important feedstock for second generation biofuel production since they do not conflict with food sources. We use non-edible cellulose-rich lignocellulosic Sunn hemp fibres – containing 75.6% cellulose, 10.05% hemicellulose, 10.32% lignin, with high crystallinity (80.17%) and degree of polymerization (650) – as a new non-food substrate for lignocellulosic biofuel production. Microwave irradiation is employed to rapidly rupture the cellulose's glycosidic bonds and enhance glucose yield to 78.7% at 160°C in only 46 min. The reactants – long-chain cellulose, ionic liquid, transition metal catalyst, and water – form a polar supramolecular complex that rotates under the dual-mode microwave's alternating polarity and rapidly dissipates the electromagnetic energy through molecular collisions, thus accelerating glycosidic bond breakage. In 46 minutes, 1 kg of Sunn hemp fibres containing 756 g of cellulose produces 595 g of glucose at 160 °C, and 203 g of hydroxymethyl furfural (furanic biofuel precursor) at 180°C. Yeast (*Saccharomyces cerevisiae*) mediated glucose fermentation produces 75.6% bioethanol yield at 30°C, and the ionic liquid is recycled for cost-effectiveness.

We also present experimental evidences of chemical chaos, which is observed when the Sunn hemp fibres are hydrolyzed using the same ionic liquid and the transition metal catalyst in well-mixed batch reactors heated to 110°C by an oil-bath instead of a microwave. The catalytic hydrolysis of lignocelluloses produces chaotic strange attractors with fractal dimensions and positive Lyapunov coefficients on the product phase spaces. All the 5 products (glucose, fructose, hydroxymethyl furfural (HMF), levulinic acid (LA), and formic acid (FA)) exhibit aperiodic (i.e., non-repetitive) temporal oscillations, peaking at 5 hours for water-addition rates ranging from 25 to 43 $\mu\text{l/gm/hr}$, when the hydrolysis system operates in the domain of chemical chaos. 37.5 $\mu\text{l/gm/hr}$ of water-addition maximizes the concentrations of glucose, LA, FA at all times, with their average yields peaking at 5 hours to 67.5%, 12.4%, and 5%, respectively. At water-addition rates of 45 $\mu\text{l/gm/hr}$ and higher, the system operates close to its thermodynamic equilibrium, resulting in the temporal oscillations to disappear completely, though the yields of glucose and HMF continue to peak at 5 hours. We show that the peak non-equilibrium yield of glucose obtained at the water-addition rate of 37.5 $\mu\text{l/gm/hr}$ is 15% higher than its corresponding peak equilibrium yield at 45 $\mu\text{l/gm/hr}$ of water addition, leading to a 15% increase in bioethanol production.

Audience Take Away:

- Which type of lignocelluloses are the ideal substrates for second generation biofuel production?
- What is the detailed chemical kinetics of catalytic hydrolysis of lignocelluloses mediated by ionic liquids?
- How does microwave-based one-pot synthesis exploit this kinetics to produce biofuel precursors from recalcitrant lignocelluloses in less than 46 minutes?
- How does the cross-catalytic nature of the kinetics engender temporal oscillations and chemical chaos in the region of thermodynamic non-equilibrium, which help increase the yields of hydrolysis products?
- What are bottlenecks in scaling up either of these two high-yield processes, and how can they be overcome?

Biography

Dr. Saikat Chakraborty is an Associate Professor in the Department of Chemical Engineering at the Indian Institute of Technology Kharagpur, with joint affiliation at the School of Energy Science and Engineering, and the PK Sinha Center for Bioenergy and Renewables. He did his PhD in Chemical Engineering from University of Houston, USA, and his post-doctoral fellowship in Pulmonary Physiology from University of Texas Medical School. His areas of research include lignocellulosic and algal biofuels, and chemical pattern formation. He has published 50 international papers and has filed for 4 patents. He has received Young Engineer Award from Institute of Engineers India, Sigma Xi Research Achievement Award from the University of Houston, and is a member of the European Federation of Chemical Engineers' Sustainability Section.

Study on biogas dry reforming using Ni catalysts and impurity effects

Yuchen Gao*, Jianguo Jiang, Aikelaimu Aihemaiti, Yuan Meng, Tongyao Ju, Siyu Han, Xuejing Chen
School of Environment, Tsinghua University, Beijing, China

Biogas is a typical renewable bio-energy derived from anaerobic digestion process, mainly composed of methane and carbon dioxide. Dry reforming is a promising technology which can utilize biogas and produce syngas. In this study, Ni catalysts using different supports were synthesized and characterized systematically via N₂-physisorption, XRD, TEM, EDS, XPS, H₂-TPR and TGA. The catalytic activity and stability of different catalysts was investigated under 600-850 °C. It was found that the Ni/MgO catalyst is a promising catalytic material which showed both good activity and stability due to the strong interaction between Ni and support. Besides, as impurities like H₂S, O₂ and N₂ exist in biogas; they cannot be ignored during biogas dry reforming. Therefore the effect of H₂S in different concentrations on biogas reforming was also focused on. Experimental results based on Ni/MgO catalyst as well as a review of recent studies concerning impurity effects are shown, suggesting that impurities even in trace amount can affect the performance of reforming. This research provides a useful reference for industrial operation of biogas dry reforming.

Audience Take Away:

- Recent developments of biogas utilization technologies.
- New progress in biogas dry reforming and impurity effect study.
- This research will allow others to expand their research or teaching and provide new information for catalyst design.

Biography

Ms. Yuchen Gao studied Environmental Engineering at Tsinghua University and achieved bachelor degree in 2016. Then she joined the research group of Prof. Jianguo Jiang at Tsinghua University for Ph. D study and will graduate in 2021. Her research interest mainly includes biogas reforming, catalysis and solid waste utilization. She has published 16 research articles in SCI(E) journals.

Improving probiotic stability to achieve product maximum efficacy

Davor J. Korčok

Research and development department and management, Abela Pharm, Belgrade, Serbia

Purpose of work: Probiotics are manufactured as pharmaceutical-dosage forms registered on the market as: drugs, food supplements, or as medical devices. The main goal of this paper was to set probiotic production stages in order to obtain high quality finished product.

Materials and methods: Viability of probiotic species (bacteria or fungi) was determined by the method of counting the number of microorganisms in suitable medium, after packaging in different packaging materials: a) PVC foil; b) PVdC foil; c) PVdC foil in laminate flow pack foil; or d) PVdC foil in laminate flow pack foil with inert gas, using the same manufacturing conditions prior to packaging phase. Manufactured product was tested under conditions of long-term stability study according to ICH guidelines. The analysis confirmed that the moisture content was important parameter of the probiotic stability, which was analysed on the same set of conditions as additional parameter that influences the probiotic viability under the following conditions: a) with air humidity control and b) without it.

Results: Analyses have presented that probiotic content was the smallest in PVC foil (under the declared value), because it has no barrier properties to temperature and humidity. The product packaged using other materials showed satisfactory results regarding the probiotic viability, whereas the best results were observed using the PVdC foil in laminate flow pack foil with inert gas. Additionally, the study confirmed the hypothesis that moisture content negatively affects the viability of probiotic, since the results obtained with air humidity control were significantly higher than without it.

Conclusion: In order to obtain quality probiotic product which is effective and safe during the declared shelf life, it is necessary to provide optimal conditions during its manufacture, which was confirmed in this study.

Audience Take Away:

- Proper definition of probiotics and difference between product that can be declared as probiotic and those who can't.
- How water activity, oxygen and other ambient conditions affect the probiotic stability.
- People will distinguish the importance of right packaging material in order to improve probiotic stability.
- This presentation will help the audience in proper judgment of many probiotic products which are placed on the market and how to minimize negative effect that ambient conditions (temperature, light, humidity and oxygen) have on probiotic efficacy and stability. Using the guidelines presented in the presentation, other faculty and industry members can use to expand this research, or to offer other solutions for delicate problem of probiotic viability.

Biography

Davor J. Korčok, PhD, specialist of Industrial Pharmacy and specialist of Food Technology, is the lead auditor in international organization standards for Quality Management Systems. He holds prestigious ECA certificate and has been appointed as internal and external consultant of the Agency for medicinal products and medical devices of Bosnia and Herzegovina, and as the visiting and accredited lecturer at the Faculty of Pharmacy, University of Sarajevo and Belgrade, and for the Health Council of Serbia. Also, he is renowned as a first author and co-author of many scientific researches all published in distinctive scientific magazines, he was an editor of scientific guidelines: "Secrets of intestinal microbiota, modern recommendation for use of probiotic products", published in 2017. He is a member of the board of directors of United Association of Serbia for Quality. In January 2019 he was elected to be president of the Scientific Technical Committee for Pharmacy. On the position of the General Manager of Abela Pharm, he has been since April, 1st 2012.

Design & synthesis of cost effective NiPMoS/Laponite and its use as a superior catalyst for hydrodeoxygenation of furfural

P. Santhana Krishnan and K. Shanthi*

Department of Chemistry, Anna University, Chennai 600 025, Tamil Nadu, India

In the near future, fossil fuel era will soon be undoubtedly wiped out in accordance with the British Petroleum statistics and International energy agency. In addition, increasing global energy demand, climate change and carbon dioxide (CO₂) emission from fossil fuels make it a high priority to search for an alternative energy resource. Hence, biomass will undoubtedly be one of the abundant, sustainable and renewable resources for future energy production. In India, 1500 lakhs tons agro waste is produced every year. Farmers are widely used to burn agricultural waste creating air pollution. Till now, many countries failed to find its productive use in the absence of enough government push, improper agro-waste management and business model to enhance rural economy for farmers. Lignocellulose waste is commonly discharged from coir and cork process, paper pulp industries as waste materials. If it is handled correctly, it can be processed efficiently over eco-friendly, cheap heterogeneous catalysts, with the production of value-added chemicals and fuels that could be used as alternative energy source to fossil fuels and would increase a bio-based economy.

Commercial solid acids such as zeolites & alumina, metal catalysts, such as for instance Mo, Pt, Pd, Re, Rh, Ru were previously investigated for hydrodeoxygenation (HDO). Microporous nature of commercial zeolites, coke formation, metal leaching on the γ -alumina (γ -Al₂O₃) and zeolite supports limit their practical applications in hydrotreating. By modifying cheap Laponite RD clay, desired textural properties and morphology in nanoscale range can be created. Hence, it can be used as a low cost support for the catalyst. Industrial hydrotreating, supported Ni (Co) promoted Mo or W sulfide catalysts were usually synthesized by post sulfidation of the oxide catalyst at high temperature with several sulfiding agents. In order to avoid high exposure of H₂S gas, the current research work has been planned to synthesize MoS₂ catalysts under hydrothermal method using thio urea as a sulfiding agent. Then, the materials has been employed for hydrodeoxygenation (HDO) of furfural (Hemicellulosic model compound) into fuel grade hydrocarbons using Ni promoted MoS₂ supported on Laponite in high pressure fixed bed reactor at 503 K – 583 °C under 20 bar H₂ pressure. To comprehend the structure activity of the catalysts, the catalysts were characterized by N₂ adsorption-desorption, XRD, HR-TEM, TGA, DRS-UV-Vis, FI-IR, TPD/TPR. Further, the stability and reusability of the catalysts have been checked thoroughly throughout the entire reaction. The hydrothermal addition of phosphorous into NiMoS has significantly improved the textural properties of both unsupported and supported catalysts by enhancing the extent of sulfidation of nickel. The promotional rate of nickel and the number of (Ni:Mo) slabs have raised up. The structure- activity relationship of the catalysts will be discussed in detail. The recyclability and stability of the catalysts were also excellent under the experimental conditions.

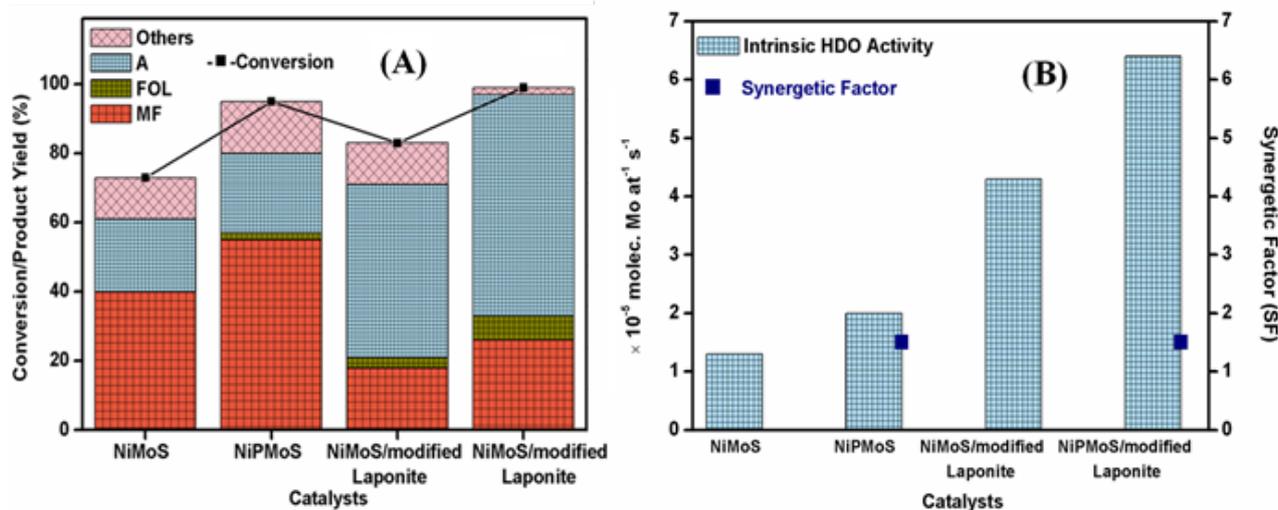


Figure (A) Conversion and Product yield of the catalysts, (B) Intrinsic HDO activity and synergetic factor of NiPMoS and NiPMoS/modified Laponite

Reaction Conditions: 2.5 wt% of Furfural (FUR) in isopropyl alcohol (IPA) and Toluene (TOL), Feed rate: 2.0 mL/h;

Time: 6-8 h; Temperature: 503 K – 583 K; H₂ pressure 20 bar; H₂ flow rate, 50 cm³/min and WHSV: 1.98 h⁻¹).

Audience Take Away:

- The importance of energy today and sustainable & Renewable energy production using biomass
- Hydrodeoxygenation of furfural over heterogeneous catalysts were performed employing cost effective Laponite clay as support for industrial NiMoS catalysts synthesized using hydrothermal method.
- Here, the presenter will discuss the structural activity relationship of the catalyst. The presentation can enable the audience to be aware of the benefits and feasibility of such low cost effective support for the conventional hydro-treating viz., hydrodeoxygenation reactions for biomass conversion to biofuels.

Biography

Prof. K. Shanthi was born in Trichy, India in 1961. She has graduated from Madras University in 1981 in Chemistry and received M. Sc. Degree in 1983. She joined the research group of Dr. Kuriacose at Indian Institute of Technology, Madras for catalysis and received Ph.D. degree in 1989. Later, she joined the Department of Chemistry Anna University, Chennai as a Lecturer in 1991 and She became a Professor in the year 2009 and now heading the Department of Chemistry. She has 75 numbers of international publications with two books at her credit. Her research interests are the surface chemistry, photocatalysis and hydrotreating catalysts for clean and bio fuel production

Preparation and coke-resistance study of Ru promoted Mesoporous Ni/Al₂O₃-CeO₂ catalyst in dry reforming of methane

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² Shaanxi Gas Storage Transportation and Comprehensive Utilization Engineering Research Center, Shannxi Provincial Natural Gas Co., Ltd. Xi 'an, China

Dry reforming of methane (DRM) is one of the most effective ways to convert greenhouse gases including methane and carbon dioxide into hydrogen/syngas. Due to the unique advantages such as economic feasibility and high activity of Ni-based catalyst, it has been widely employed in the reforming reaction in the past decades. However, Ni-based catalysts have several shortcomings including carbon deposition and thermal sintering, which tended to hinder its industrial application. In this work, ruthenium is introduced in the Ni/Al₂O₃-CeO₂ catalyst to overcome these defects effectively. Compared with conventional impregnation method, the sol-gel method is used to prepare Ni-xRu /Al₂O₃-CeO₂ which can enhance both activity and stability of the expected catalysts. Different ratios of Ru to Ni are investigated to validate the catalytic activity and coke formation for the prepared catalysts and Ni-0.3% Ru/Al₂O₃-CeO₂ is confirmed to own the top catalytic performances. Under the space velocity (27000 mL·g_{cat}⁻¹·h⁻¹) and reaction temperature (1073 K), the CH₄ and CO₂ conversions of 0.3% Ru promoted Ni-based catalysts could reach 90% and 96% respectively, which are 10% and 6% higher than Ni/Al₂O₃-CeO₂ catalyst. The XRD and SEM results show that the Ru addition can increase the interactions between active components and supports; meanwhile the Ru doping can decrease the Ni particle size and uniform the active metals, leading to the large specific surface area of catalysts. The H₂-TPR characterization indicates that Ni-0.3%Ru/Al₂O₃-CeO₂ possesses stronger reducibility and more nickel active sites than Ni/Al₂O₃-CeO₂. Although TEM and TG illustrate that Ru doped catalyst samples perform invisible morphology change of the deposited carbon, the Ni-0.3%Ru/Al₂O₃-CeO₂ with Ru addition can improve the anti-coking ability significantly, which is bound to have a promising application in the future.

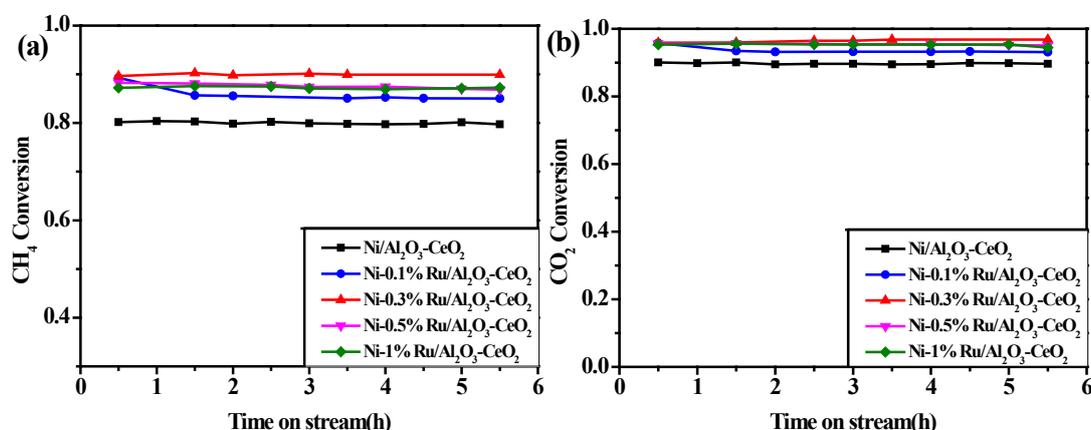


Fig. 1: Catalytic performances based on different ratios of Ru to Ni for DRM: (a) CH₄ conversion, (b) CO₂ conversion
Reaction conditions: WHSV 27000 mL·g_{cat}⁻¹·h⁻¹, 1073 K.

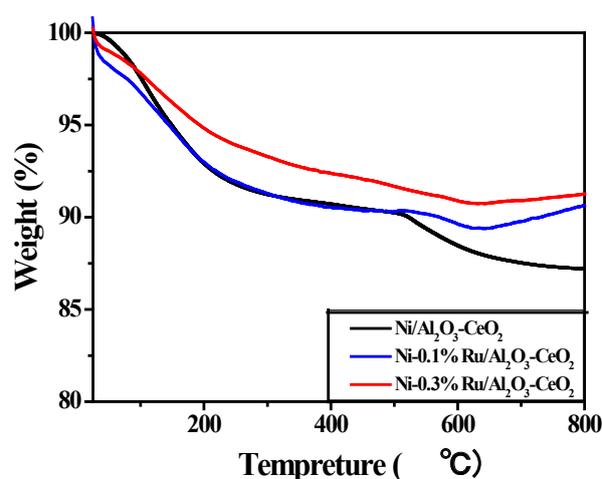


Fig2. TG profiles of the spent catalysts after 6 h reaction.

Audience Take Away:

- Ru doped Ni/Al₂O₃-CeO₂ is prepared through sol-gel method
- Ni-0.3%Ru/Al₂O₃-CeO₂ catalyst exhibits high specific surface area and small nickel particles
- Ni-0.3%Ru/Al₂O₃-CeO₂ catalyst confirms its remarkable coke resistance capability in DRM

Biography

Dr. Yuqi Wang studied Chemical Engineering and got his BS and MS at Northwest University (China). In 2006, he received his Doctor's degree from Xi'an Jiaotong University (China). In 2009, he was awarded China Young Backbone Teacher Scholarship and worked as a research scholar in Low Carbon Green Technology Laboratory, University of Nevada (Reno). He has been engaged in research fields including catalytic reaction engineering, chemical engineering and hydrogen energy for over 20 years. He has undertaken over 30 research projects and published 110 academic papers, authorized 20 China invention patents, and he was awarded 22 teaching and scientific research prizes.

Acknowledgment:

The authors thank the financial support by the National Natural Science Foundation of China (21276209), State Key Laboratory of Chemical Engineering (No. SKL-CHE-18A02), and Shannxi Provincial Natural Gas CO., LTD

Anode electrode catalyst for liquid fueled solid alkaline fuel cells (SAFCs)

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³Core Research for Evolutionary Science and Technology, Japan Science and Technology Agency (JST-CREST), Japan

The R&D center of Noritake Company Ltd. is actively involved in the development of materials for FC application (PEMFC, SOFC and SAFC) with advanced properties. Highly porous, anion conducting, flexible substrates, consisting of an anionic clay (Mg-Al LDH) coated PVDF substrates were made for applications like, in the development of anion conducting pore filling membranes (1-2). In collaboration with IIR of Tokyo Institute of Technology, novel electro catalyst materials for liquid fuel oxidation are being developed by the rational selection of conditions leading to morphology control of the catalyst and the substrate material. As an alternative fuel resource to hydrogen, liquid fuels such as ethanol, ethylene glycol, liquid formate etc., an ambient temperature fuel with advantages like easy handling, storage and transportation definitely scores over hydrogen. Out various liquid fuels, Formate (HCOO-) is considerably less toxic and environmentally benign compared to other liquid fuels such as methanol and liquid ammonia. Furthermore, HCOO- can be regenerated by the electro-reduction of CO₂, making formate a viable fuel for liquid fuel cell application. Several palladium based electrocatalyst nano alloys are being developed with superior activity and stability towards liquid fuel oxidation in alkaline medium (3-5). Some of the materials and technologies developed for alkaline fuel cells will be detailed in the presentation.

Biography

Present position: Deputy General Manager, R&D Center, Noritake Co., Ltd., Japan. (2006 ~)

Research Experience : >20 years of R&D experience in the field of ceramics/materials chemistry

Ph. D (*Chemistry*) : Council of Scientific and Industrial Research (CSIR) -NIIST, India (1999)

Post Doctoral : The University of Tokyo, Japan (2003) ; Korea Advanced Institute of Science and Technology (KAIST), Korea (2002) ; KOSEF Fellow, South Korea (2001)

International Publications: > 50, Patents: 15 ; Presentations- National/International: >50

DAY 1

BREAKOUT HALL

5TH EDITION OF GLOBAL CONFERENCE ON

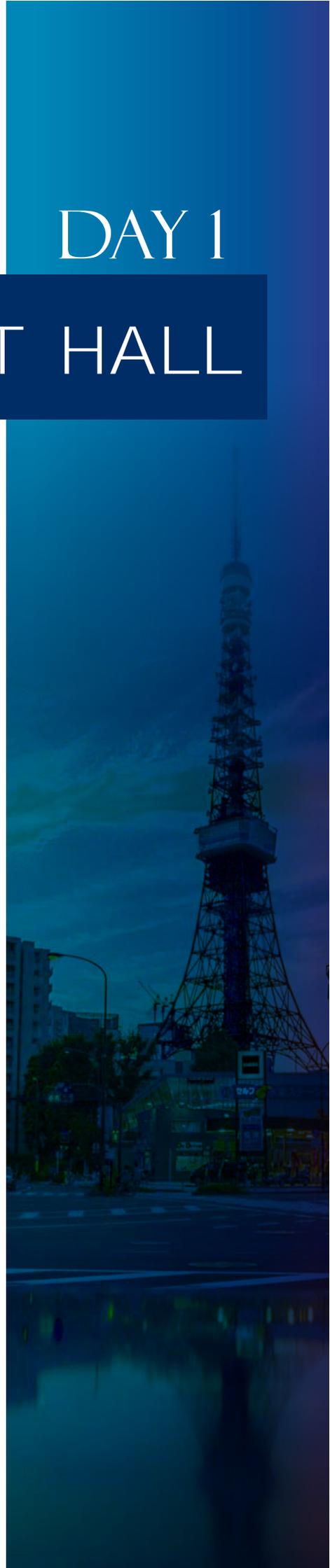
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The mechanism of the base-free Ru(PTA)₄Cl₂ catalyzed hydrogenation of CO₂ to formic acid

Edward N. Brothers,^{1*} Rajesh K. Raju,¹ and Salvador Moncho¹

¹A&M University at Qatar, Department of Chemistry, Doha, Qatar

Catalytic hydrogenation of CO₂ to fuels is an ideal strategy that offers solutions to two major concerns of the 21st century: global warming due to anthropogenic CO₂ emissions and the rapid depletion of nonrenewable fossil fuel reserves. Of the many possible CO₂ products, formic acid (HCOOH) has been attained recent attraction as a low-toxic liquid hydrogen storage material with a volumetric hydrogen density of 53 g of H₂ per litre. Despite the progress in the development of homogeneous catalysts for the hydrogenation of CO₂ to formic acid, none of these reactions could achieve industrial level applications due to the complications arises from the base additives. Even though base-free hydrogenations could evade the issues in the separation of formic acid, little efforts have been taken in this research direction. Recently, Laurency and co-workers have reported a robust ruthenium catalyst Ru(PTA)₄Cl₂ (PTA=1,3,5-triaza-7-phosphaadamantane) for the base-free hydrogenation of CO₂ to HCOOH in acidic media without the need of any bases, additives or buffers [*Nature. Commun.* 2014, 5, 4017]. In water, the catalyst affords to form 0.2 M formic acid with a turnover number of 74 whilst the same catalyst produces 1.9M formic acid in DMSO, an almost 10 times increase in the HCOOH formation. Employing density functional theory (DFT) calculations, we studied in detail the various mechanistic pathways for the hydrogenation of CO₂ to formic acid for this novel catalysis. We found that the solvent itself act as a base and assist in the heterolytic cleavage of H₂ to form the Ru-monohydride species Ru(PTA)₄(Cl)(H) from the Laurency's catalyst Ru(PTA)₄Cl₂. The computed enthalpic changes (ΔH) of 20.9 kcal/mol and 19.8 kcal/mol are in excellent agreement with the experimental activation enthalpies of 22.9 kcal/mol and 17.5 kcal/mol in water and DMSO, respectively. We have also explored the reaction pathways for the hydrogenation of CO₂ to formic acid by the key species Ru(PTA)₄(Cl)(H). The explicit role solvent in the reaction pathways were also investigated. We have found that the formation of the Ru-monohydride species from the Laurency's catalyst is the rate-determining step of the reaction. Unraveling the thermodynamic and kinetic aspects of the reaction pathways for the hydrogenation of CO₂ for this novel catalysis can aid the further development of novel robust catalysts for the hydrogenation of CO₂ in base-free reaction conditions.

Biography

Prof. Brothers did his PhD at Penn State, a postdoc at Rice University, and has been at Texas A&M University at Qatar as a professor since 2008, where he also served as the Program Chair of Science for five years. His research focuses on understanding the reaction mechanisms of metal bearing homogeneous catalysts.

Structural and electrochemical study of IrO₂ and NiO-coated Ni anode by atomic layer deposition (ALD)

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¹Basic Research and Scanning, Research and Development Division, Industrie de Nora S.p.A., Milan, Italy

²Department of Chemistry and Materials Science, School of Chemical Engineering, Aalto University, Aalto, Finland

Atomic Layer Deposition (ALD) is a special type of Chemical Vapor Deposition (CVD) technique that could grow conformal and uniform thin films on the surface of a substrate through alternate self-limiting surface reactions. The development of this technique has been successfully demonstrated in thin film electroluminescent display production, but the industrial use of this technique remained marginal for more than two decades.¹ On the other hand, hydrogen is one of the promising solutions for the sustainable and green energy problem, but the process is still not optimal because of the sluggish kinetic of the anodic oxygen evolution reaction (OER) due to the well-known scaling relation restriction.² In this study, iridium dioxide (IrO₂) and nickel oxide (NiO) thin films were deposited on industrial Ni coarse mesh (and Si [100] for reference) as an anode for alkaline water electrolysis. ALD operating parameters such as the number of deposition cycles, amount of O₃ flow, deposition and sublimation temperatures, and pulse and purge rates were varied to determine the effect of changing these parameters on the electrochemical performance of the material. Total deposition time took approximately 14 hours (for 1000 cycles) and 21 hours (for 1500 cycles).

To establish the structure-catalytic behavior relationship, materials were characterized using: Grazing Incidence X-ray Diffraction (GIXRD), X-ray Reflectivity (XRR), Scanning Electron Microscopy (SEM), and iR-corrected Single Electrode Potential Test (CISEP). As seen on the GIXRD patterns (Figure 1a), variation on the operating parameters did not affect the crystalline phases of IrO₂ (tetragonal) and NiO (cubic) present on the thin films. OER was investigated in industrial conditions (high temperature and high KOH solution) at varying high current densities of 1 to 12 kA/m²). Results from the electrochemical tests (Figure 1b) showed the catalytic activity of IrO₂ and NiO thin film (approx. 25 to 60 nm). Overpotential values, η , of the coated Ni mesh were 20 to 60 mV lower than the uncoated Ni mesh. In summary, the study has demonstrated the feasibility of using ALD technique to deposit conformal, uniform and electroactive thin films on industrial metallic substrates as an anode for alkaline water electrolysis.

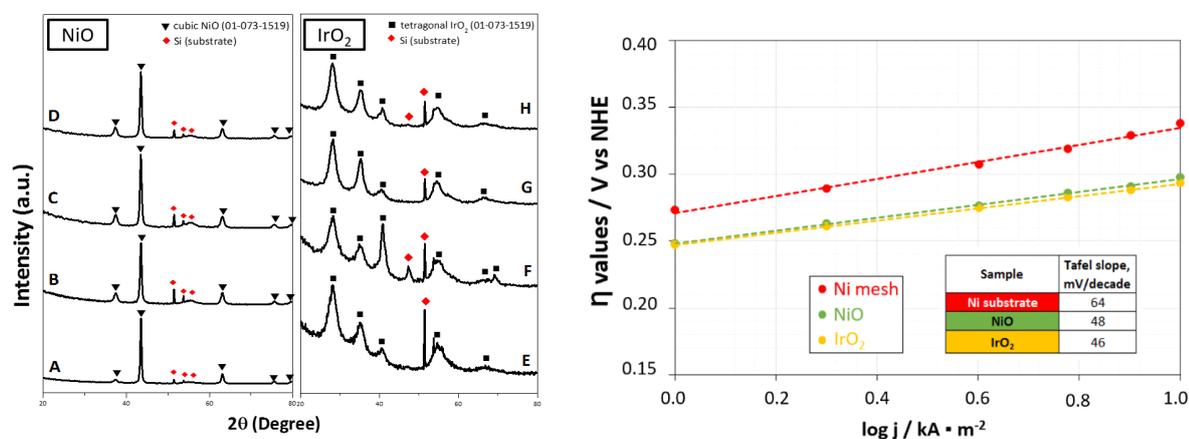


Figure 1. (a) GIXRD patterns of NiO and IrO₂ on Si [100]; and (b) Tafel plots of anodic overpotentials η .

Audience Take Away:

- Through this oral presentation, the audience could have an insight on the application of the ALD technique in the field of electrochemistry under industrial conditions. Eventually, this would be helpful for them to have an idea for further research especially on the case of the people interested also on thin film technologies. Also, they could learn different characterization techniques suitable for this type of materials. Initial results of the study would be helpful for those studying the same materials (e.g., metal oxide, substrate, water electrolysis) but with different deposition technique to have a comparison on the structural, morphological and electrochemical characteristics of the different materials.
- This oral presentation demonstrates the advantages of ALD technique on depositing conformal, uniform and pin-hole-free thin films. Initial results showed that these thin films are electroactive in terms of lower oxygen overpoten-

tial values (vs. uncoated substrates) in alkaline water electrolysis. Since this study is an initial attempt on using thin film electrodes for oxygen evolution reaction in alkaline water electrolysis, a lot of improvement on the work could be done especially on the academia part. Different studies could be done on correlating ALD operational parameters with the obtained characteristics of the thin film. The presentation could also help the presenter and the audience to start a scientifically-deep conversation on the points that could be improved or the things that could be tried to continue the study. Since the presenter has an industrial point of view, the study could also benefit other industry partners interested on thin film technology as well as people from academia who has more experience on the theory of the technique. With this, the presentation could provide certain practical solutions to some limitations on the field or on the technique.

Biography

DJ Donn is currently a Junior Researcher at Industrie de Nora under a European Training Network program, fully funded by the EU and dedicated to the education of Early-Stage Researchers within the field of “Electrochemical Conversion of Renewable Electricity into Fuels and Chemicals”. He was awarded with the Erasmus Mundus Master in Chemical Innovation and Regulation in 2017 from the University of Bologna and University of Barcelona and a Bachelor's Degree in Chemical Engineering from the University of the Philippines. Before obtaining his MS, he made some internships and worked for 3 years as Process Engineer at Petron Corporation (Philippines).

Laccase-electrospun materials as biocatalytic systems for application in environmental protection

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Over recent years, there has been a significant increase in the use of immobilized biocatalysts in many fields of science, life and industry, mainly due to the improvement of the stability and activity of enzymes at harsh reaction conditions as well possibility of their reuse. The immobilized biocatalysts are used, among others in the synthesis of pharmaceutically active substances, in the food industry, as well as in the processing and conversion of biomass components. However, it is also becoming increasingly common to use biocatalytic systems based on immobilized enzymes in the conversion processes (biodegradation) of selected compounds present in wastewater, which pose a potential threat to life and health of living organisms. This is possible due to the immobilization of such enzymes as laccase, tyrosinase or peroxidases, which can be immobilized, among others on the surface of composite oxide materials, biopolymers, or materials produced by the electrospinning technique. As a result, it is possible to obtain systems with a characteristic that enables effective application of the developed solutions.

In the presented study poly(l-lactic acid)-co-poly(ϵ -caprolactone) and poly(methyl methacrylate) with incorporated magnetite nanoparticles were used for immobilization of laccase from *Trametes versicolor* and further, obtained biocatalytic systems were applied for removal of naproxen, diclofenac and tetracycline from model water solutions. Effect of various process conditions, such as pH, temperature, and its duration on the biodegradation efficiency of pharmaceuticals were studied in details. Moreover, storage stability as well as reusability of the immobilized enzymes were evaluated and compared. Obtained results clearly show that immobilization of laccase using various electrospun materials results in production of highly active systems capable for effective removal of environmental pollutants.

Audience Take Away:

- In the presented study, for immobilization of laccase, novel electrospun support materials have been used, which might be also applied for immobilization of other enzymes.
- We demonstrate a proof-of-concept for the obtaining and application of novel biocatalytic systems capable for effective biodegradation of hazardous compounds from water solutions.
- Optimal process conditions for removal of pharmaceuticals have been examined that facilitate effective removal of pharmaceuticals.

Biography

Received the Ph.D. at the Faculty of Chemical Technology, Poznan University of Technology in 2017. From 2017 to 2018 was a postdoc researcher at Center for BioProcess Engineering at DTU Chemical Engineering, Technical University of Denmark and now works at the Faculty of Chemical Technology, Poznan University of Technology. Research area focuses on enzyme immobilization using various types of support materials and different groups of biocatalysts. During doctoral studies, participated in numerous programs that supported scientific carrier and mobility including Opus, Preludium and Etiuda financed by National Science Center Poland. During last 5 years he published over 40 peer-reviewed articles.

Acknowledgements:

This study was funded by Ministry of Science and Higher Education (Poland) as financial subsidy to PUT under the grant no. 03/32/SBAD/0915.

Low-temperature synthesis and inkjet printing of photoactive TiO₂ on polymeric substrates

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A low-temperature method was used to prepare and inkjet-print photoactive TiO₂ films on polymeric substrates using a commercial inkjet printer. The as-prepared substrates were used in a microfluidic device fabricated with selective transmission laser welding. The catalytic activity of the printed nanolayers was studied in a microreactor based on the photodegradation of methylene blue as a standard pollutant. The overall process is cost-effective and efficient in manufacturing flexible lightweight microreactors coated with tunable catalytic films for catalysis and photocatalysis applications.

Many attempts have been made to immobilize photocatalytic particles in continuous reactor systems such as using optofluidic devices or coated microchannels manufactured on ceramics, glass or silicon. In spite of the progress on material deposition techniques into macro and microfluidic devices, there are still limitations due to complex fabrication procedures and low performance. Among different coating techniques, material printing or inkjet printing has emerged recently. This novel technique is suitable for non-contact uniform coating of functional metal oxides such as TiO₂.

In this work, the TiO₂ sol was prepared from hydrolysis of TiCl₄ at 100 °C and directly dispersed in ethylene glycol for ink formulation. The ink printability and colloidal stability were assessed by rheological and interfacial properties. X-ray diffraction spectrum of the synthesized TiO₂ confirmed the crystallized phase of pure anatase with an average particle size of 4.2 nm. The synthesized TiO₂ exhibited higher activity ($k = 0.021 \text{ min}^{-1}$) compared to the commercial standard powder ($k = 0.011 \text{ min}^{-1}$). Furthermore, the microreactor showed promising performance and stability, and the inkjet printing method proved to be a customizable technique for coating active nanocatalysts.

Audience Take Away:

- A calcination free route to synthesize active TiO₂ nano catalyst below 100 °C.
- Immobilize catalyst particles on polymeric substrates without high temperature heat treatment.
- Manufacture flexible lightweight microreactors using a cost-effective method.
- Lower operational costs and more material choices due to low temperature process.
- Scalability and flexibility for various catalysis applications.

Biography

Mr. Hesam Maleki received his BSc and MSc in chemical engineering from Sharif University of Technology, Iran. He worked on the synthesis of new nanocatalysts for biodiesel production in the Catalysis and ThermoKinetics research group. He started his PhD project in 2017 funded by Low Carbon Eco-Innovatory. Currently, he is a second year PhD student at the University of Liverpool. His research is on miniaturizing the chemical reactions for environmental applications. He has 4 scientific papers in peer-reviewed journals.

Pyrazole as a corrosion inhibitor for carbon steel in aqueous media

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The inhibitory impact of pyrazolin derivative (Pz) on corrosion of carbon steel in 1 M HCl was examined by potentiodynamic polarization method and electrochemical impedance spectroscopy (EIS). The hindrance effectiveness of Pz on corrosion of carbon steel in 1 M HCl arrangement increments on expanding in convergence of the P2. Potentiodynamic Polarization estimation demonstrates that Pz goes about as a blended mixed inhibitor. The idea of adsorption of the Pz on carbon steel surface is found to comply Langmuir adsorption isotherm. EIS estimation result is likewise associated with the consequence of polarization. DFT ponder affirmed the adsorption of inhibitor particles on mellow steel surface. The surface morphology of the mild steel surface was examined using ScanningElectron. Density Functional Theory calculations and molecular dynamic simulations were used to give basic insights into the action mode of inhibitors as well as to substantiate the experimental results.

Using polyisobutylene-supported sulfur ligands for metal sequestering

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Whether it is industry, agriculture, research experiments, or just ordinary activities, modern societies in the 21st century produce unwanted waste. In some cases, this waste is concentrated and can be easily dealt with. In other cases, such waste can be minimized; this has been demonstrated in the development of environmentally benign syntheses that have used polymer-bound metal catalysts to minimize chemical waste in homogeneous catalysis. However, waste most often cannot be completely eliminated. Even if it is minimized, unwanted by-products from industrial or agricultural endeavor or from a modern city often end up in organic or aqueous waste streams in a highly diluted form. Herein, we report the use of Polyisobutylene (PIB) as a polymeric support for metal sequestration in organic solutions. PIB is functionalized to convert its terminal C=C into metal sequestering groups (carboxylic acid, thiol or amine group). The use of a cleavable linker to regenerate the PIB-sequesterant is also studied.

Audience Take Away:

- Learn about homogeneous catalysis
- Learn about the use of PIB as a homogeneous support
- Learn about sequestration of metals

Biography

Dr. Hassan S. Bazzi is the associate dean for research and professor of chemistry at Texas A&M University at Qatar, a branch campus of Texas A&M University. Dr. Bazzi received his bachelor's and master's degrees in chemistry and organic chemistry, respectively, from the American University of Beirut (1996 and 1998), and his Ph.D. in polymer chemistry with Dean's Honor List from McGill University (2003). He worked briefly with the United Nations as a chemical weapons inspector in Iraq before doing a postdoctoral research fellowship at Université de Montréal. He joined Texas A&M at Qatar as assistant professor in 2004, was promoted to associate professor (2009), and then to full professor (2014).

Inorganic oxide systems with immobilized laccase as tools for dyes decolorization

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Wastewaters containing dyes are toxic pollutants released to environment, which can be dangerous for living organisms and human health. They can cause various diseases, for example cancers, allergies and neurological disorders. Many industries, such as textile and automotive industries generate huge amounts of wastewaters, in which huge amounts of dyes are presented. There are a number of methods used to remove dyes from aqueous solutions, such as adsorption, sedimentation, coagulation, membrane techniques or photocatalysis, however biodegradation deserves special attention. It is a dyes removal technique in which the main degradation factors are microorganisms and/or enzymes. Especially for dyes conversion, enzymes such as laccases, tyrosinases and peroxidases are the most frequently used. These oxidoreductases, which are widespread in nature, catalyse the oxidation of a wide variety of substrates, such as dyes, pharmaceuticals and other phenolic compounds. Nevertheless, in order to increase the biodegradation efficiency and improve enzymes stability, the immobilization process is carried out using support of various origin. It should be emphasized that selection of the suitable support material is a crucial step in enzyme immobilization.

In the presented work, the Remazol Brilliant Blue R (RBBR) textile dye was degraded using laccase from *Trametes versicolor* immobilized inorganic onto oxide systems such as: $\text{TiO}_2\text{-ZrO}_2$, $\text{TiO}_2\text{-ZrO}_2\text{-SiO}_2$, $\text{ZrO}_2\text{-SiO}_2$ and $\text{ZrO}_2\text{-SiO}_2$ modified by copper ions. Based on the obtained results, it was confirmed that the laccase was immobilized successfully. Furthermore, effect of the support type, concentration of dye solution as well as pH and temperature conditions on the efficiency of enzymatic decolorization were evaluated using UV-Vis spectroscopy. What is more, it was found that obtained biocatalytic systems might be reuse in successive degradation cycles due to the improvement of the laccase stability.

Audience Take Away:

- The novel inorganic oxide systems may find applications in various fields of science and industry, such as carriers for laccase immobilization.
- Laccase immobilized onto synthesized oxide materials may be used for removal of various phenolic compounds, among others dyes, from aqueous solutions.
- The presented results suggest that dye was removed due to simultaneous adsorption and bioconversion.

Biography

Katarzyna Jankowska studied Chemical Technology at Poznan University of Technology and graduated as MSc in 2017. She joined the research group as a PhD student of Prof. Jesionowski at the Institute of Chemical Technology and Engineering at the same university. She is awarded by Polish National Agency for Academic Exchange in form of Iwanowska scholarship. Biotechnology, enzyme immobilization and electrospinning technique are her main scientific interests.

Acknowledgement:

This work was funded by research grant funds from the National Science Centre Poland (DEC-2018/29/N/ST8/01026).

Optimal design and sensitivity analysis of Gas-solid reactor for efficient H₂ storage

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Metal hydride (MH) has large hydrogen storage capacity and mild operation conditions, which is considered to be a promising method for utilization. Since the hydrogenation/dehydrogenation is reversible chemical reaction with strong thermal effect, the design and optimization of gas-solid reactor is crucial to storage and transportation. Based on the bionic optimization and constructal theory, a new bionic duplex DNA elliptical-tube reactor (B-D (DNA)-ER) is developed to descend the maximal axial temperature difference (ΔT_{ax}) by 5.1 K/5.6 K for absorption/desorption inside the gas-solid reactor. The sensitivity analysis results of B-D (DNA)-ER indicate that the effect sequence of structural parameters (optimal value) on reaction rate should obey: major diameter (10 mm) > major axis (4 mm) > minor axis (2 mm) > pitch (6 mm) > installation angle (45°), which is consistent with the effect order of heat transfer tubes on the radial distribution in B-D (DNA)-ER. Therefore, the radial distribution of the heat transfer tubes was proved as the major factor to reaction performance compared to the axial direction. According to the theory of constructal entransy dissipation rate, a novel radiation mini-channel reactor (RMCR) is proposed to further improve the heat transfer and reaction performance through the arrangement of radial tubes. The calculation results illustrate that RMCR can significantly accelerate the absorption rate in radial direction, which may complete the hydriding process within 1200 s, causing the 11.4 K reduction of maximal radial ΔT_{rad} than B-D (DNA)-ER. The 7 reactors are extensively investigated and compared, revealing that the gas-solid reactor with radiation tubes own the best performance than others, which can save 77%, 52% and 37% reaction time than tank reactor, straight tube reactor and spiral tube reactor, respectively. The sensitivity analysis results indicated that axial pitch was the most sensitive structure factor for RMCR.

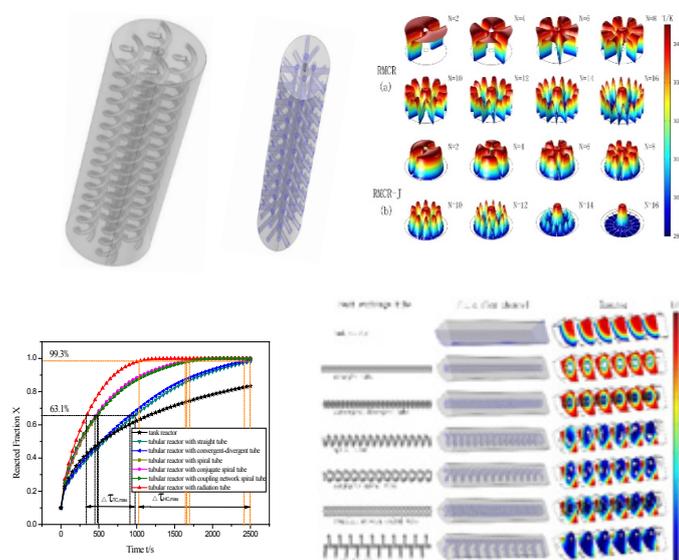


Fig.1 the structure of (a) B-D (DNA)-ER and (b) RMCR; Effects of heat exchange tube numbers on the temperature distributions of RMCR & RMCR-J at $t=1000$ s based on constructal entransy dissipation rate maximization (c);The comparisons of reacted fraction (d) and bed temperature distributions at $t=1000$ s (e) during hydrogenation process.

Audience Take Away:

- This presentation will provide new design ideas (bionic optimization and constructal theory) for gas-solid reactors and introduced an efficient method of parameter sensitivity analysis for scholars.
- This presentation will express a conclusion that the radial distribution of heat exchange tube was the dominant factor of reaction performance instead of axial distribution of heat exchange tube and heat exchange area.

- This presentation will introduce 3 types of gas-solid reactors including B-D (DNA)-ER, RMCR and RMCR-J, and the comparison results indicate that B-D (DNA)-ER can improve the reaction rate along axial direction of reactor, and RMCR can improve the reaction performance along radial direction of reactor. RMCR-J demonstrated an outstanding and stable performance than all other reactors.

Biography

Dr. Di Wang studied Process equipment and control engineering at Northwest University (China) and graduated as Bachelor of Engineering in 2016. She is recommended for admission to be a PhD in Chemical Engineering at Northwestern University (China). She has been engaged in research fields including chemical engineering and hydrogen energy for 5 years, meanwhile she has undertaken 1 and participated in 3 research projects. She has published 1 academic paper in SCI(E) journal and authorized 4 China patents.

Acknowledgment:

The authors thank the financial support by the National Natural Science Foundation of China (21276209), State Key Laboratory of Chemical Engineering (No. SKL-ChE-18A02), and Shannxi Provincial Natural Gas CO., LTD.

The effect of ionic liquids on the photocatalytic activity of BiOX semiconductors in cytostatic drug degradation

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The effect of ILs cation type (imidazolium, pyridinium and pyrrolidinium) on the morphology, surface properties and photoactivity of BiOX type semiconductors obtained by solvothermal method, has been systematically investigated. The physicochemical properties of BiOX photocatalysts were characterized by means of X-ray diffraction (XRD), Scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Fourier transform-infrared spectroscopy (FT-IR), Brunauer-Emmett-Teller (BET) method, UV-vis diffuse reflectance spectra (UV-vis/DRS) and photoluminescence spectra (PL). Rhodamine B and 5-fluorouracil were used as the model compounds to evaluate the adsorption capacity and photooxidation performance of studied BiOX. Removal of chromium (VI) from acidic solution was demonstrated photoreduction ability of BiOX.

The obtained results indicate a significant influence of the ionic liquid on the morphology and photocatalytic activity of bismuth-based semiconductors prepared by the solvothermal method. The loosening of the structure and increasing the particle size of the photocatalysts due to ILs use were observed. Changes of the obtained bismuth oxyhalides structures were also associated with the increase of their BET specific surface area and pore volume. The beneficial influence of the use of ionic liquids in the solvothermal synthesis process on the energy band gap value of the obtained bismuth semiconductors was noticed. The extension of energy band gap in the bismuth oxybromides and oxyiodides, and the reduction of energy band gap in the bismuth oxychlorides prepared by IL-assisted solvothermal method were obtained. Using the ionic liquid assisted solvothermal method well-formed crystalline structures (XRD) without residues of ILs on their surface (XPS, FT-IR) were synthesized.

Moreover, the BiOX samples synthesized with ionic liquids were applied to remove of some cytostatic drugs from water. Based on the identified intermediates of drugs degradation and photogenerated oxidants participated in drug degradation under BiOBr. The degradation pathway of some cytostatic drugs was proposed.

The obtained results indicate that the use of ionic liquids as a halogen source can increase the photocatalytic activity of bismuth oxyhalides. The materials effectively purified the water from micropollutants such as cytostatic drugs. However, their beneficial effects should be considered individually in relation to particular micropollutant and an oxidation or reduction processes.

Audience Take Away:

The problem with the cytostatic drugs in environment will be presented.

- The structure and activity of BiOX semiconductors and the methods of its preparation will be discussed.
- The effect of ILs used for preparation of BiOX on its photocatalytic activity will be shown
- The correlation between the halide ion precursor used for preparation BiOX and its morphology and photoactivity will be explained
- The mechanism of photocatalytic removal of cytostatic drugs under BiOX will be explained
- The influence of actual effluents from WWTP and surface water on the photocatalytic removal of drugs will be presented

Biography

Prof Ewa M. Siedlecka studied Chemistry at the University of Gdansk in Poland. She received her PhD degree (peptides chemistry) in 1994 at the same institution. She then changed her research interest to Advanced Oxidation Processes. She received Doctor of Science (habilitation) degree in chemistry in 2011, and title of full professor in 2018. She is a chef of Advanced Oxidation Processes Lab at the Department of Chemistry University of Gdansk. She has published more than 70 research articles in SCI(E) journals. She is interested in photocatalytic and electrochemical removal of pollutants from water.

Preparation of activated carbon derived from arecanut shell agro waste using phosphoric acid catalyst: Estimation of ferets diameter

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In this work, activated carbon was produced by chemical activation using phosphoric acid catalyst. Activated carbon derived from agricultural waste of arecanut shell. Activated carbon is produced by chemical activation at temperature of 4000C by slow pyrolysis. Impregnation ratio maintained is 1:1, 2:1, 3:1, 4:1 (Phosphoric acid: Biomass) by stichiometry. Optimized results obtained at 3:1 impregnation ratio. The BET surface area and iodine number surface area was calculated and compared. The TGA investigation revealed that activated carbon is thermally stable at 4800C. SEM images reveal morphological change caused on surface. Ferets diameter is estimated to know the circularity of particle. Iodine number surface area, iodine number, methylene blue number results proved 3:1 is optimized impregnation ratio is important in determining the quality of activated carbon obtained.

Audience Take Away:

- Explain how the audience will be able to use what they learn?
- Audience will able learn manufacture process of the activated carbon from agrowaste.
- Audience will able to learn characterization of the prepared activated carbon.
- Audience will able to learn how to calculate the ferrets diameter of activated carbon particle.
- How will this help the audience in their job?
- Once audience learn manufacturing process ,they can prepare the activated carbon from any agrowaste, and will able to sale as per application or end use product say for waste water treatment etc.
- Is this research that other faculty could use to expand their research or teaching?
- Yes definitely other faculty can use this for futures expand.
- Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient?
- Yes definitely, because this will simplify environment related problem.
- Will it improve the accuracy of a design, or provide new information to assist in a design problem? List all other benefits.
- Accuracy in design of manufacturing process is need of time as this process is carried by slow pyrolysis at 4000C. Accuracy in design of muffle furnace will help to increase the yield of activated carbon by reducing volatile by product.

Biography

Mr A S Jadhav studied Chemical Engineering at the Shivaji University, Kolhapur, INDIA and post graduated as ME in 1994. He then. Joined at the Khopoli Polytechnic, Pen Engineering College Pen. He is presently working at AISSMS COE Pune as Assiatant Professor in Chemical Engineering. He received BEST RESEARCH PAPER AWARD in 2008 by Deccan Sugar Technological Association, Pune, Phd Scholarship for research of Rs 60000/- by SAKAL INDIA FOUNDATION, Pune, INDIA, BEST REASERCH PAPER AWARD by Carbon Science Technology journal Pune in 2018. He has published 8 research articles in SCOPUS, Web of Science and UGC approved journals.

Plasma surface activation of fibers for immobilization of enzymes on conductive and non-conductive textiles: Application to various processes

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Porous textiles are flexible fibrous materials having high porosity (80-99%) and providing low pressure drop, a high surface-to-volume ratio for enzyme immobilization and allowing easy diffusion of reactant mixture (substrate and products). Monitoring of fiber diameter and pore size is possible using different techniques and the choice of chemical nature of the fiber is important to resist processes and to immobilize enzymes. Most enzyme immobilization methods are still facing challenges in terms of health hazards and high environmental impact. Thus, it is important to find eco-friendly approaches to achieve efficient enzyme immobilization with optimal bioactivity. Plasma treatments are eco-friendly processes which can be used to activate durable PET –polyethylene terephthalate or conductive carbon fiber nonwovens for appropriate enzyme immobilization at fiber surfaces. Not all plasma treatments using dielectric barrier discharge can be used to activate conductive carbon fiber surfaces.

Results of immobilization of β -galactosidase and glucose oxidase (GOx) on PET and/or conductive carbon fibers will be presented.

In the first part, the effect of 3 different surface plasma treatments on the immobilization of β -galactosidase on a fibrous PET nonwoven membrane by gel-film entrapment and direct sorption methods will be described. β -galactosidase is an important enzyme biocatalyst used in food industry for the hydrolysis of lactose necessary for lactose-intolerant people. In addition, this enzyme catalyzes the formation of galacto-oligosaccharides, which are prebiotic additives for the so-called “healthy foods”. With the optimized sorption method using N_2/O_2 CRP plasma, no decrease in enzyme activity was detected, and the immobilized enzyme could be used over more than 15 cycles.

This study provides a novel method for enzyme immobilization under mild and controllable conditions, which can be interesting for use in food processing

In the second part, the effect of plasma treatments on GOx enzyme immobilization on electrically conductive supports will be described. Immobilization which allows enzyme bioactivity and stability improvement, for use and re-use in different applications, is important. Carbon-based textiles, are robust materials to be used as alternative for expensive rigid metals, since they possess good electrical conductivity and good resistance to corrosion in different media. They are however hydrophobic and their surface has to be activated using appropriate plasma dielectric barrier discharge. The results obtained showed that specific Cold Remote Plasma, was efficient in functionalizing the surface of carbon felts and PEDOT:PSS coated felts. This increased carbon surface energies facilitated the immobilization of GOx by physical adsorption with maintained bioactivity and improved reusability and interesting bio-electrochemical response. Finally, the obtained bio-functionalized carbon textiles were primarily evaluated for use in sustainable applications for wastewater treatment such as Bio-Fenton (BF) and enzymatic Bio-Electro-Fenton (BEF).

Audience Take Away:

- Audience will learn about different eco-friendly plasma treatments which can be used for textile supports and those which enable to activate surface of both conductive and nonconductive surfaces, for enzyme immobilization and efficient bioactivity.
- Knowledge and comparison of enzyme immobilization methods using plasma eco-technologies. Other faculty could use the results to expand their research or teaching. These techniques can be tested in a huge field of applications where the use of enzymes –supported on porous textiles, is required. It does provide practical solutions that could simplify or make a designer's job more efficient, for example in the field of waste water treatment, food processing and in innovative textiles.

Biography

Associate Professor N BEHARY studied Organic and Textile Chemistry at ENSAIT and Lille University, France and graduated as MS in 1995. She then joined the research group of Prof. Caze at GEMTEX laboratory, and received her PhD degree in 2000 at the same institution. She worked in International Relations at ENSAIT between 2002-2006, and joined research laboratory of the PhD institution in 2006. She has carried and supervised research work in the field of ecotechnologies/biotechnologies for functionalization of textiles, and got her “habilitation to direct PhD research” in 2014. She has published more than 40 research articles in SCI (E) journals.

Hydrogenation of Dibenzo-18-crown-6 ether using γ -Al₂O₃ supported Ru-Pd and Ru-Ni bimetallic nanoalloy catalysts

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Ruthenium-palladium (Ru-Pd) and ruthenium-nickel (Ru-Ni) bimetallic nanoalloy particles with various metal compositions were synthesized by microwave irradiated (MWI) solvothermal technique using PVP (poly-N-vinyl-2-pyrrolidone) as capping agent and ethylene glycol as a solvent as well as reducing agent. Synthesized bimetallic nanoalloy particles were subsequently impregnated onto γ -Al₂O₃ support to obtain supported nanoalloy catalysts. Agglomeration of nanoalloy particles were restricted by using excess solvent during synthesis, then distilled and recovered after completion of reaction. Hydrogenation of Dibenzo-18-crown-6 ether (DB18C6) was carried out at 9 MPa, 120°C and 3.5 h using synthesized bimetallic nanoalloy catalysts. It was observed that bimetallic nanoalloy catalyst synthesized by MWI using Ru:Pd 3:1% (w/w), exhibited higher catalytic activity and resulted 98.9% conversion of DB18C6 with 100% selectivity towards cis-syn-cis dicyclohexano-18-crown-6 ether (CSC DCH18C6).

Thermodynamic modeling for the carbonate system $\text{Na-K-HCO}_3\text{-CO}_2$ in alkanolamines solutions: An extended application for CO_2 scrubbing

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CO_2 is considered as the major contributor to the Earth's global warming. Though the cause of emission is driven by regional dynamics, the growth of CO_2 concentration in atmosphere has been around 40% since the beginning of the 21st century. In recognition that coal-fired power plant is a single large source of CO_2 emission makes the post-combustion capturing (PCC) an optimal solution. Furthermore, the presence of acidic gas tends to result in equipment corrosion and pipeline clogging, so that ensuring the security of adsorption process must be in focus. Over the past decades, scientists and researchers are on the lookout for techniques to fasten the CO_2 adsorption process; many have found that amine additives such as monoethanolamine (MEA), diethanolamine (DEA) as well as other blended amine solutions are capable of improving the adsorption efficiency. It is well-known that potassium carbonate (K_2CO_3), aka. hot potash solutions, are among the most prevalent solid sorbents particularly effective to improve the overall performance of CO_2 stripping process. Here the biggest challenge presents is the low in the rate of reaction, thus resulting in poor CO_2 mass transfer if the solution is used alone. By the addition of amine promoters such as MEA or DEA, the rate of adsorption can be greatly enhanced. For example, a study had concluded that when K_2CO_3 aqueous solution is promoted by DEA (20 wt.%), the absorption performance could reach equilibrium enhanced by a factor of 5. Due to its physical nature, K_2CO_3 presents thermal stability, thus capable of serving as an inert, solid sorbent even when temperature exceeds 373 K.

CO_2 absorption technology involves in-depth analysis of chemical equilibrium for all three phases. As such, the aim of this study is to develop a comprehensive thermodynamic model which can be used to forecast the solid-liquid-gas (SLV) equilibrium system that contains $\text{Na-K-HCO}_3\text{-CO}_2$ in alkanolamines solutions, so that this model can be further applied for the calculation of partial pressure of CO_2 under different temperature, loading of solid sorbents, and/or contents of solvent composition. We consider a model reliable for the direct calculation of CO_2 solubility in the promoted, hot potash solution only if both SLE and VLE parameters are accurate. As for preliminary study, we have found an ample of references that reports on the vapor-liquid equilibrium (VLE) data for both systems: $\text{MEA-CO}_2\text{-H}_2\text{O}$ and $\text{DEA-CO}_2\text{-H}_2\text{O}$. However, we can hardly find any relevant data pertaining to the SLE system that reports on the solubility of K_2CO_3 , KHCO_3 in alkanolamine solutions. As such, another objective of this work is to conduct solubility experiments for the proposed, solid-liquid system: $\text{K}_2\text{CO}_3\text{-KHCO}_3\text{-MEA-H}_2\text{O}$, $\text{K}_2\text{CO}_3\text{-KHCO}_3\text{-DEA-H}_2\text{O}$, from the temperature range of 283 – 353 K at atmospheric pressure; this was achieved by adjusting the solubility parameters using the Mixed-Solvent Electrolyte model. All these should aid in the effort for the development of a comprehensive model, which can be applied to forecast the CO_2 solubility in the promoted, potash solution.

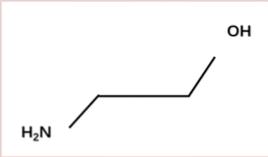
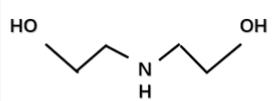
Amine Solvent	Structure	Systems Studied	A List of Species
Monoethanolamine (MEA)		MEA - H_2O (VLE) MEA - H_2O - CO_2 (VLE) MEA - H_2O - K_2CO_3 (SLE) MEA - H_2O - KHCO_3 (SLE) MEA - H_2O - K_2CO_3 - CO_2 (SLV)	H^+ HCO_3^- OH^- K^+ MEA^{H^+} MEACOO^- CO_3^{2-} H_2O MEA (aq) $\text{CO}_2 \text{ (aq)}$ KOH (aq)
Diethanolamine (DEA)		DEA - H_2O (VLE) DEA - H_2O - CO_2 (VLE) DEA - H_2O - K_2CO_3 (SLE) DEA - H_2O - KHCO_3 (SLE) DEA - H_2O - K_2CO_3 - CO_2 (SLV)	H^+ HCO_3^- OH^- K^+ DEA^{H^+} DEACOO^- CO_3^{2-} H_2O DEA (aq) $\text{CO}_2 \text{ (aq)}$ KOH (aq)

Fig 1. A list of amine solvents used, systems studied, and species involved for parameterization.

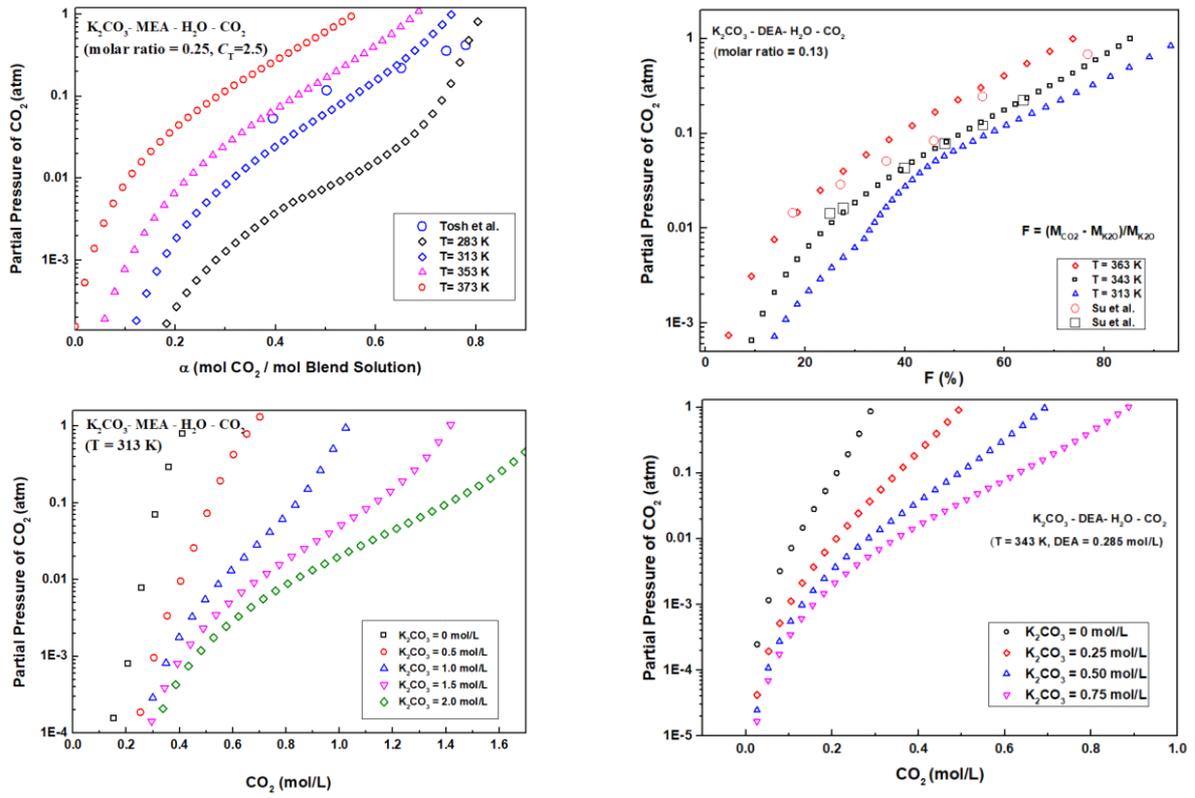


Fig 2. Solubility modeling of CO₂ in quaternary systems: K₂CO₃-MEA-H₂O, K₂CO₃-DEA-H₂O.

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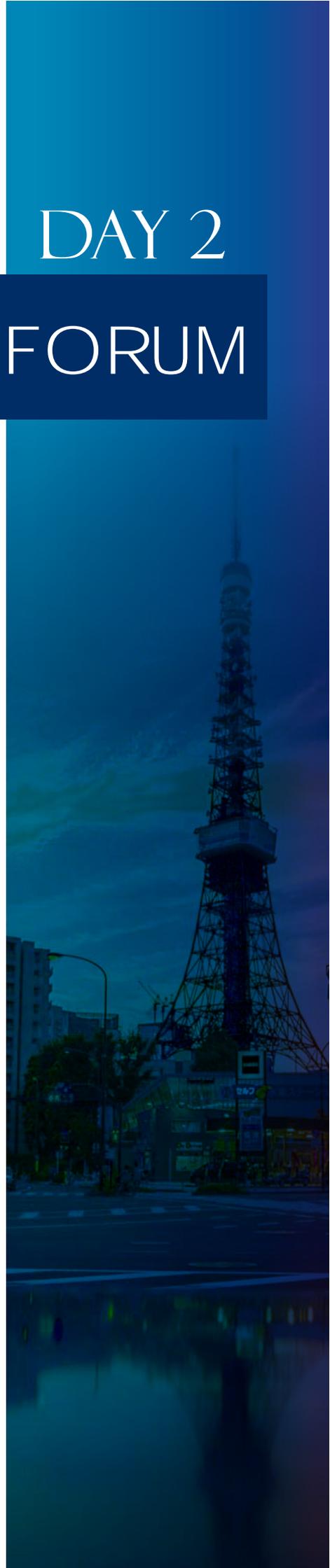
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Biography

Dr. Díaz López (Ciudad Real, 1986) received his PhD degree in Chemical Engineering in 2014 at the University of Castilla – La Mancha (UCLM, Spain). He worked in R&D projects of heterogeneous catalysis and reactor engineering at the Institut de Recherches sur la Catalyse et l'Environnement de Lyon (France) and the Institut de Recerca en Energia de Catalunya (Spain). Recently, Dr. Díaz López obtained a position as a Lecturer at Technical University of Madrid (Spain). He has published 18 research articles in SCI(E) journals and participated in more than 20 conferences.

Passivation by atomic layer deposition to increase the lifetime of Co/Al₂O₃ catalysts in the Fischer-Tropsch synthesis

José Antonio Díaz López

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² Universidad Politécnica de Madrid (UPM), Department of Mechanical, Chemical and Industrial Design Engineering, ETSIDI, 28012 Madrid, Spain

Nowadays, Fischer-Tropsch synthesis (FTS) has regained interest motivated by the development of the biorefinery concept, which is focused on producing chemicals and fuels from biomass sources. Despite being discovered more than a century ago, FTS is still facing some challenges, which hinder its consolidation as a viable alternative to produce synthetic fuels from renewable sources. In this regard, deactivation is a major issue [10.1016/j.cattod.2010.02.077]. In this work, Atomic Layer Deposition (ALD) was used as a passivation technique in cobalt-based catalysts to prevent from deactivation during FTS. This technique has been proven to be feasible in other reactions [10.1021/ar300229c], but not in the FTS.

Starting from a Co/ γ -Al₂O₃ reference (REF, Johnson Matthey), three catalysts have been passivated by Al₂O₃-ALD at different levels (3, 6 and 10 cycles -3ALD, 6ALD, 10ALD, respectively-), then characterized (N₂ physisorption, XRD, TPR, Oxygen titration) and tested in the FTS (230 °C, 20 barg, 8400 NmL/gh, H₂/CO 2 (v/v)). Characterization results revealed that the number of ALD cycles did not affect the cobalt particle size, but led to important changes in reduction properties. In this sense, the higher the number of ALD cycles, the harder the cobalt particles to reduce. These differences were also observed in FTS tests, so that initial catalytic activity of 3ALD (A/A_{REF} = 0.99) and 6ALD (A/A_{REF} = 0.95) was practically the same as the reference, whereas it was lower in sample 10ALD (A/A_{REF} = 0.71). After 100 h of experiment, activity of 3ALD was higher than that of the reference (A/A_{REF} = 1.02), which confirmed the positive effect of ALD as a way to increase the resistance of Co-based catalysts against deactivation in the FTS. Extrapolation of 100 h results to one-year operation (8000 h) led to a significant increase in catalytic resistance against deactivation (Figure 1).

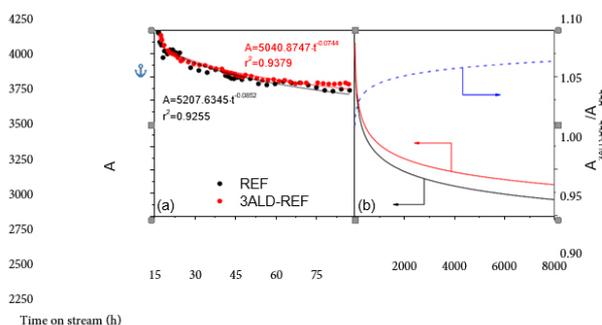


Figure 1. Comparison between REF and 3ALD-REF results and power fitting (a) / Extrapolation of fitted results to 8000 h operation (b). $A = X(\%) \cdot GHSV/100$

To understand the deactivation phenomena and the prevention role of ALD, post-mortem characterization studies will be carried out. Sintering is one of the main causes of catalyst deactivation in the FTS [10.1016/j.cattod.2010.02.077], although other causes such as carbon deposition and cobalt re-oxidation cannot be ruled out.

Further studies will be focused in two pathways: optimize the ALD variables (temperature, number of cycles, ALD precursor) and evaluate the catalytic performance in FTS with real syngas mixtures (H₂/CO/CO₂). This work is part of the European project Heat to Fuel [www.heattofuel.eu], which aims to deliver cost-competitive biorefineries to produce synthetic fuels from biomass residues.

Audience Take Away:

- The current status of fuel market in the European Union and the potential role and benefits of biorefinery processes.
- The renewed interest in the Fischer-Tropsch synthesis and the role of this process to produce synthetic fuels from biomass residues.
- The concept of Atomic Layer Deposition and the application of this technique to increase the resistance of catalysts against deactivation.
- The use of Atomic Layer Deposition as a technique to increase the lifetime of cobalt based catalysts in the Fischer-Tropsch synthesis.



Biography

Q.B. (Rinus) Broxterman (1956) got his PhD degree in 1985 at the University of Groningen (The Netherlands) on an organic chemical topic. He worked for 3 years at an F & F company. From 1988 to April 2017 he worked for DSM in Geleen (NL) in several R&D functions. For more than 10 years he has been Corporate Scientist Chemistry & Catalysis. From May 01, 2017, he is CTO of InnoSyn B V. InnoSyn BV is –since May 01, 2017 - an independent chemical process R&D company in Geleen.

Industrialization of (catalytic) chemistry in flow

Q.B. Broxterman

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InnoSyn B V is a chemical process R&D organization located at the Brightlands Chemelot Campus in Geleen , The Netherlands . InnoSyn performs ‘invention’, ‘improvement’ and ‘implementation’ R&D services for its customers and strategic partners (www.innosyn.com)

Organic chemistry combined with several types of catalysis and supported by modern chemical engineering constitutes the technological competences of InnoSyn.

This presentation will focus on activities in and results of industrializing (catalytic) chemistry in flow.

The purpose of the vast majority of lab/academic work on flow chemistry (mostly with micrometer wide channels) is generation of knowledge, rather than output of (significant) quantities of chemicals. In contrast (and as a consequence) , few reports exist on challenges in and solutions for manufacturing larger amounts of chemical products using flow chemistry (typically few kg/hr and higher).

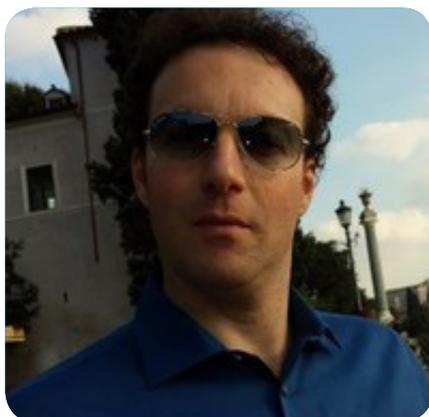
We report here InnoSyn’s results in 3 domains of flow chemistry: the l, l/l, g/l domain, the s/l domain and the g/l/s domain.

The technical challenges are increasing in this order:

- The l, l/l, and g/l domain: cost-performance (flow should be more cost-effective than batch), and handling of fast and highly exothermic chemistry. Organometal cryogenic flow chemistry is an example. The fundamental issues are largely solved.
- The s/l domain: the same challenges as above. On top of this: issues around solids like potential clogging or deposition of solids in the (flow) system. Additionally, dosing solids as slurry is certainly in the R&D phase not trivial. Examples include Grignard and Reformatsky chemistry (formation and use). This domain is under active development.
- The g/s/l/ domain: On top of the challenges above: mass- and heat transfer limitations in the flow system , as a consequence of typical chemistries in this domain, have to be overcome. 3-Phase hydrogenation using a heterogeneous catalyst is a prominent example. This domain is under active development.

Audience Take Away:

- Learn to understand the real life scale-up barriers in modern flow chemistry, and how they depend on the various reaction phases (#, and type).
- Learn why modern flow chemistry is very useful for pharmaceutical and other fine/chemical industries.
- Learn what is new in modern flow chemistry (despite the fact that bulk chemistry already applies continuous manufacturing for a very long period).
- Learn how these challenges were solved for some specific important, but technologically difficult synthetic methods.



Biography

Eng. Eugenio Meloni studied Chemical Engineering at the University of Salerno (Italy) and graduated in 2001. He then joined the research group of Professor Vincenzo Palma at the Department of Industrial Engineering of the same University, as research fellow in the field of Catalysis and Industrial Chemistry. His researches involve the formulation, preparation, characterization and testing of structured catalysts for (i) soot abatement emitted by diesel engines or bio-mass combustion plants, and (ii) the intensification of different catalytic processes, also by means of alternative energy sources. He published about 47 research articles on international peer reviewed journals, with h-index 10.

Process intensification: New perspectives for Chemical Engineering

Eugenio Meloni

University of Salerno, Department of Industrial Engineering, Via Giovanni Paolo II, 132 – 84084 Fisciano (SA)

The European Union, through the SET-Plan, aims to reduce greenhouse gas emissions by 20%, to have a 20% share of energy from low-carbon energy sources and to have a 20% reduction in the use of primary energy by improving energy efficiency by 2020, with a long-term ambition to reduce emissions by 80-95% by 2050. In particular EU suggested that in the future energy system, H₂ should be produced from renewable feedstock using renewable energy in order to be considered “zero CO₂”, so resulting in a practically closed carbon cycle with no impact (in terms of anthropogenic emissions) to the environment. In this way, a process intensification is mandatory. The approach to process intensification regards process-intensifying equipment, characterized by designs that optimize mass, heat, and momentum transfer (e.g. monolithic catalysts) and process-intensifying methods, involving the application of alternative energy sources, so leading to compact, safe, energy-efficient, and environment-friendly sustainable processes. In particular, the use of structured catalysts with high thermal conductivity, could overcome the heat transfer limitations that occur in both endothermic and exothermic reactions. For example, in the case of Methane Steam Reforming (MSR) reaction, the limiting step is the heat transfer towards the reaction volume, since its high endothermicity requires high heat fluxes, so resulting in complex reactor geometries and very high temperatures of heating medium. Therefore, very expensive construction materials, very high reaction volumes and very slow thermal transients are present. The structured catalysts could allow achieving a very uniform temperature profile, resulting in a more effective and selective exploiting of catalyst surface, minimizing the catalyst mass, making the system more attractive in terms of cost and compactness.

Furthermore, the appropriate catalyst carrier selection is a key point for the equilibrium-limited exothermic reaction, such as Water gas Shift (WGS). A flattened temperature profile, i.e. higher inlet temperature and lower outlet temperature, may be realized enhancing the heat back-diffusion in the solid structure of a high conductive catalyst carrier, so allowing higher reaction rates at the inlet sections and higher CO conversion at the outlet section, minimizing the overall reaction volume.

Audience Take Away:

- The presentation could allow the audience to view Chemical Engineering in a new point of view, by identifying the limiting step of a process and consequently generating alternatives in order to implement an innovative process.
- The presentation could help in a sustainable process design, and in a scale-down of an existing industrial process, with the aim for example of a distributed H₂ production.



Biography

Dr. Kukueva studied Chemistry at the Cherkassy National University of Bohdan Chemelnizky, Ukraine and graduated in 1989. She then joined the research group of Prof. Minaev B.F. at the State Technological University, Cherkassy, Ukraine. She received her PhD degree in 1996 at the institute of Physical Chemistry of Pissar-gevsky of Ukrainian Academy of Science (Kiev, Ukraine). Recently Kukueva Vitalina has received three years postdoctoral fellowship supervised by Prof Lisichenko at the Institute of Environmentally geochemistry Ukrainian Academy of Science (Kiev, Ukraine). She has published more than 50 research articles in SCI(E) journals.

Predictions of chemical reactivity with theoretical calculations

Kukueva Vitalina

Cherkassy State Technological University, Cherkassy, Ukraine

Today, organic phosphorus compounds (OPC) are actively exploring all the main scientific centers of the world, as determined by their chemical benefits, the importance of the activity of organisms and great potential practical use in industry, fire safety, agriculture and everyday life. There are some different points of view on the reaction mechanisms of inhibiting action of OPC on the combustion, that can be presented as number of different reactions with active centers of flame $H\cdot$, O^{\bullet} , $OH\cdot$ participation. In the experimental work showed that the OPC has extinguishing properties, but the mechanism at the elementary reactions not yet finally clarified. In the work of Werner and Cool, a reaction path of OPC destruction to form a molecule of CH_3PO_2 . In this channel is secondary. On the contrary, it is argued that the destruction occurs mainly through methylphosphonate and further to phosphoric acid. A model for the study is the following. First of all we have calculated energy gap corresponding chemical bonds in the molecule of researched extinguishing agent then gradually have calculated the interaction energy of each of the products formed from the degradation with the active centers of the flame. For the development of mechanisms of the inhibitory effects of OPC on the flame possible ways of thermal degradation of this compound quantum chemical ab initio (6-31 G⁺) method have been examined. The research has showed that the thermal degradation of OPC molecules occurs by gradual elimination of atoms and groups of atoms. It is Werner-Cool point of view on the OPC destruction mechanism. So, theoretical calculations helped us to predict the most probably reaction ways in the complicated chemical processes.

Audience Take Away:

- I think that anybody from the audience will be able to make identical calculations in their own researches.
- Presented materials allow opening peculiarities of reaction mechanisms. It will help to penetrate in the researched processes deeper. This research can be useful for direction of experimental investigations to predicted more preferable reaction ways. Theoretical calculations provide a practical solution to a problem that could make a designer's job more efficient, because the number of experimental tested samples could be minimized? It will improve the accuracy of a design and provide new information to assist in a design problem.
- Preliminary theoretical calculations minimize the economic costs of experimental studies.

SPEAKERS

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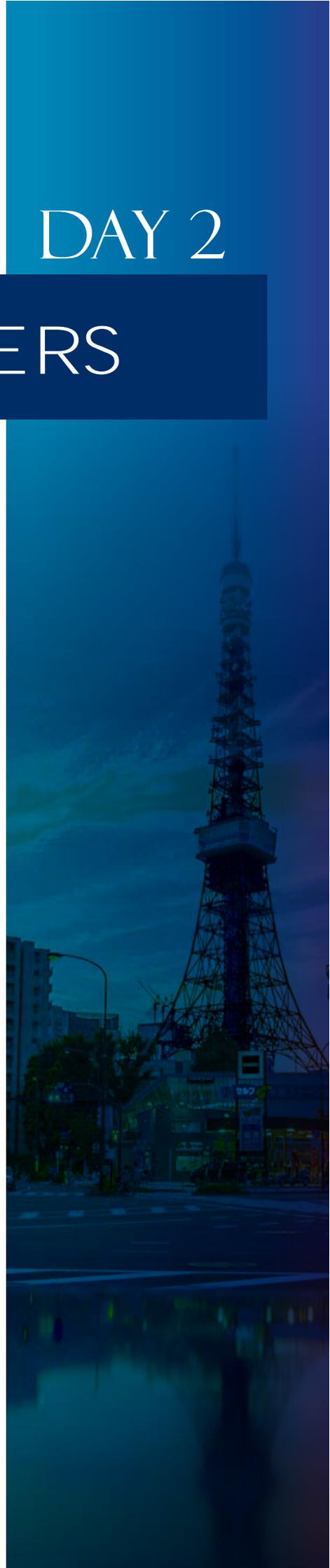
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Photoelectrocatalytic removal of anticancer drug from water solution

Aleksandra Pieczyńska¹, Paweł Mazierski¹, Patrycja Wilczewska¹, Agnieszka Fiszka Borzyszkowska¹, Anna Białk-Bielińska², Adriana Zaleska-Medynska¹, Ewa Maria Siedlecka¹

¹Department of Environmental Technologies, University of Gdańsk, Gdańsk, Poland

²Department of Environmental Analysis, University of Gdańsk, Gdańsk, Poland

Chemotherapy drugs are considered a group of emerging pollutants which can possibly impact the aquatic life in the water bodies receiving effluents from wastewater treatment plants. Therefore, the search for alternative methods that will enable the effective removal of drugs from pharmaceutical wastewater and hospital or/and municipal sewage is still a top priority. Photoelectrochemical oxidation is one of the promising method for degradation persistent and toxic organic pollutants from aqueous phase. Based on the literature data and own experience, it could be concluded that the efficiency of the photoelectrochemical treatment system depends mainly on activity of the photoelectrode materials. Thus, one of the challenges in this field is the development of photoactive materials, in the form of thin layer, activated by low powered and low cost irradiation sources (such as sunlight). So far, in such processes, as photoelectrodes were used various types of semiconductors, among which the most frequently used was TiO₂. However, pure TiO₂ nanostructures are active only under UV radiation. One of the method to enhance the photocatalytic activity under visible light is sensitization of TiO₂ nanostructures with narrow-gap semiconducting materials. Sensitization of TiO₂ nanostructures with quantum dots (QDs) of narrow-gap semiconductors, such CdS, PbS, SnS will allow for obtain a new materials with photoelectrochemical activity under visible light. The activity of these nanocomposites will depend on their surface and structural properties like type of semiconductors, size and amount QDs.

In the presented study, we prepared photoanodes based on TiO₂ nanotubes which were sensitized with QDs of CdS, PbS, SnS and applied them for photoelectrocatalytic removal of selected anticancer drugs. The photoelectrodes differed in type of semiconductor, amount and size of QDs. The structure and morphology of photoelectrodes were investigated. The PEC degradation activity of the prepared electrodes at different values of electric potential, irradiation intensity, pH and drug was determined. The participation of individual oxidants in anticancer drugs degradation was studied based on reactions with scavengers. Moreover, the photoelectrocatalytic degradation pathway of anticancer drugs and the ecotoxicity of the effluents against *Lemna minor* were investigated.

Audience Take Away:

- Correlation of surface, optical and electrochemical properties with photoelectrochemical activity of nanocomposites Ti/TiO₂(NTs)/XaSb
- Better understanding of the mechanism of nonocomposite formation and dependence between parameters of SILAR method and surface properties of obtained nanostructures
- The efficiency and mechanism of photoelectrocatalytic degradation of anticancer drugs

Biography

Dr Aleksandra Pieczyńska studied Environmental Protection at University of Gdańsk (Poland) and graduated as MS in 2009. She also completed Engineer degree at Gdansk University of Technology in 2011. She then joined the research group of Prof. Siedlecka at the Department of Environmental Technologies, University of Gdańsk. She received her PhD degree in 2014 at the same institution. In 2013 she started work as Research Assistant at Department of Environmental Technologies, University of Gdańsk and since 2015 she obtained the position of Assistant Professor at the same institution. She has published 20 research articles in SCI (E) journals.

Acknowledgement:

Financial support was provided by the Polish National Science Center [grant number 2015/19/D/ST5/00710].

Design and fabrication of hybrid Nano-Filters for waste water remediation

Qurat Ul Ain Nadeem ^{1,2*}, Rohama Gill ², Dmitry Shchukin ¹

¹Stephenson Institute for Renewable Energy, University of Liverpool, UK

²Fatima Jinnah Women University, the Mall, Rawalpindi, Pakistan

Deterioration in the drinking water facilities is one of the major and life threatening concerns of the developing world. A number of scientific studies have been conducted to resolve the issue while numerous are in pipeline to attain a cost-effective method for the particular issue. Present research also highlights the scientific efforts done in the similar field to resolve this devastating issue. Promising results were obtained by synthesizing photocatalytic nano-coatings comprised of mixed-metal oxides of ZnO-CdO and ZnO-MnO₂ via co-precipitation method followed by their inclusion in multi-layered thin polymeric films using Layer-by-layer (LbL) deposition. FTIR and XRD analyses confirmed the appropriate chemical bonding (503.44 cm⁻¹ and 472.56 cm⁻¹), crystallographic characteristics (ZnO-CdO ~ 36.2nm and ZnO-MnO₂ ~ 29.0nm), and phase identification of the subject moieties, respectively. Raman studies also confirmed the presence of specific bonding in relation to each type of mixed-metal oxide thin film setup. Multi-layered thin films deposition for PEI(PSS/ZnO-CdO)_n and PEI(PSS/ZnO-MnO₂)_n layers was also recorded at 375 nm for 10 bilayer of PEI(PSS/ZnO-CdO) and PEI(PSS/ZnO-MnO₂), respectively, with increasing absorbance per layer pair. While testing their pollutant removal/degradation potential, the two multilayer systems were found highly effective to remediate an organic pollutant i.e. Methyl Blue from wastewater systems with photocatalytic degradation capabilities of up to 95% along with an appropriate re-cycling efficiency of upto several cycles. Moreover, the designed setup has also shown adsorption efficiency for inorganic pollutants e.g. heavy metals and 92% adsorption of 20ppm Cu is seen when tested against polluted water.

Audience Take Away:

- Present research highlights an innovative design of nano-filters that can cater both organic and inorganic pollutants from aquatic environment in one go.
- The design of the study is quite simple and easy to operate, as well as the product formed is quite cost-effective in terms of its wide spread usage for environmental remediation. Moreover, the particular methodology has enough room to study and fabricate nano-filters of the same kind using different mixed metaloxides.

Biography

Ms. Qurat Ul Ain Nadeem is an active environmentalist who is pursuing her Doctoral research in Environmental Chemistry from Fatima Jinnah Women University, Pakistan and from Stephenson Institute for Renewable Energy, University of Liverpool under a sandwiched scholarship program funded by Higher Education Commission (HEC), Pakistan. Her research advisors include Dr. Rohama Gill and Prof. Dmitry Shchukin, the two renowned names in these particular fields. Ms. Nadeem has also worked as a research associate in HEC (Pakistan) funded Project No. 5461/Punjab/NRPU/R&D/HEC/2016. She has published quality research works in reputed journals and is working enthusiastically to contribute her energy into the environment of sciences.

Structure & performance of Li/MgO supported molybdenum oxide for oxidative cracking of N-Hexane

Cassia Boyadjian^{1*}, Leon Lefferts²

¹Baha and Walid Bassatne Department of Chemical Engineering and Advanced Energy, Maroun Semaan Faculty of Engineering and Architecture, American University of Beirut, Beirut, Lebanon

²Catalytic Processes and Materials, MESA+ Institute for Nanotechnology, University of Twente, Enschede, the Netherlands

Oxidative cracking of n-hexane, as a model compound to naphtha, is studied as an alternative to steam cracking for production of light olefins. Li/MgO is a potential oxidative cracking catalyst due to its non-redox properties and high selectivity to olefins. In this work, we further study the possible enhancement of properties of Li/MgO through promotion with molybdenum. Structural details of molybdenum promoted Li/MgO are investigated with XRD, XPS, TPR and Raman spectroscopy. Catalytic oxidative cracking experiments are performed in 4mm alumina reactor packed with 0.4-0.6mm catalyst particles. Reactant gas consisting of 10 mol% of hexane vapor, 8 mol% of O₂ and balance helium is fed to the reactor at a rate of 100ml/min. Reactions are studied at temperature of 575 °C and WHSV between 154 – 385h⁻¹.

Structure-performance study of Mo-Li/MgO catalyst indicates the presence of three types of molybdate species, the formation of which depends on Mo loadings. (i) Isolated tetrahedral [MoO₄]²⁻ species, (ii) monomeric Li₂MoO₄ phase in which MoO₄ is tetrahedrally coordinated and (iii) polymeric Li₂Mo₄O₁₃ phase in which Mo is octahedrally coordinated. These phases are present in low concentrations, below the detection limit of XRD and their formation becomes significant with the increase in atomic ratio of Mo/Li. We show that these molybdate phases are inactive for C-H bond scission in the alkane, yet result in considerable improvements in both catalyst surface area and stability.

Improvement in catalyst surface area is explained by the formation of Li₂MoO₄ and Li₂Mo₄O₁₃ phases from reaction of MoO₃ with various lithium phases (Li₂O and Li₂CO₃) during catalyst preparation reducing the amount of Li₂CO₃ originally present in Li/MgO and responsible for catalyst sintering when exposed to high temperatures. Catalyst stability is improved due to increased acidity of the Li/MgO upon promotion with molybdenum, preventing CO₂ adsorption on Li⁺O⁻ active sites of the catalyst, hence inhibit sintering and loss of low coordinated Mg²⁺LCO²⁻LC sites.

It is concluded that minimal Mo loadings (0.3wt%) is sufficient to bring considerable improvements in the catalyst, while high Mo loadings lead to enhanced redox activity and CO₂ formation. 0.3 wt% Mo promoted Li/MgO catalyst is efficient for the selective conversion of hexane to olefins, giving olefin yield up to 24%, and very good stability with time on stream.

Audience Take Away:

- Li/MgO catalyst is already well studied in literature for applications such as oxidative coupling of methane, oxidative dehydrogenation of alkanes. The following paper further investigates the performance of the catalyst for the oxidative cracking of n-hexane.
- The paper proposes molybdenum promoted Li/MgO as potential catalyst for oxidative cracking of naphtha, as an alternative to steam cracking. The catalyst seems to be promising for the production of light olefins from naphtha. The proposed catalyst could be further studied for cracking of renewable feedstock such as bio-oil, pyrolysis oil etc.
- The paper presents detailed characterization on the various oxide phases present in the catalyst and their role in enhancing catalytic properties.

Biography

Cassia Boyadjian has a master's degree (2005) in chemical process engineering and PhD (2010) in heterogeneous catalysis from the University of Twente in the Netherlands. She performed her PhD work at the group of Prof. Leon Lefferts on catalytic cracking of n-hexane. In 2011–2013 she worked at BASF in Ludwigshafen as research scientist of petrochemical catalysts. In 2013–2014 she worked at BASF-Antwerp as process engineer. In 2014 she joined the American University of Beirut as assistant professor of chemical engineering. Her research interests are in catalytic conversion of waste and renewable carbon sources into chemicals and fuel.

The conversion of poly aromatic hydrocarbon into fine chemicals and fuels over molybdenum phosphide supported on various acidic and porous materials

Muhammad Usman*, Aasif Helal, Abuzar Khan, Oki Muraza, Zain H. Yamani

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The search for the cheap, efficient and highly selective catalytic process of heavy aromatics for fine chemicals and fuels is currently a popular research direction. Coal tar is the major byproduct during the coal carbonization process, which are the major and important feedstocks composed of various chemicals and carbon-based materials. Naphthalene which is a major component in coal tar could be converted into a useful product i.e., Tetralin by controlled partial hydrogenation. The quest for finding an appropriate catalyst in this direction is the topic of this work. In this study, the hydrogenation of polyaromatic hydrocarbon-naphthalene was conducted over metal phosphide catalysts (MoP) supported on three different acidic zeolite (Hbeta, HZSM-5, and HY) and inert activated carbon (AC) to know the effect of different acidic density and pore size on the conversion of polyaromatic hydrocarbon into fine chemicals and fuels. These results revealed that the MoP/Hbeta having the highest pore size and strong acidity cause deep cracking and are highly selective to low carbon fuels. The selectivity to ring opening product decrease by decreasing the acid density. Lowest cracking and high selectivity to tetralin were found on the MoP/AC due to the weak acidity, microporous structure, and low reduction temperature which don't allow the reactant feed to react effectively to the catalyst surface. It was concluded that the coal and coal tar aromatics can be converted selectively to various chemicals and fuels by selecting the optimum metal phosphide supported on zeolites having appropriate acidity and porous structure.

Audience Take Away:

- The audience will learn about the design and application of highly selective and stable heterogeneous catalysis for petrochemicals.
- The lecture will cover to solve a problem from fundamental lab work to industrial scale. This work will also cover the backbone of heterogeneous catalysis (conversion, selectivity, and stability).
- The audience will learn how to achieve high selectivity and stability using heterogeneous catalysis. This will help the audience to design material for targeted applications.
- Industrial catalyst requires long term stability which will be covered during this speech. This speech will provide a perspective on how to convert environmentally hazardous chemicals into useful chemical products through heterogeneous catalysis.

Biography

Dr. Muhammad Usman received Master degree in Chemistry from the University of Peshawar, Pakistan in 2009. Dr. Usman earned Ph.D. in 2014 from Institute of Process Engineering, Chinese Academy of Sciences, China. He has four years of postdoc research experience from Tsinghua University China and Berkeley Global Science Institute at KFUPM. At present, Dr. Muhammad Usman is serving as a Research Scientist (~ Assistant Professor) in the Center of Excellence in Nanotechnology, King Fahd University of Petroleum and Minerals, Saudi Arabia. Dr. Usman expertise included zeolite for heterogeneous catalysis, adsorption kinetics, catalytic modeling designing & application. Dr. Usman holds two US patents, published > 20 peer-reviewed international journals (like ACS catalysis, J Mat Chem A, Chemical Eng J, AIChE) in addition to several conference proceedings/presentations.

Confinement effect of alcohols and water in MFI Zeolite from Ab Initio molecular dynamics simulations

Mal-Soon Lee

Institute of Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington, USA

Zeolites are one of the most promising solid acid catalysts for chemical conversion of renewable biomass-derived alcohols into fuels and chemicals through alcohol dehydration condensation and alkene oligomerization. Dehydration of alcohols to alkenes is a well-known prototypical acid catalyzed reaction, where confinement and entropic effects impact the rates of these reactions. For such conversions, H-ZSM-5 zeolite is commonly used as a platform for acid catalyzed reactions due to its strong acidity and enhancement of reaction rates due to confinement in pores. One grand challenge is to understand how confinement and solvent influence entropic effects and ultimately impact the rates of these reactions. In this talk, I will present the structure and thermochemistry of ethanol and water adsorption on the Brønsted acid site of H-ZSM-5 by means of ab initio molecular dynamics (AIMD) simulations. Structural and spectroscopic properties obtained from simulations will be discussed and directly compared with *in situ* infrared (IR) and NMR spectroscopy. Entropic component of free energy is strongly influenced by the confinement and solvent effect. We will discuss entropy and enthalpy of adsorption estimated from the computed vibrational density of states (VDOS) using a quasi-harmonic approximation. Our results show a good agreement with available experimental measurement. This enables us to take into account enthalpic and entropic effects caused by the dynamics of the motion of the reaction intermediates. AIMD simulations show that hydrogen transfer from the zeolite scaffold to water/ethanol occurs as temperature and water/alcohol content increases. In the simulations with only ethanol g, proton transfer occurs via relay between H-bonded ethanol molecules. When water is present the excess proton becomes soluble at a mobile $\text{H}_3\text{O}^+[\text{H}_2\text{O}]$ cluster. Overall, this study exemplifies how anharmonic effects, as captured by AIMD, are critical for the quantitative modeling of the free energetics of zeolite-catalyzed processes.

Audience Take Away:

- Confinement and solvent effect on adsorption enthalpy and entropy and hence adsorption free energetics on zeolite
- Influence of water on alcohol adsorption on zeolite
- Anharmonic effects, as captured by AIMD, are critical for the quantitative modeling of the free energetics of zeolite-catalyzed processes

Biography

Mal-Soon Lee is a senior scientist at Pacific Northwest National Laboratory, USA. She has been working in the field of computational physics/chemistry with an emphasis on studying the phase behavior and reactivity at complex interfaces using a variety of statistical mechanical tools. Her areas of application include studies of catalysis, CO_2 sequestration, nuclear waste disposal. She employs large-scale high-performance computing techniques such as ab initio molecular dynamics to understand materials' properties and free energetics at high temperature/pressure. With statistical mechanical techniques, she calculates enthalpies/entropies of reaction, spectroscopic properties, which can be directly compared with experimental observations.

Synthesis, characterization, and application of MOF@clay composite as a visiblelight-driven photocatalyst for environmental remediation

Radheshyam Rama Pawar* and Keiko Sasaki

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In the past two decades several hundreds of new Metal-Organic Frameworks (MOFs) have been reported for diverse applications (such as adsorption, separation, magnetism, photoluminescence, drug delivery including catalysis & photocatalysis, etc.). Whereas till this time, very few of them also have been commercialized; nevertheless, a large number of MOFs show limitations such as high production cost, poor chemical stability, obstructing their practical applications. Compositing of MOFs with other materials is a very new research avenue that appears to offer the solution to issues mentioned above. Besides, established composites show improved performances in the targeted areas of applications due to developed synergistic structural and textural properties effect. So far, plenty of MOF composites with organic polymers and carbon matrices have been developed for targeted applications. Surprisingly, there are scarce reports on composting of MOFs with clay minerals, which are naturally abundant, highly stable, low-cost containing variable elements (including of iron, magnesium, silica and other cations) which has a potential to offer not only superior aquatic stability and surface area suitable for adsorptive removal of organic and inorganic contaminants from water bodies, but also charge carrier in photocatalytic composites. In this regards in the present investigation, novel MOF@clay composites were fabricated *in situ* with most water stable $Zr_6O_4(OH)_4(ABDC)_6$ (where ABDC = 2-aminobenzene-1,4-dicarboxylic acid) and by varying the natural sepiolite (Sp) content in MOF@Sp_{1,2} and 3 composites. The amino-functionalized MOF is selected due to its high light absorption ability in the visible light region and, natural sepiolite was used due to its fibrous morphologies, which offer rigid and active surfaces for the adsorption of cationic dye molecules through electrostatic interaction. The original and fabricated composite materials were systematically evaluated by PXRD, FTIR, N_2 adsorption-desorption, XPS, TGA, and elemental composition measurements to investigate the alteration in the structural and textural properties. The zeta potential measurement confirmed that the surface coverage of fibrous Sp with completely developed MOF particles through strong electrostatic interaction between the positively charged MOF and the negatively charged sepiolite. The N_2 adsorption uptake, especially at the low-pressure in MOF@Sp₂, was observed higher than the original MOF and Sepiolite. This might be because the assembly of the MOF nanoparticles is expected to increase the actual number of neighboring framework atoms. Additionally, composite MOF structures enhanced thermal stability due to the incorporation of stable Sp. The optimized MOF@Sp₂ composite validates the high dispersion of MOF particles on the Sp matrix which serves as an efficient photocatalyst for degradation of Rhodamine B (RhB) as a model of organic pollutants under visible light irradiation due to their synergistic effect. Also, the reason can be explained by the fact that the well-dispersed MOF particles on the surface of sepiolite enhanced to degrade RhB by avoiding the recombination between photogenerated electrons and holes in MOF@Sp₂ composite. The optimized composites were also examined under several batches of photocatalysis experiment to optimize the solution pH and amount of catalyst loading. The developed composite was observed highly stable in under highly acidic and basic pH conditions. The possible mechanism of RhB degradation was proposed, where a superoxide radical is mainly responsible for RhB degradation, confirmed by scavenger test. Overall the present study delivers a novel approach for the construction of highly effectual MOF@clay based composites for visible light-driven photocatalysis for environmental remediation.

Audience Take Away:

Environmental concerns such as water pollutions are of paramount importance in front of the global research community today that has driven enormous efforts to develop cost-effective and sustainable technologies offering rapid and reliable removal of contaminants from water. These research efforts have offered partial solutions to water pollution and related problems with their pros and cons. Therefore, we anticipate the research outcome in terms of the new and efficient materials for adsorptive removal of toxic inorganic and organic water contaminants as well as efficient photocatalysts for the degradation of organic pollutants. The present study has the potential to offer new methodologies and technologies for *in-field* bodies such as industrial effluents and naturally contaminated waters. These research studies provide a very new research avenue to expand interdisciplinary research applications by using MOF@clay composite. This research topic is also useful to many different faculties to improve the understanding of MOF@clay composite materials in the concern areas of application. Moreover, it would result in the generation of intellectual properties such as scientific patents and publications.

Biography

Dr. Radheshyam R Pawar studied Chemistry at the North Maharashtra University, India and graduated as Master of Science in 2006. He then joined the CSIR-CSMCR-research institute in Bhavnagar, India as a research fellow and worked for India Government funded projects for four years. In

2011 he registered for his doctoral study under the guidance of Prof. Dr. H C BAJAJ. At the same institute in the Department of Inorganic Material and Catalysis. He received his Ph.D. degree in Chemical Science in 2014 from AcSIR-CSIR New Delhi-India. Then he joined as a postdoctoral fellow with Prof. S M Lee at Kwangdong University, South Korea for three years. Presently he is working as a JSPS postdoctoral research fellow in the research team of Prof Keiko Sasaki, Department of Earth Resources Engineering, Faculty of Engineering, Kyushu University, Fukuoka, Japan. Dr. Pawar has published more than 30 research articles in refereed international journals.

Cluster beam deposition of preformed metal clusters for liquid and vapour phase catalysis

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The deposition of preformed cluster beams onto suitable supports represents a new paradigm for the precise preparation of heterogeneous catalysts. Compared with traditional chemical methods, it exhibits a range of unique advantages including good size (and composition) control, no toxic reagents needed, absence of chemical ligands etc. However, for a long time the feasibility of cluster-beam deposited catalysts for reactions under realistic conditions has been limited by the low production rate. Based on our successful scale-up of the cluster flux, we present here two experimental validations of cluster catalysts, for liquid phase and vapour phase reactions, respectively. i) Au/Cu nanoalloy clusters of variable compositions on MgO powder supports, created by a dual-magnetron sputtering gas condensation cluster source, are found to be highly active for the catalytic reduction of 4-nitrophenol in solution. The interplay between the Au and Cu atoms at the cluster surface appears to enhance the catalytic activity via the binding energies of product and reactant. In addition, the physically deposited clusters with Au/Cu ratio close to one show a 25-fold higher activity than a Au/Cu reference sample made by chemical impregnation. ii) Size-controlled Pd clusters deposited on diced graphite tapes from the Matrix Assembly Cluster Source (MACS) are found to be much more active (per unit weight) than a Pd reference sample made by wet impregnation in the vapour phase 1-pentyne selective hydrogenation reaction. Cluster size evolution before and after reaction suggested that the superior activity derived from the smaller cluster size and better stability against sintering compared to the Pd reference sample. In addition, no synergetic effect was found in Pd/Au cluster catalyst. The observed similar activity (per surface atom) from the Pd and Pd/Au cluster catalysts could be attributed to surface oxidation, which can drive the Pd atoms to the cluster surface, thus forming a similar Pd surface as pure Pd clusters.

Audience Take Away:

- In my presentation, I will introduce a method to prepare solvent-free cluster catalysts by cluster beam techniques.
- The active site of Au/Cu binary clusters for nitrophenol reduction is Au/Cu two atom site.
- The catalytic performance of the cluster catalysts (Pd clusters supported on diced carbon tapes) made with a new type of cluster beam source, MACS, is demonstrated in selective hydrogenation of 1-pentyne to 1-pentene in vapour phase, which shows a higher activity (per unit weight) than the reference sample made by traditional impregnation.

Biography

Rongsheng Cai is currently a Research Officer in the Nanomaterials Lab, College of Engineering, Swansea University. He obtained his M.S. degree in Materials Science from Qingdao University (2014) and undertook a PhD supervised by Prof. Richard Palmer at the University of Birmingham (2014–2018). His research interests focus on transmission electron microscopy and catalytic properties of deposited metal clusters. He has published more than 30 research articles in SCI journals.

NMR Methods for operando analysis of heterogeneous catalytic processes

Mojtaba Mirdrikvand¹, Wolfgang Dreher

¹The University of Bremen, Department of Chemistry, In vivo MR group, Leobener Str. 7, 28359 Bremen, Germany

The in situ analysis of catalysed gas phase reactions offers not only an accurate characterisation of the reactions, but also the possibility to validate numerical simulations. The latter allows optimizing operational performance and reducing industrial costs as well as predicting possible risks at scaled up reactors. Nuclear Magnetic Resonance (NMR) can be used as a non-invasive method for the in situ analysis of velocity, diffusion, temperature, and concentration of species in heterogeneously catalysed systems. The possibility of monitoring the crucial reaction parameters online and simultaneously in opaque reactors turns NMR into a powerful toolkit for the operando analysis of reactions. To determine each parameter, optimised NMR techniques are required. This contribution shows practical and methodological examples of NMR methods in the fields of in reaction engineering with emphasis on methanation reaction. The talk includes NMR Velocimetry (MRV) of methane gases in foam catalyst carriers followed by an analysis of diffusion and dispersion of gas in monolithic structures. Furthermore, NMR spectroscopic imaging (MRSI), and NMR Thermometry will be discussed in order to show how the temperature profile of catalyst bed can be determined in highly exothermic reactions such as methanation or Fischer-Tropsch reaction. Finally, the analysis of tortuosity, NMR relaxation times and diffusion in micro- and macropores illustrates to which extent NMR can characterise heterogeneous catalysts coated on foams or pellets. The obtained results may directly improve numerical micro- or macroscale simulations.

Audience Take Away:

- Explain how the audience will be able to use what they learn?
- The talk will give an insight into NMR approaches for measurements of velocity, diffusion, temperature, and concentration of substances in gas/liquid phase heterogeneous reactions.
- How will this help the audience in their job?
- The proposed NMR methods can be applied to ongoing or future studies in reaction engineering groups participating in the conference.
- Will it improve the accuracy of a design, or provide new information to assist in a design problem? List all other benefits. Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient?
- The results directly benefit numerical pseudo-heterogeneous simulations of reactors by giving precise information on
- Full field velocity analysis in monoliths structured catalysts
- Temperature profile in catalyst bed
- Axial and radial dispersion of gas in monolithic structured catalysts

Biography

Mojtaba Mirdrikvand has completed his master studies in chemical and energy engineering at the University of Magdeburg in Germany. He is currently as research assistant at the University of Bremen. He has been also working as visiting scholar at the School of Chemical Engineering and Analytical Science at the University of Manchester in 2018. His current research aims at process analysis using NMR techniques to characterise mass transport and reaction processes.

Environment management and advancing technological processes for technical lead production

Ahmet Haxhijaj

University of Mitrovica, Republic of Kosova

In this talk we aim to present the analyses of the composition of agglomerate that is used in Shahte-water-jacket furnace in Trepça. It is also analyzed the theoretical and real consumption of the coke for technical lead produced. The aim of the research is to optimize the parameters of the technological process in order to increase quantity of the technical lead produced by minimizing the quantity of lead in agglomerate and gases in the furnace. The data presented are supported in the work of Shahte furnace and are a result of the theoretical and experimental study of the quantity of scoria and the percentage of the lead in the scoria. The presentation especially emphasizes the increase of the technical lead and minimizing the quantity of the lead in the scoria. The research also emphasizes the reduction in energy consumption and the improvements in the environment protection. The Insitiute Vniicvetrnet has concluded that the future of the lead metallurgy and lead production with economic and environmental sustainability stands on the processes with direct reactive melting in the Kivcet Process. The research has analyzed Kivcet processes for the possibility of utilizing it in the lead production in Trepça Company.

Biography

Professor Ahmet Haxhijaj was entitled PhD by University of Prishtina, Faculty of Mining and Metalurgy, with topic "Intensify and Optimize the Reductive Process of Melting the Lead Agglomerate in Port-Piri Furnace" in 2003. In 1989 he finished post-graduate studies at University of Zagreb, Faculty of Metallurgy, Sisak. He studied Metallurgy Science and presented a master thesis in "Materials and Heat Balance in Port-Piri Furnace". In 1978 graduated in the topic "Indium Composition in Products and Inter-products of Lead and Zinc, and Seperation Process of Extracting Indium in Trepça. He currently lectures in the Department of Metallurgy and Materials, Faculty of Geoscience, University of Mitrovica and Faculty of Applied Arts at University of Peja. He published more than 42 papers and is a member of the Alb-shkenca board. Since 2016 is the Editing Chief on IJMPEM "International Journal Minerals Processing Extractive Metallurgy. In 1983-1993 he worked in the Zastava laboratory in Peja në thermal processing and was the manager of four projects in this field. In 1978-1983 he worked in the Lead Metallurgy in Zveqan, Trepça.

Novel efficient Pd-free catalyst for Suzuki C-C coupling reaction: Green protocol

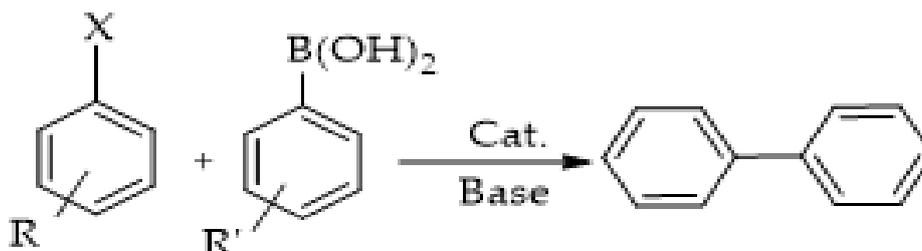
Ghalia Alzhrani¹, Nesreen S. Ahmed², Elham S. Azam¹, Tamer S. Saleh^{2,3}, Mohamed Mokhtar^{1,2*}

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Suzuki cross-coupling reaction has developed one of the furthestmost effectual approaches for the synthesis of biaryls or substituted aromatic moieties from aryl halides and arylboronic acids with a palladium-catalyst in the past two era's. Herein, Pd-free layered double hydroxide containing nickel catalysts were prepared by co-precipitation method under ultrasonic irradiation and N₂ atmosphere with different molar ratios of Ni: Mg: Al and coded as (1NiLDHs-Dr), (1.5NiLDHs-Dr) and (2NiLDHs-Dr). A series of reduced catalysts under 5% H₂/N₂ at different temperatures were coded as 1NiLDHs-R200, 1.5NiLDHs-R200 and 2NiLDHs-R200. As-synthesized 2NiLDHs-Dr was the superlative catalyst when coupling different aryl halides with different boronic acids derivatives. Deep investigation of all catalysts was done using different techniques such as inductively coupled plasma optical emission spectroscopy (ICP-OES), x-ray photoelectron spectroscopy (XPS), powder x-ray diffraction (XRD), thermogravimetric analyses (TGA), Fourier transfer infrared (FTIR), scanning electron microscope (SEM) connected with energy dispersive x-ray (EDX) and N₂-physisorption at -196 °C. The results attained verified that α-Ni(OH)₂ was fashioned for 2NiLDHs-Dr catalyst and the enclosure of nickel ions in the cationic sheet of layered structure were responsible for the fascinating catalytic efficacy rather than the basic nature of material. The Ni-containing LDHs catalysts encourage forthcoming studies in Pd-free catalyzed C-C coupling reactions.



Audience Take Away:

- I will introduce some fundamentals in carbon-carbon coupling reaction.
- The audience will be updated with the most up to date research in layered double hydroxide catalysts.
- It provides the audience with new technologies in organic synthesis and application in different fields

Biography

His dual roles as Professor of Physical Chemistry, Surface Chemistry and Catalysis Lab in the Physical Chemistry Department of the National Research Centre (NRC) in Egypt, as well as my "delegation", since 2004, to King Abdul-Aziz University (KAU) in Saudi Arabia, are just the latest in a string of leadership roles he has held in the academic and scientific research field for almost 30 years. His research interests in advanced materials, nanomaterials with special interest in their application in heterogeneous catalysis. Solid acids and solid bases for liquid phase and gas phase reactions. In addition, he is specialist in catalyst and adsorbent characterization with particular expertise in adsorption measurements. He has also served as journal reviewer for over 100 articles, as a member of journals' editorial boards, and in academic and industrial collaboration on projects in various parts of the world. His scientific and research career includes contributions and participation in over 30 workshops and conferences, close to 100 publications and 10 patents registered in Japan and the USA and distinctions from numerous professional and major global bodies. He was cited in Marquis Who's Who in Science in 2013 and was awarded an outstanding research award in 2011-2017 from the deanship of scientific research at KAU.

Novel synthesis of mesoporous alumina by hydrothermal technique & their role as catalyst support for valuable chemicals

Sujatha Parmeswaran^{1*}, Dhaval Kathvadiya^{1,2}, Deep Ka.Patel^{1,2} & Yogeshwar Suryawanshi¹

¹ Technical & Applied Chemistry Department, Veermata Jijabai Technological Institute (VJTI), Matunga, Mumbai 40001, India.

² Institute of Science and Technology for Advanced Studies & Research (ISTAR), Sardar Patel University Vallabhvidhyanagar, Gujarat. India.

In recent years, inorganic materials with different shapes and microstructures have received considerable attention owing to the obvious dependence of their properties on their shape and texture. The materials with hierarchically macro-mesoporous structures are of great interest as potential catalyst supports, catalysts and adsorbents, which is due to their large specific surface area and, more important, their texture mesopores and intrinsic interconnected macropore network being able to efficiently transport guest species to framework catalytic sites. In addition, inorganic materials with hollow spherical structure show several advantages such as high mobility, good surface permeability, large specific area and low density. So, synthesis of such mesoporous assemblies and inorganic hollow spheres with hierarchically macro-mesoporous structures which are good candidates as **catalyst supports can be discussed during the presentation**. The synthesis and utility of γ -Al₂O₃, as well as other transition aluminas, can be traced to a favourable combination of textural properties (i.e., surface area, pore volume, and pore size) and acid base characteristics. Conventional forms of γ -Al₂O₃ typically exhibit a BET surface area below 250 m²/g and a pore volume less than 0.50 cm³/g. Various methods have been reported on the synthesis of AlOOH and γ -Al₂O₃ used as adsorbents, filters, catalysts, and catalyst supports. Mesoporous aluminium oxides have been prepared using different surfactants as structural directing reagent. The use of mesoporous alumina as support with loading of different transition metal catalyst will lead to form a new platform in fine chemical industries to get high yield of product.

Audience Take Away:

- Explain how the audience will be able to use what they learn?
- Audience will be benefited after the talk regarding in the terms of the do and don't during the synthesis procedures.
- We believe that it will a great opportunities two way opportunity to know more about the "spillover" because of more surface area which is hot topic in catalysis.
- It would be great opportunity and fruitful discussion for audience as well as learners.
- How will this help the audience in their job?
Yes by the experience more correct approach will learnt from the presentation.
- Is this research that other faculty could use to expand their research or teaching?
YES, they can expand their area in Advanced Materials.
- Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient?
Yes, partially it may provide after appropriate design.
- Will it improve the accuracy of a design, or provide new information to assist in a design problem? List all other benefits.
YES, Synthesis strategies would be an additional part for informative design.

Biography

Dr. Sujatha Parmeswaran after completing B.Sc. in Chemistry (1986), done B. Tech. in Polymer Science & Rubber Technology (1989) and M.Tech. (1991) in Polymer Technology both from Cochin University of Science and Technology, Cochin, Kerala, India. Later she joined in a project group in the Department of Chemistry of the University of Kaiserslautern, Germany in (1992-93). Completed Phd. (Technology) in Chemical technology, in the area *Polymer Supported inorganic Catalysts*, from Institute of Chemical Technology (ICT), Mumbai (1997). In 2000 joined in the Technical & Applied Chemistry Department, Veermata Jijabai Technological Institute (V.J.T.I), Mumbai, India, as Assistant Professor and currently holding the position as the Head of the Department, V.J.T.I. Her research area includes Catalysis, Nanomaterials, Nanocatalysis, Composites and other Advanced Materials.

Supercritical fluids as reaction media for scalable production of carbon nanomaterials

Haider Hassan A. Almkhelfe

Ph.D. Chemical Engineering/Catalysis and Nanotechnology Midland Refineries Company_Daura Refinery

We have demonstrated scalable and selective synthesis of carbon nanotubes (CNTs), carbon nanofibers (CNFs), and onion-like carbons (OLCs) in a batch reactor using supercritical fluids (SCFs) as reaction media. The process utilizes toluene and alcohols (ethanol, propanol, and butanol) as carbon precursors in combination with ferrocene. Growth with supercritical toluene at 600 °C in the absence of water yields large diameter CNTs while introduction of 92.5 mmol/L of water enhances product yield by 50%, promoting formation of smaller diameter CNTs and decorating the exterior surface of CNTs with Fe nanoparticles. At 400 and 500 °C, in the absence of water, supercritical toluene produces mainly OLCs and CNFs, respectively. For alcohols, a gradual evolution of the morphology of nanocarbons forms from mainly OLCs to tube-like structures as the ratio of C/O atoms increases, possibly due to a decrease in the tendency of graphitic sheets to minimize their energies by curling into onion-like structures as chain length increases. This study provides a framework for utilizing SCF reaction media in a batch reactor to achieve scalable and selective growth of different nanocarbons and nanocarbon-metal nanocomposites

Synergistic catalysis of nano-metal and semiconductor (metal oxides) molecular/atomic-layer film coated on the support of Novel Hybrid complex nano-structured Pt Catalyst prepared by photochemical route

Zhou Jicheng^{*}, Zhang Yanji, Wang Fei, Xu Wentao, Kai Li, Mengdie Lv

Key Laboratory of Green Catalysis and Chemical Reaction Engineering of Hunan Province, School of Chemical Engineering, Xiangtan University, Xiangtan 411105, Hunan Province, China.

Herein, we report a novel strategy, which combine nano-metal with semiconductor (metal oxides) atom layer film coated on the support, to fabricate Novel Hybrid Complex Nano-structured Pt/@-MeOx/SBA-15 Catalyst prepared by photochemical route. This Hybrid Complex Nano-structured Pt/@-MeOx/SBA-15 Catalyst is a novel Hybrid nano-structured catalysts, which nano-metal were anchored on the semiconductor (metal oxides) atom-layer film coated on the support.

The novel Hybrid complex nano-structured Pt Catalyst exhibited remarkable catalytic activity in the selective hydrogenation of benzaldehyde, conversion exceeding 99.9% was achieved with >99% selectivity. No decay in the activity was observed by 12 cycles. for the Chemoselective hydrogenation of nitro compounds by 0.1wt% Pt/@-MeOx/SBA-15 Catalyst, Conversion achieved up to more than 99% with the selectivity of more than 99%. For the selective hydrogenation of p-chloronitrobenzene, it also obtained high selectivity(>99%) at complete conversion, the catalyst yields a TOF of 57588 h⁻¹, about 2 orders of magnitude higher than that of the traditional Pt catalysts and 11.5-fold higher than the best result reported in the literature.

More importantly, the Novel Hybrid Complex Nano-structured Pt Catalyst exhibited the Synergistic Catalysis of nano-metal and semiconductor (metal oxides) atom-layer film coated on the support for the Chemoselective hydrogenation of nitro compounds by Pt/@-MeOx/SBA-15 catalysts and for the selective hydrogenation. The superior performance can be attributed to the Synergistic Catalysis of nano-metal and semiconductor (metal oxides) atom-layer film coated on the support and the unique properties of hybrid nano-structure.

Biography

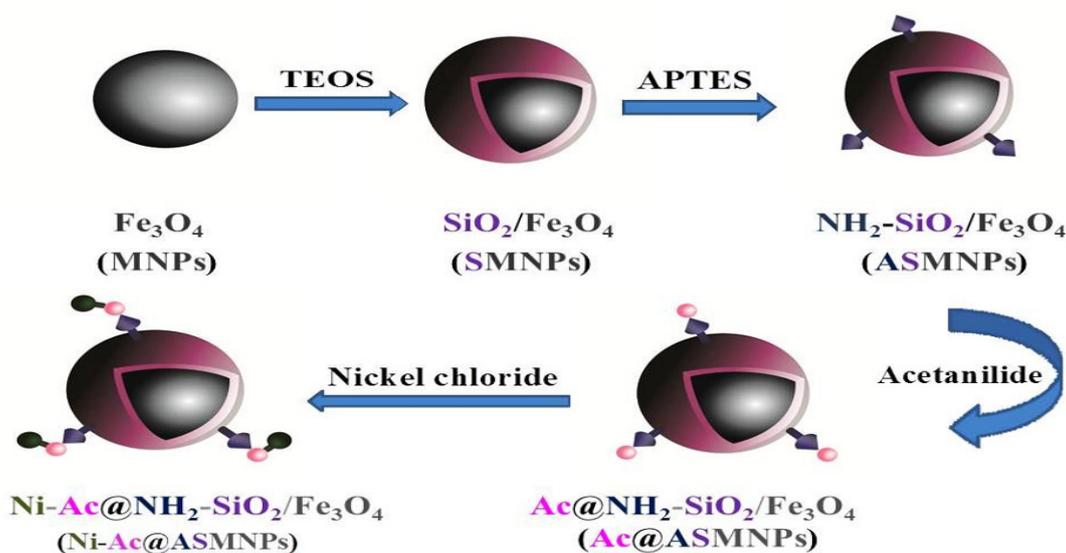
1985 Bachelor Xiangtan University, China
1993 Master Zhejiang University, China
1999 Ph.D. Dalian University of Science and Technology, China
2003-2004 Visiting Prof. University of Waterloo, Canada
Since 2002 Prof. School of Chemical Engineering, Xiangtan University, China

Nanocomposites with different metals as magnetically separable nanocatalysts for oxidation of aldehydes

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Department of Chemical Engineering, North Tehran Branch, Islamic Azad University, PO Box 19585/936, Tehran, Iran

In this study, two metals were chosen for composing two different nanocatalysts. Zinc acetate and nickel chloride anchored acetanilide that was attached to functionalized magnetic nanoparticles (Fe_3O_4) coated by silica and made two complexes. Their identification were presented by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and gas chromatography mass spectrometer (GCMS). These nanocatalysts were used for oxidation of aldehydes: 3-hydroxybenzaldehyde, 4-methoxybenzaldehyde and 3-nitrobenzaldehyde. High efficiency, stability, recoverability, recyclability and selectivity were achieved by these nanocatalysts.



Scheme 1. Route for the synthesis of magnetic nanocatalyst with Ni as metal.

Biography

Akbar Esmaili has completed his Ph.D at the age of 47 years from Islamic Azad University, Tehran, Iran. He is the Prof. Department Chemical Engineering North Tehran Branch, Islamic Azad University. He has published more than 100 papers in reputed journals, more 13 books, referee for more 100 papers and serving as three editorial board member of repute.

Pd Nanoparticles supported on copper oxide prepared via microwave – Assisted synthesis: An efficient catalyst for suzuki cross-coupling

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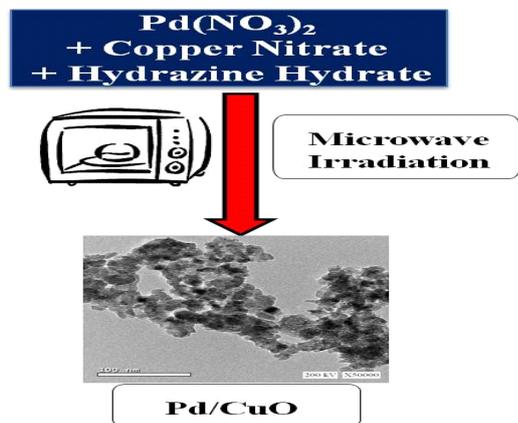
⁴PhD, Cairo University, EGYPT

Transition metal nanoparticles have been widely investigated as a potentially advanced pathway in catalysis field due to their distinctive properties. The precise optimization through controlling the particle size is one of the key factors to obtain unique physical and chemical properties. Recently, Copper based nanoparticles have a huge impact in the field of catalysis research as they have been tested in several major reactions such as Suzuki-Miyaura cross-coupling.

The previously mentioned research studies have revealed the high catalytic activity of metallic and bimetallic nanoparticles through using copper oxide as an ideal support in C-C cross-coupling reactions which are considered as one of the most relevant processes in Organic Synthesis. The importance of those kinds of nanomaterials are not only because they are covering the research area of cross-coupling reactions which are widely used in several strategic industries like cosmetic, pharmacy, agriculture, and natural products; but also as they cover other potential applications in sensors, catalysis and energy conversion.

It is important to notice that there is also a main advantage of using copper oxide as a support as it significantly increase the surface area of the active ingredient of the used catalyst, hence causing a huge enhancement of the contact between reactants and catalyst to be nearly like that of the homogeneous catalysts. This also led to some innovative ideas regarding the use of nano-catalysis for green chemistry development including the possibility of using the concept of microwave assisted synthesis combined with nano-catalysis.

In this manuscript, we report on a green efficient method to prepare highly active Pd nanoparticles supported on copper oxide as a highly efficient catalyst for potential use in Suzuki cross-coupling.



Biography

Prof. Shahir Sadek earned his B.Sc. in Chemical Engineering in 1971 from Military Technical College (MTC), followed by minimum CSc. in 1977 from Brno Academy (VAAZ), CSSR. Prof. Shahir earned his Ph.D. in June 1981 from the University of Orsay, Paris, France, in Organic chemistry. He worked as a lecturer, associate professor and professor in the Chemical Engineering Branch at the Military Technical College in Egypt from 1981 to 1996. Prof. Shahir led the chemical Engineering Department in Higher Technological Institute, 10th of Ramadan City (HTI) from 1996 to 2004. In September 2004, He worked as Associate Dean for October branch of HTI, Associate Dean for Education & student affairs in HTI, and as Dean of HTI till October 2012. In September 2013 Prof. Shahir joined the British University in Egypt as Head of Chemical Engineering and Vice Dean for research, postgraduate studies and Community Services till now.

POSTERS

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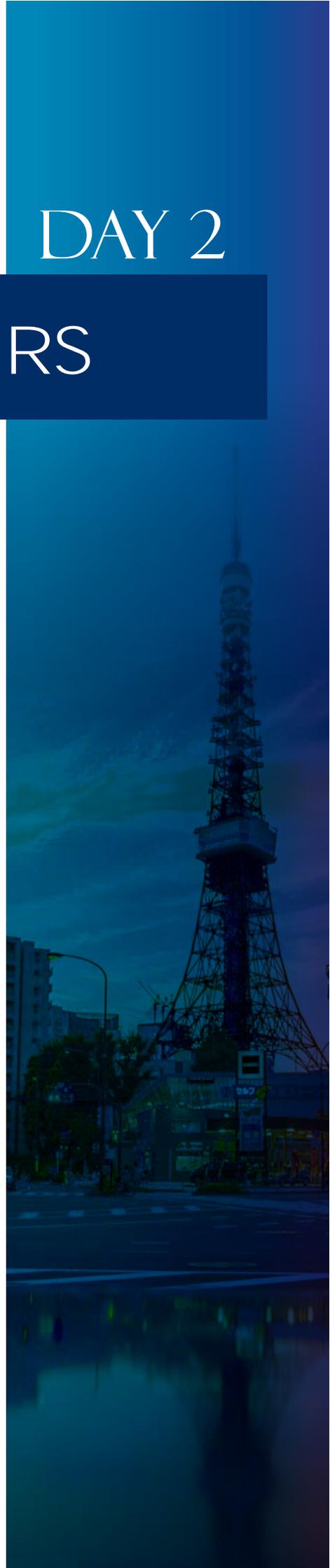
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Heteropoly acid supported on silica catalyst for dehydration of methanol to dimethyl ether

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¹Department of Chemistry, Taibah University, Medina, Saudi Arabia

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Dimethyl ether (DME) is used as an eco-friendly aerosol propellant and intermediate in the production of chemicals (e.g. olefins and dimethyl sulfate). Recently, DME has attracted interest as a clean fuel alternative to diesel due to its good burning characteristics, low NO_x emissions and high cetane number (55–60). DME is produced by dehydration of methanol in the gas phase at 250–360 °C over solid-acid catalysts, typically γ -Al₂O₃. Here, it was studied the dehydration of methanol to DME over the bulk and SiO₂-supported H₄SiW₁₂O₄₀ (HSiW) catalysts on at 5–60 wt% loading, prepared by wet impregnation method. Silica was chosen as the support due to its large surface area and weak interaction with HPA. The catalysts were characterized by several techniques such as BET, XRD, FTIR, ICP, TG-DSC and NH₃ adsorption microcalorimetry. Dehydration of methanol was studied in a continuous flow fixed-bed reactor with on-line GC analysis described previously in the temperature range of 100–150 °C at 3.8–21.8 kPa methanol partial pressure using N₂ as a carrier gas. We observed that the catalyst surface area and pore volume decrease with increasing HSiW loading from 260 m²/g for 5%HPA/SiO₂ to 7.8 m²/g for pure HSiW. It was found that methanol conversion increased with increasing the HPA loading, passing a flat maximum between 25–60% HPA loading. This can be explained by increasing the strength of catalyst active sites and decreasing the surface area, which cause the opposite effect on methanol conversion. In addition, the reaction time courses are studied at different methanol partial pressures. These results also show significant catalyst deactivation at a low methanol pressure of 3.83 kPa. With the methanol pressure increasing, a more stable catalyst performance was observed, with practically no deactivation at 16.7 kPa methanol pressure for 24 h on stream.

Audience Take Away:

This Poster Presentation promising in the field of heterogeneous catalysts techniques using heteropoly acid and the topic related to dehydration of methanol to dimethyl ether.

Biography

Rawan AL-Faze is currently a PhD student in Chemistry Department at the University of Liverpool, UK. She has a scholarship holder sponsored by the Government of Kingdom of Saudi Arabia. She completed her BSc degree in Science & Education Chemistry in 2010 from Taibah University, Saudi Arabia. Master degree of Science in physical chemistry was finished in 2014 from Taibah University, Saudi Arabia. Her research interest's center around the study of multifunctional catalysis for the conversion of biomass-derived molecules, such as alcohols, ketones and carboxylic acids, to value-added organic chemicals and transportation fuels, using heterogeneous catalysis.

Solution plasma synthesis of catalytic carbon composite materials for oxygen reduction reaction

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²Graduate School of Materials Science and Engineering, Faculty of Engineering, Shibaura Institute of Technology, Tokyo, 135-8548, Japan

In recent years, theoretical calculations and experiments demonstrated that introducing nitrogen into carbon lattices could induce charge redistribution and result in the creation of the net positive charge on the adjacent carbon, which enhance the adsorption of O₂ molecules and thus become an effective ORR catalyst. However, rational design of a new catalyst system based on nitrogen-doped carbon materials is still present intriguing challenges in ORR catalysis research. Herein, a new kind of nitrogen-doped carbon nanoparticle–carbon nanofiber (NCNP–CNF) composite with advanced ORR catalytic activity has been developed via a new approach assisted by solution plasma process. The carbon composite nanomaterials were synthesized by growing nitrogen-doped nanoparticles through 2-cyanopyridine (C₆H₄N₂) on CNFs. This integration led to a unique morphological feature and modified physicochemical properties. Firstly, the incorporation of nitrogen atoms in the carbon composite nanomaterials synthesized was confirmed by elemental analysis and the nitrogen content of NCNP–CNFs was found to be approximately 1.35 atom %. SEM and TEM observation revealed that most of NCNPs attach to the CNF surface throughout almost area investigated, giving rise to a unique morphology with an interconnected porous structure. The onset potential of ORR for NCNP–CNFs composite was estimated to be at –0.14 V vs. Ag/AgCl, which is 70 mV more positive than that of CNFs (–0.21 V). From linear sweep voltammetry (LSV), CNFs demonstrated a two-step reduction process with low current density whereas NCNP–CNFs showed a single-step wide plateau of higher limiting current density compared to CNFs. The calculated electron transfer number (*n* values) of NCNP–CNF composite were estimated to be 3.21–3.51. The enhancement in ORR activity of NCNP–CNF composite can be attributed to the synergistic effects of good electron transfer from highly graphitized CNFs as well as abundance of exposed catalytic active sites originated from meso/macroporosity in NCNPs.

Audience Take Away:

- Solution plasma process (SPP) is a novel material synthesis method. Using SPP, synthesis process of functional nanomaterials such as nanoparticles will be established.
- This presentation shows estimation method of electrocatalytic properties for oxygen reduction reaction (ORR) using electrochemical methods.
- The audience can learn that heteroatom-doped carbon composite materials can function effectively as catalytic materials for ORR.

Biography

Dr. Ishizaki received his PhD degree from Waseda University, Japan in 2004. He served as a postdoctoral research associate at Nagoya University (2004–2006), as an assistant professor at the Nagoya University (2006–2007), and as a research scientist at Materials Research Institute for Sustainable Development, National Institute of Advanced Industrial Science and Technology (AIST) (2008–2012), Japan, respectively. Presently, he is a professor in Department of Materials Science and Engineering, College of Engineering, Shibaura Institute of Technology, Japan. He has published more than 100 research articles.

Diethylaminoethyl cellulose (DEAE-C): A catalyst for applications in heterocyclic synthesis

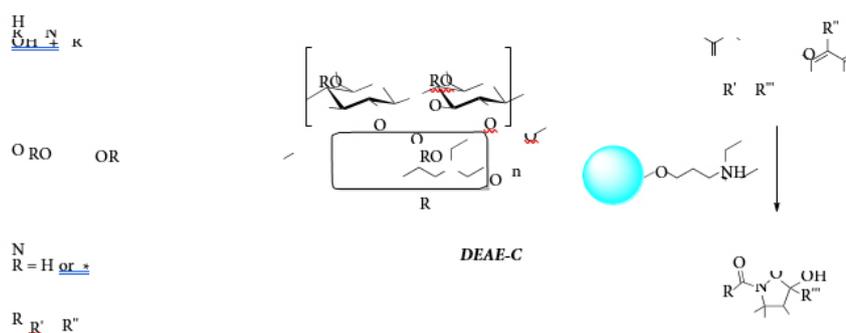
Karzan Khaleel Aljaf,^{1*} Ahmed Anwar Amin,² Faiq H. S. Hussain,³ and Paolo Quadrelli¹

¹Department of Chemistry, University of Pavia, Viale Taramelli 12, 27100 – Pavia, Italy

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³Research Centre-Ishik, University of Erbil, (Iraq)

A new attention has recently driven to the extension of the use of DEAE-C to organic reactions, and in particular for the preparation of heterocyclic compounds as scaffold for biological active molecules. Being DEAE-C an ammonium salt, it can be considered as a potential mild acid catalyst or a proton donor and these features could in theory catalyze standard acid-promoted organic reactions or other processes. In addition, the resin nature of DEAE-C could suggest the way to perform organic reactions in the solid state.



Very few examples can be found regarding DEAE-C organic synthesis applications. It is difficult to say if this is due to the failure of attempts made to use DEAE-C or just to forgetfulness or distraction of the organic chemistry investigators. The reported examples deal with the synthesis of isoxazolidines and the selectivity results could be quite interesting and worth for further investigations, as the methodology seems to be a valuable alternative especially for the opportunity that offers to extend the application to a variety of hydroxamic acids and unsaturated carbonyl compounds.

The Diethylaminoethyl cellulose (DEAE-C) is a positively charged resin typically used in ion-exchange chromatography, for the separation and purification of proteins and nucleic acids. DEAE-C is a weakly basic anion exchanger with tertiary amine functional groups bound to a hydrophilic matrix.

Biography

Dr. K.K. ALJAF studied Chemistry at the Salahaddin University, Kurdistan region-Erbil/Iraq and graduated as MS in 2010. He then joined the research group of Prof. Paolo Quadrelli at the Department of Organic Chemistry, Pavia University. In current time he is Ph.D. student since 2017. He has published four research articles in different journals, his main research interests are heterocyclic chemistry, antiviral synthesis, and solid phase synthesis.

Catalytic impact of Red Mud and metal oxides on the upgrading of fast pyrolysis vapour of biomass

Jyoti Gupta*, Yi Lin, Konstantinos Papadikis, Ivan V. Kozhevnikov, Elena Yu. Konysheva

Department of Chemistry, Xi'an Jiaotong-Liverpool University, Suzhou, China

Renewable bio-oil constitutes a more sustainable and long term solution to the world energy needs. Bio-oil is a complex mixture of oxygenated organic compounds derived from the depolymerisation of cellulose, hemicellulose, and lignin. Its high oxygen content, acidic nature, instability, and immiscibility with petroleum derived fuels make the bio-oil a low grade liquid fuel. Catalytic fast pyrolysis is the efficient way to remove these oxygenated compounds by converting them into useful products that fall into the fuel range or by selective conversion to valuable compounds. Red mud is a industrial solid waste residue formed during the production of alumina and is a complex mixture of oxides such as Fe_2O_3 , Al_2O_3 , TiO_2 , SiO_2 and other minor inclusions. Thermal pre-treatment of Red Mud at 950 °C was found to be effective in catalysis, as during the thermal treatment unstable components ($\text{FeO}(\text{OH})$, $\alpha\text{-AlO}(\text{OH})$ and hydrous aluminium silicates) of the initial Red Mud transformed into more stable oxide phases, resulting in a higher selectivity of pyrolysis products. Red Mud catalysis increased the yield of valuable chemicals, such as furfural and acidic compounds. Alkaline earth oxide promoted ketonisation reactions. Ketones are highly stable, higher energy and desirable molecules since they can easily couple with other bio-oil products (via aldol condensation and hydrogenation/alkylation) to create longer chain molecules that fall into the fuel range. Phenols yield was decreased in both of the catalysis. Catalysis by Red Mud and Alkaline earth oxide can provide significant economic and ecological benefits. The effect of catalysts on the fast pyrolysis vapour upgrading was analysed by Pyrolysis-Gas chromatography-Mass spectrometry technique. X-ray powder diffraction (XRD), Scanning electron microscopy with Energy Dispersive X-ray analysis (SEM/EDX), IR-spectroscopy, Brunauer-Emmett-Teller (BET) and Thermogravimetric analysis (TGA) were applied for catalyst characterisation.

Audience Take Away:

- Audience will learn about the conversion ways of problem causing oxygenated compounds into valuable chemicals.
- This is the heterogeneous catalysis. Audience can try different type of catalysis to look over the results.
- The research is good for economic and ecological point of view.

Biography

Mrs Jyoti Gupta studied Chemistry at the Jiwaji University, Gwalior, India and post graduated as Master of Science in 2006. She joined the research group of Chemistry, Xi'an Jiaotong-Liverpool University, Suzhou, China in 2015. Now she is working on Catalysis and in the final year of PhD. She has published research article in JAAP-Elsevier journal.

Gas-phase hydrotreatment reactions of 2,5-Dimethylfuran using bifunctional metal-acid catalysts

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Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK¹

In the last few decades, there has been a growing interest in green chemistry. As fossil fuel reserves become depleted, considerable attention is being given to the use of biomass as a sustainable feedstock. Wide range of chemicals and fuels can be synthesised using furanic compounds which are a family of cellulosic and hemicellulosic platform compounds. These compounds, however, require upgrading (deoxygenation) to produce chemicals and fuels. Bifunctional catalysis is widely used in upgrade strategies to achieve high activity and selectivity. Recently, several groups have focused on the direct ring opening of the aromatic furans. The use of noble metal-based bifunctional catalytic systems can enhance ring opening. The aim of this work is to study the hydrogenation and hydrogenolysis of furan derivatives over bifunctional metal-HPA catalysts containing Pt and Pd together with acidic Keggin heteropoly salt Cs_{2.5}H_{0.5}PW₁₂O₄₀ (CsPW). The reactions were studied using a fixed-bed continuous flow reactor with on-line gas chromatographic (GC) analysis in the temperature range of 60–100 °C and ambient pressure. The catalysts were characterized by BET, ICP, XRD, TEM and H₂ chemisorption. It is demonstrated that the bifunctional hydrotreatment pathway is more efficient than the monofunctional metal-catalysed pathway. The Pt/C + CsPW physical mixture, as compared to the impregnated catalyst 1% Pt/CsPW, was found to be a very efficient catalyst for the selective one-step hydrodeoxygenation of 2,5-DMF under mild conditions via the metal-acid bifunctional catalysis, providing almost 100% yield of n-hexane at 90 °C. The reaction did not proceed at all in the absence of Pt or in the presence of CsPW alone. The higher activity of the mixed Pt/C + CsPW catalyst, having Pt and H⁺ sites far apart, compared to the impregnated Pt/CsPW catalyst with Pt and H⁺ in close proximity may be explained by catalyst coking, which would affect stronger the Pt/CsPW catalyst.

Audience Take Away:

- This Poster Presentation promising in the field of biomass feed stocks instead of fossil resources.
- Data present here may help to develop completely new kind of reusable catalysts suitable for wide application in academic and in industry.
- Our research could be useful to other faculty to expand their research or teaching in the field of heterogeneous catalysis.
- They will see the role of metal-acid bifunctional catalysis in reaction mechanism.

Biography

Hanan Althikrallah is currently a PhD student in Chemistry Department at the University of Liverpool, UK. She has a scholarship holder sponsored by the Government of Kingdom of Saudi Arabia. She completed her BSc degree in Science & Education Chemistry in 2005 from King Faisal University, Saudi Arabia. Master degree of Science in Advanced Chemical Sciences was finished in 2017 from University of Liverpool, UK. Her research interest's center around the study of multifunctional catalysis for the conversion of biomass-derived molecules to value-added organic chemicals and transportation fuels, using heterogeneous catalysis. As the catalysts, oxides and oxide-like compounds possessing acid-base properties modified by platinum group metals will be investigated. This has economic and environmental feasibility, which is to reduce the cost of production and energy consumed.

Palladium nanocatalyst supported on chitosan and its catalytic performance in Suzuki- Miyaura coupling reactions

Hamad M. Al-Matar*, Wael Tohamy

Chemistry Department; Faculty of Science; University of Kuwait; P.O. Box 5969; Safat; 13060 Kuwait.

Biopolymers were used as supports for the preparation of palladium-based nanoparticles (pd- NPs). The chitosan-based Pd (II) catalyst (non-toxic, cheap, eco-friendly) were structurally characterized using a range of methods such as Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), Differential scanning calorimetry (DSC), Differential thermal analysis (DTA), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), scanning electron microscopy (SEM). (Fig 1,2)

Palladium is commonly known as best catalyst in the Suzuki–Miyaura coupling reactions due to its very high efficiency therefore, using the recently chitosan-based Pd (II) catalyst in the Suzuki–Miyaura coupling reactions, will be described. The reaction optimization and substrate scope will be discussed, and role of rapid catalyst activation in achieving mild reaction conditions will be emphasized.

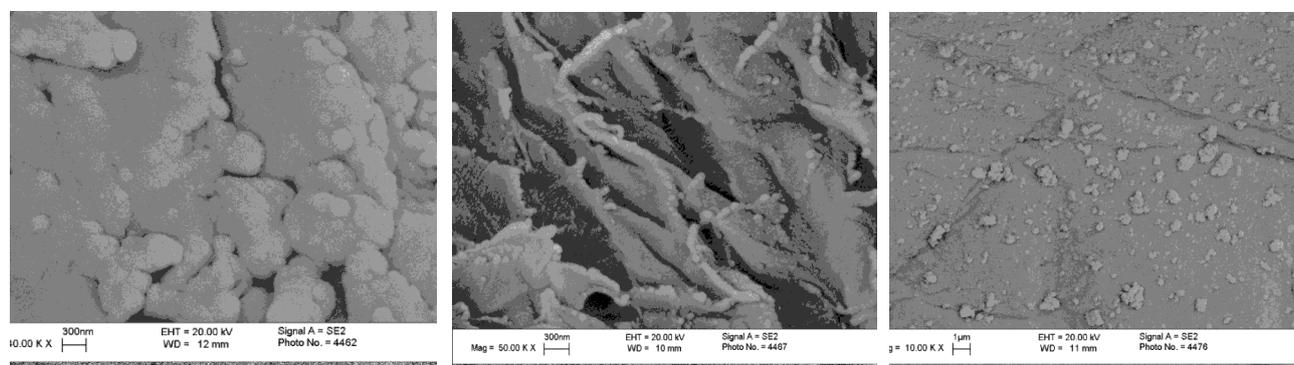


Fig 1. SEM spectra of (a) chitosan, (b) chitosan-schif base (c) chitosan-pd

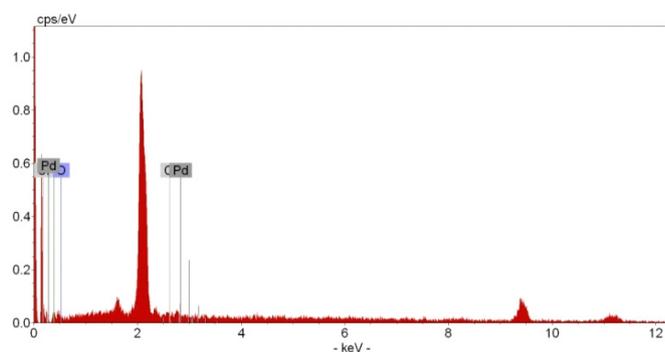


Fig. 2. EDS spectra of chitosan-based Pd (II) catalyst

Audience Take Away:

- I think the audience will surely get benefited by the work presented herein as the methodology developed is quite simple, advantageous and easy to handle.
- The researchers will be able, after my talk, do their own catalyst preparation using similar method.
- The different applications in industry, medicine and ecology will be discussed.
- Catalysts can be applied to Suzuki–Miyaura coupling reactions.

Biography

Hamad Al-Matar is Associate Professor in Organic Chemistry at Kuwait University, Kuwait. In the year 2009, he completed PhD in Organic Chemistry from University of Sussex, Brighton, UK. In the year 1997, he completed his MSc in Organic Chemistry from Howard University, Washington DC, USA. he has published more than 25 research articles in SCI(E) journals.

Synthesis of nitrogen-doped nanocarbons by solution plasma process using cyano-aromatic molecules for catalyst of oxygen reduction reaction

Ai Serizawa¹, Takeo Koike², Kazuki Yoshida², Daiki Numata², and Takahiro Ishizaki¹

¹Department of Materials Science and Engineering, College of Engineering, Shibaura Institute of Technology, Tokyo, 135-8548, Japan

²Graduate School of Materials Science and Engineering, Faculty of Engineering, Shibaura Institute of Technology, Tokyo, 135-8548, Japan

Oxygen reduction reaction (ORR) is the most important process occurring at the cathode in fuel cells. Pt/carbon catalysts have long been known as the most efficient materials for cathode due to its excellent ORR activity. However, their high cost, scarcity, poor long-term durability, and methanol crossover effect have hindered the performance and large-scale production of fuel cells in the coming decade. Nitrogen-doped carbons have recently emerged as a promising material for next-generation fuel-cell cathode instead of Pt/carbon owing to highly efficient ORR activity and excellent durability without methanol crossover. Solution plasma process (SPP) has been gaining a considerable interest in the various synthesis and applications of nanomaterials owing to its several advantages, such as simple equipment, short-time synthesis, ambient condition, and ability to scale up. Very recently, SPP has shown a great potential for the synthesis of carbon nanomaterials by using small organic molecules as precursors such as benzene, toluene, and ethanol. It can also be potentially extended for the synthesis of heteroatom-doped carbons simply by changing the organic precursors. Our previous report has shown that the nitrogen-doped carbons have been successfully synthesized by SPP using the mixture of benzene and pyrazine. However, the ORR performance of synthesized nitrogen-doped carbons was far from that of Pt/carbon. Therefore, further development of nitrogen-doped carbons by SPP is still challenging and highly desirable. In this study, cyano-aromatic molecules, including cyanobenzene (CNBZ), cyanopyridine (CNPD), and cyanopyrazine (CNPZ), were used as the precursors for synthesis. For comparison, undoped nanocarbons were also synthesized from benzene (BZ). The results demonstrated that the nitrogen doping content directly related to the amount of nitrogen atom in the precursors, which varied in the range of 0.6-1.5 at%. The electrocatalytic activity toward ORR in an alkaline medium in terms of onset potential and limiting current density were found to be improved in the order of CNPZ > CNPD > CNBZ > BZ. The ORR tended to proceed via four-electron pathways at -0.4 V for the nitrogen-doped carbons synthesized CNPZ. Moreover, they possess long-term durability and excellent tolerance to methanol crossover effects. Acknowledgement: This research was supported by Japan Science and Technology Agency (JST) under Program on Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA) (No. 18072116).

Audience Take Away:

- Solution plasma process (SPP) have a great potential for the synthesis of carbon nanomaterials by using small organic molecules with its advantage such as simple equipment, short-time synthesis and ambient condition.
- SPP was applied to synthesize the nitrogen-doped nanocarbons for catalyst of oxygen reduction reaction which is the most important process occurring at the cathode in fuel cells.
- The nitrogen-doped carbons synthesized cyanopyrazine (CNPZ) synthesized by SPP showed long-term durability and excellent tolerance to methanol crossover effects.

Biography

Dr. Serizawa received her PhD degree from Tokyo Institute of Technology, Japan in 2008. She served as a Postdoctoral Research Associate at Oak Ridge National Laboratory, USA (2009–2010), and as an Assistant Professor at Osaka University, Japan (2011–2013) and at Shibaura Institute of Technology (2006–2007). Presently, she is an Associate Professor in Department of Materials Science and Engineering, College of Engineering, Shibaura Institute of Technology, Japan. She focuses on materials design of metallic and inorganic materials by means of microstructure control and surface modification. She has published more than 50 research articles.

Ammonia synthesis activity of nanostructured $\text{Ni}_2(\text{W},\text{Mo})_3\text{N}$ and $\text{Co}_3(\text{W},\text{Mo})_3\text{N}$ compounds

S. Al Sobhi*, A. L. Hector

School of Chemistry, University of Southampton, Southampton, UK

The Haber –Bosch process is very successful development, and great achievements in the twentieth century for the production of ammonia. The process involves combining pure H_2 and N_2 directly over a promoted iron catalysts at temperatures of 450-500 °C and reaction pressures of over 100 atmospheres. This process produces over 150 million metric tons of ammonia each year and consumes over 1 % of the world's energy supply. Furthermore, the process is estimated to generate ca. 3 % of global greenhouse gas emissions. Thus, it would be desirable to develop alternative catalytic materials that could operate at lower temperatures and pressures in order to reduce the energy consumption. Metal nitride materials have shown a significant activity for ammonia synthesis under ambient pressure. There is a significant literature of ternary materials including $\text{Co}_3\text{Mo}_3\text{N}$ and $\text{Ni}_2\text{Mo}_3\text{N}$ but few studies exist of varying the electronic structure of these materials by substitution. In this work a series of different compositions in the form of $\text{Ni}_2(\text{W},\text{Mo})_3\text{N}$ and $\text{Co}_3(\text{W},\text{Mo})_3\text{N}$ were prepared and investigated for ammonia synthesis activity. Ammonia synthesis from 75% H_2 and 25% N_2 was carried out at ambient pressure.

All of the materials were found to be active at higher temperature.

Audience Take Away:

This research focuses on the synthesis of nanostructured metal nitride materials. The audience will learn about the new efficient nitride materials that allow the production of ammonia under mild conditions. This could enable further approaches to materials development and discovery.

Biography

Samia Al Sobhi is a PhD student at the University of Southampton, UK, under the supervision of Prof Andrew Hector. Her project revolves around the development of complex metal nitride catalysts for ammonia synthesis, funded by the Saudi Ministry for Higher Education. She graduated with honors from Taibah University, KSA, with a BSc in Chemistry, and obtained an MSc in Chemistry with Nanotechnology from Hull University, UK.

Surface property-activity relations of Co/Sn oxide nanocatalysts evaluated using a model reaction: Surface characterization study

Ndzondelelo Bingwa¹, Matumuene Joe Ndolomingo, Tafadzwa Mabate, Sifelani Dube, Reinout Meijboom

¹Department of Chemical Sciences, University of Johannesburg, Johannesburg, Gauteng, South Africa

Herein we report on the synthesis, characterization and catalytic evaluation of cobalt (Co) and tin (Sn) oxide catalysts synthesized via the sol-gel approach. Preliminary characterization using nitrogen sorption measurements show the materials as mesoporous with relatively high surface area. The catalyst with the least amount of Co had the highest surface area (146 m²/g) compared to the catalysts with the highest amount of Co. Furthermore, temperature-programmed reduction (H₂-TPR) was used to study the redox properties of the catalysts. The H₂-TPR analysis revealed that the catalysts are only reduced at relatively high temperatures (> 300 °C). While the temperature-programmed desorptions using ammonia (NH₃-TPD) and carbon dioxide (CO₂-TPD) results suggest that the total amount of acidic and basic sites is the function of different amounts of metal content in the catalytic materials. The catalyst with the least amount of Co appeared to have the highest number of acidic sites compared to other catalysts. Evaluation of the catalytic activity was studied using oxidation of morin as model reaction. The catalyst with the least amount of Co, (Co_{0.3}Sn_{0.7}O_x) appeared to be the most active catalyst.

Audience Take Away:

- The work in this poster presentation will be of great importance in the development of heterogeneous catalysts that do not consist of precious metals. The use of tin (Sn) in heterogeneous catalysis plays a significant role in unveiling catalytic properties of acidic metals which are less expensive.
- The study of heterogeneous catalytic surfaces provides information which is crucial in the development of catalysts that are highly active and highly selective to certain products in catalytic organic transformations. The relationship of certain surface properties and the catalytic activities unveiled so far provide information that help in elucidating catalytic mechanisms at the surface and this then hints at properties to fine tune for development of specific catalysts for specific reactions.

Biography

Ndzondelelo Bingwa graduated in chemistry in 2012 from Walter Sisulu University (Eastern Cape, South Africa) and received his PhD at the University of Johannesburg (Johannesburg, South Africa) in 2018. He is working as a lecturer in the department of Chemical Sciences of the University of Johannesburg since his Ph.D graduation. His research focus is mainly on the synthesis of reducible mesoporous metal oxides for use as catalytically active supports for immobilization of various nanoparticles. Ndzondelelo is the author of several international peer-reviewed articles.

Oxidative desulfurization of diesel fuel catalyzed by carbon-supported polyoxometalates

Reem Ghubayra*, Charlotte Nuttall, Sophie Hodgkiss, Coral Rogers, Michael Craven, Elena Kozhevnikova, Ivan Kozhevnikov

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Due to increasingly strict environmental regulations, further reduction of sulfur content in transportation fuels is a challenging task. Hydrodesulfurization (HDS) is the most widely used technology for removing sulfur from diesel fuels, which is usually operated at high temperature (300-400 °C) and pressure (30-130 atm) using alumina-supported Co-Mo or Ni-Mo sulfided oxides as catalysts. The main drawbacks of HDS are severe operating conditions and low desulfurization efficiency in the case of refractory benzothiophenes. Oxidative desulfurization is a promising method for removing refractory aromatic sulfur compounds. Typically, it involves liquid-phase biphasic oxidation of organosulfur compounds with H₂O₂ at 60 °C and atmospheric pressure to yield sulfoxides and sulfones, which can be separated from the fuel by precipitation, extraction or adsorption. This work demonstrates that Keggin-type polyoxometalates (POM) supported on activated carbon, POM/C, are effective solid catalysts for oxidative desulfurization of diesel fuel under mild conditions in a biphasic system composed of a model diesel fuel (heptane) and aqueous 27.9% H₂O₂.

Audience Take Away:

- Carbon-supported HPAs are active catalysts for oxidative desulfurization of diesel fuel.
- HPMo/C outperforms other recently reported heterogeneous ODS catalysts
- Easy catalyst/product separation enables catalyst reuse without loss of activity

Biography

Mrs. Reem ghubayra studied Chemistry at the Central Michigan University, United State and graduated as MS in 2017. She then joined the research group of Prof. Ivan at the University of Liverpool, United Kingdom for PhD. She has published two research articles in Springer and Applied Catalysis B: Environmental journals.

Catalytic CO oxidation by Fe doped penta-graphene: A density functional study

Donglin Li, Wenliang Li*, Jingping Zhang

Faculty of Chemistry, Northeast Normal University, Changchun, Jilin, China

Single atom catalysts (SAC) have been investigated extensively for CO oxidation, and penta-graphene (PG) as a new allotrope of carbon has been studied due to its excellent physical and chemical properties. In order to explore the mechanism of CO oxidation and develop the application of PG in the field of SAC, series of metals doped PG were examined to catalyze CO oxidation with the aid of first-principles calculations. Fe doped at 3-coordinated carbon site of PG is found favorable with large binding energy of -12.73 eV, more importantly, exhibits high affinity to the CO and O₂. Furthermore, CO oxidation via Eley-Rideal (ER) mechanism is prior compare with Langmuir-Hinshelwood (LH) mechanism, the first CO molecule oxidation is the rate-determining step (RDS) with the energy barrier of 0.51 eV, which is comparable with other catalysts. In the case of Fe doped at 4-coordinated carbon site, ER and LH mechanisms are almost the same because of the similar energy barrier (0.60 eV and 0.59 eV). On the basis of reasonable first-principles calculations, the proposed Fe doped PG is believed to be a promising single atom catalyst for CO oxidation, and our results provide deep insights to design new heterogeneous catalysts based on PG.

Audience Take Away:

- Our theoretical results show Fe doped at 3-coordinated carbon site of PG favorable with large binding energy of -12.73 eV.
- CO oxidation via Eley-Rideal (ER) mechanism is prior compare with Langmuir-Hinshelwood (LH) mechanism.

Biography

Dr. Wenliang Li studied Chemistry at the Northeast Normal University, China and graduated as PhD in 2012. He then joined the research group of Prof. Jingping Zhang at Northeast Normal University. He obtained the position of Associate Professor at Northeast Normal University. He has published more than 30 research articles in SCI journals.

Controlling the regio- and stereoselectivity of hydrosilylation reaction catalyzed by platinum(0) complexes bearing bulky N-heterocyclic ligand

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Hydrosilylation, which usually refers to addition of silanes to double or triple C-C bonds, is one of the most powerful synthetic methods of production organosilicon compounds. This reaction gives possibility for simple functionalization of many organic compounds and for synthesis wide spectrum of silanes derivatives. Although there are many different catalytic systems characterized by good activity, regio- and stereoselectivity still remains as a great problem of this process. The reaction can lead to a several different products and can also be accompanied by several side-processes like hydrogenation, isomerization, dehydrogenative silylation, olefin oligomerization or redistribution of silanes. The number of potential products increases when we use secondary silanes instead of tertiary, because of the possibility of bis-hydrosilylation. The situation gets also more complicated when we use substrates containing more functionality which can react, for example enynes, dienes or diyenes.

Presented research deals with the problem of selectivity of the hydrosilylation reaction. Using platinum (0) complex bearing bulky N-heterocyclic carbene ligand and by careful tuning of the reaction conditions such as temperature and substrates ratio, we were able to control course of the reaction and obtain desired products with good yields and selectivity. The research concern hydrosilylation of terminal acetylenes with disubstituted silanes as well as hydrosilylation of dienes, diyenes and enynes with trisubstituted silanes.

Audience Take Away:

- On the presented poster audience will be able to see fully selective method of synthesis of mono- and divinylsilanes with E configuration around double C-C bond in the presence of platinum-N-heterocyclic carbene complex.
- There will be also presented the method of hydrosilylation of multi-unsaturated compounds with tertiary silanes. Synthetic methods contain also one-pot hydrosilylation with two different silanes.
- The information presented can significantly expand the range of methods used for synthesis of organosilicon compounds.
- Catalyst used in presented research showed tolerance to the wide scope of functional groups, which proves its versatility and means that it can be potentially used in many branches of industry and science.

Biography

Małgorzata Bołt recently obtained her master degree in chemistry at Adam Mickiewicz University in Poznań. Her current research interests focuses on synthesis of transition metal catalysts and use obtained compounds in catalytic systems such as hydrosilylation and terminal acetylenes dimerization. Her current research concerns mainly on platinum(0) catalysts bearing bulky N-heterocyclic carbene ligands. Steric hindrances around metal center caused by the presence of the bulky ligand have a great influence on activity and selectivity in the studied reactions.

Acknowledgment:

The research was financed by the National Science Center (Poland) under the SONATA Project No. UMO-2016/23/D/ST5/00417.

A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: is the cyano group better than the classical carbonyl group for the addition of NHC?

Shanshan Cao, Haiyan Yuan[†] and Jingping Zhang

Department of Chemistry, Northeast Normal University, Changchun, China

Density functional theory (DFT) computations have been utilized to investigate the N-heterocyclic carbene (NHC) catalytic reaction mechanism when carbonyl and cyano compounds co-exist. The results suggested that both the carbonyl and cyano compounds can be activated by NHC, while the order of activation by the NHC depends on the substituents of the two compounds. In the model reaction of NHC catalyzed cyclocondensation of cyclohexanone with 2-aminobenzonitrile, two key activation modes were explored, the new NHC activation carbon of the cyano-group (Mode II) is found to be preferred over the activation of carbonyl carbon (Mode I); this is remarkably at variance from the previous reports. More importantly, water molecules can improve the catalytic activity of NHC to some extent, especially in the Dimroth rearrangement process. The cooperative participation of the NHC and H₂O catalyst is identified. Moreover, the strong quadruple hydrogen bonding interactions between water/NHC and substrates are proposed to be the origin of the high activity of NHC-H₂O co-catalyzed Mode II. Additionally, these interactions stabilize the generated negative charge on carbonyl oxygen and further strengthen the nucleophilicity of the -NH group in the NHC-H₂O co-catalyzed key transition state structure, which is further confirmed by AIM and NCI analyses.

Audience Take Away:

- Density functional theory (DFT) computations
- N-heterocyclic carbene (NHC) catalytic reaction mechanism
- The importance of non-covalent interactions in novel organic reactions.

Biography

Dr. Haiyan Yuan has completed her PhD from Northeast Normal University and continued the postdoctoral studies in the school of physics in 2015. The research interests of Dr. Yuan disclose the effect of assistant (catalyst), solvent, and counterion on the organometallic and organocatalytic reactions to optimize the experimental conditions using DFT method. She has published more than 20 papers in *Angew. Chem., Int. Ed.*, *ACS Catal.*, *Green Chem.*, *Chem. Commun.*, *Org. Chem. Front.*, *J. Org. Chem.*, *J. Comput. Chem.*, etc.

Applying unreacted-core model analysis for delignification during a water/1-butanol co-solvent treatment

Yuki Kawamata*¹, Hiroya Ishimaru¹, Hiromi Aoki¹, Takuya Yoshikawa¹, Yoshihito Koyama², Yuta Nakasaka¹ and Takao Masuda¹

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²Idemitsu Kosan Co.,Ltd., Advanced Technology Research Laboratories, Sodegaura, Chiba, Japan

Lignocellulose is attractive as carbon resource for substituting fossil resource because of their carbon neutrality. In utilizing lignocellulose, fractionation of its components, such as cellulose, hemicellulose, and lignin, is necessary to accomplish high valuable use of them. Cellulose and hemicellulose are polysaccharides, and lignin is polymer of alkyl phenols. As usual, the fractionation is carried out by kraft method, in which lignin and hemicellulose is removed, but the strong base employed in the method converts lignin into residual material, which is difficult to be depolymerized and utilized as high-value added products. Thus, novel technique for the fractionation is desired for utilization of lignin. On the other hand, our previous study revealed that lignocellulose could be fractionated via water/1-butanol co-solvent treatment at around 473 K. Lignin with less structure changes is recovered in the treatment compared with that from kraft method, so the co-solvent treatment is expected the novel fractionation technique. In present work, we tried to analyse kinetics of delignification of cedar wood during the co-solvent treatment by applying unreacted-core model. This model is used to express situations in which solid particles are being consumed by reactions with forming product layer, and the amount of the reactant material being consumed is shrinking, and the model used for predicting the rate-controlling step, such as reaction on the unreacted core, diffusion of the product molecule within the product layer (remained cellulose layer) between unreacted core and film, and diffusion of the molecule within the film. As a result, the diffusion within the remained cellulose layer was indicated to be the rate-controlling step. Moreover, the result was could be supported by following results; there were no isotope effect on hydrolysis of lignin and no rotation speed effect on the delignification. These results mean the reaction and diffusion within film were not rate-controlling step. On the other hand, the size of lignin molecule obtained the delignification was approximately 3.8 nm and the pore size of remained cellulose layer was 3-10 nm, indicating diffusivity of the molecule within the layer seemed to be enough low that the diffusion step could be the rate-controlling step.

Audience Take Away:

- Analyzing technique of unreacted-core model for solid-liquid phase reactions.
- New insight to delignification on the view point of mass transfer.
- Importance to consider the mass transfer effects of chemical species in solid-liquid phase reactions.

Biography

Yuki Kawamata received master degree of Chemical Science and Engineering from Graduate school of Chemical Science and Engineering, Hokkaido university, Japan in 2017. He is currently Ph.D.student at the same graduate school and his research topics are lignocellulose conversions, especially fractionation of lignocellulosic components via organosolv treatment and lignin conversion into useful chemicals via catalytic cracking.

Acknowledgment:

This work was supported by the Advanced Low Carbon Technology Research and Development Program (ALCA, Grant Number: JPMJAL1206) from the Japan Science and Technology Agency (JST).

Application of catalytic hydrogenation in the synthesis of hydroxylated Pillar[5]arene-based amphiphiles

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A new approach was employed for the synthesis of Hydroxylated pillar[5]arene-based amphiphiles by a co-cyclization strategy followed by catalytic hydrogenation to remove the pillar[5]arene-bearing benzyl group(s). Conformational mobilities of the units and host-guest complexation with n-octyltrimethylammonium hexafluorophosphate of the synthesized perbenzylated pillar[5]arenes were studied. Different cavity sizes of amphiphilic pillararenes have been reported based on pillar[5]arenes, pillar[6]arenes, pillar[7]arenes, and pillar[10]arenes. They are divided into three main categories, cationic, neutral, and anionic amphiphiles. Nonsymmetrical amphiphilic pillararenes with different hydrophilic and hydrophobic groups were synthesized. For example, sugar-functionalized amphiphilic pillar[5]arenes have been applied in bacterial cell agglutination and hydrophilic lysin head group amphiphilic pillar[5]arenes were self-assembled into bimolecular micelles in water and used to stabilize gold nanoparticles by reducing HAuCl₄ with ascorbic acid. Many of these amphiphilic pillar[5]arenes were synthesized based on bromo or propargyl derivatives, however, recently we reported the synthesis of mono-, di- and penta-hydroxylated pillar[5]arenes by introducing benzyl groups followed by selective removal via catalytic hydrogenation. This approach provides a platform to access pillararenes with countless structural variations.

We report the synthesis of perbenzylated-pillar [5]arenes through the condensation of hydroquinone derivatives of 1,4-dibenzyloxybenzene. Co-cyclization with 1,4-dibenzyloxybenzene and hydroquinone derivatives with mono- or di-octyl group(s) followed by selective removal using catalytic hydrogenation resulted in the formation of amphiphilic pillar[5]arenes. Host-guest complexation with n-octyltrimethyl ammonium hexafluorophosphate (OMA) was investigated by ¹H nuclear magnetic resonance (NMR) titration and mass spectroscopy. The conformational mobilities of the units were studied by variable ¹H NMR. The use of easily and selectively removable benzyl protecting groups enables a wide range of structural manipulations of the pillararene system. Amphiphilic hydroxylated-functionalized pillar[5]arenes reported in this study were synthesized by co-cyclization of hydroquinone derivatives followed by catalytic hydrogenation over palladium in charcoal using anhydrous ethyl acetate as a solvent. Further studies, modification, application and self-assemblies of these amphiphilic hydroxylated-functionalized pillar[5]arenes are underway in our laboratories.

Audience Take Away:

- This approach unlocks the synthesis and the design of a wide range of structural manipulations to the hydroxylated amphiphilic pillararenes.
- This presentation demonstrates an alternative route for the synthesis of Hydroxylated pillar[5]arene-based amphiphiles via catalytic hydrogenation.
- This approach enhances the synthetic methodologies of functionalized supramolecular-pillar[5]arenes.

Biography

Dr. Abdirahman A. Mohamod studied Chemistry at the Kuwait University, Kuwait and graduated as MSc in 2013. He then joined the research group of Dr. Talal Al-Azemi at the University of Kuwait, Kuwait. His research work focuses on establishment of a new class of supramolecular organic compounds that have unique structural features such as an interesting cavity which encapsulate guest molecules to form host-guest complexation compounds. He received his PhD degree in 2018 at the same institution under the supervision of Dr. Al-Azemi. In his PhD dissertation, he developed new approach to synthesize mono- and A1/A2-dihydroxy-substituted-pillar[5]arenes via the selective removal of benzyl groups by catalytic hydrogenation. Also, he studied the host-guest complexation abilities for the synthesized pillar[5]arenes with long-chain-alkyl alcohols by ¹H nuclear magnetic resonance (NMR) titration and X-ray-single-crystal diffraction techniques. Currently, he works as teaching assistant staff at the chemistry department in Kuwait university and he has published more than 15 research articles in SCI(E) journals.

Magnetic composite for wastewater treatment and control with visible light

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Global environmental pollution and energy shortage are becoming increasingly prominent and have a significant impact on the living space of human beings. At present, the researches on photocatalytic semiconductor materials in photocatalytic degradation of organic pollutants in wastewater have attracted much attention from scholars at home and abroad. Ta₂O₅ has been proved to have higher photocatalytic activity than TiO₂, so it is recognized as a photocatalytic material with great application prospects. Graphite-like carbon nitride is characterized by its large specific surface area, good adsorption, good chemical stability, high electron conductivity, and narrow band gap width (2.7eV). Therefore, the composite of g-C₃N₄ Ta₂O₅ and Fe₃O₄ photocatalytic materials based on the modification mechanism of semiconductor composite technology will be conducive to expanding the visible light response range, improving the quantum efficiency and enhancing the visible light catalytic performance. The poor dispersion and repetition stability of the materials prepared by the above method affect the catalytic performance of the composites. Proposed in this paper one step of hot solvent was prepared with different contents of g-C₃N₄ composite photocatalytic materials, based on the analysis of the structure and morphology of the composite photocatalytic materials, research sulphonamide wastewater in visible light catalytic degradation, analysis of the different content of g-C₃N₄ effect on the photocatalytic properties of the composite material, and further study of mechanism of photocatalytic decomposition of photocatalytic materials. Composite photocatalytic materials with visible light photocatalytic activity were prepared by thermal solvent method. The main results are as follows: a) The composite photocatalyst has a hollow spherical structure. The results of ultraviolet-visible diffuse reflectance show that the composite photocatalyst has a certain visible light response characteristics. b) The photocatalytic activity of the composite photocatalyst for the degradation of sulphonamide wastewater was tested. The results showed that the photocatalytic activity of the composite photocatalyst was the best when the light time was 120min and the content of g-C₃N₄ was 40wt%, and the degradation rate reached 99.8%. c) The photocatalytic degradation mechanism of the composites was further studied by capturing the active species. The results showed that superoxide radicals were the main active species. The cyclic photocatalytic experiments showed that the photocatalytic activity of the composites was stable under visible light irradiation.

Audience Take Away:

- Understanding the performance and mechanism of photocatalytic materials.
- Understanding the application of photocatalytic properties of photocatalysts in water environment treatment and solar cell conversion.
- Source of sulphonamide wastewater and its pollution and harm to water environment.
- Eutrophication control of water body

Biography

Prof/A. Xie studied Environmental Engineering at the Beijing Institute of Technology, Beijing, China and graduated as Dr in 2007. She then worked at the School of Chemistry and Chemical Engineering, Chongqing Institute of Technology, Chongqing, China. She has published more than 30 research articles in various journals including SCI(E).

Activation of peroxymonosulfate by magnetic nitrogen-doped graphene for the degradation of organic pollutants in water

Qilong Xie*, Dekui Sun, Yan Liu, Litao Jia, Bo Hou, Debao Li

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Developing efficient, low-cost and environmental-friendly catalysts is of great significance for heterogeneous activation of peroxymonosulfate (PMS) degradation of organic pollutants in environmental remediation and protection fields. In this study, the Co@N doped porous graphene shells structure (Co@NC) with different carbonization temperature (700, 800, 900 °C) was prepared using a simple pyrolysis process.

Benefited from the rationally structural design of the carbon precursor and post-treatment with surface engineering, the derived Co@N-C can efficiently activate PMS for fast decomposition of organic pollutants with trace cobalt leaching in aqueous solution. 99.5% of TC degradation at 10 min were achieved over Co@N-C with PMS, which was faster than most carbocatalysis. Co@N-C also has an excellent long-term stability and good performance toward the pollutants degradation at a wide pH range of 3.0–9.0. Additionally, the singlet oxygen (1O_2) was identified as the dominant reactive species rather than sulfate radicals in Co@NC /PMS system based on the trapping experiment and EPR analysis. Finally, possible degradation pathways were proposed based on LC-MS analysis of the reaction intermediates. The excellent performance can be attributed to the synergetic effect of N-doped graphene, underlying Co nanoparticles, and the encapsulation structure in which carbon shells protect Co from leaching and aggregation. The embedded Co NPs also afford the carbocatalysts to be magnetic for an easy recycling. This study provided a new insights in catalyst design for PMS-based advanced oxidation for organic pollutants degradation in wastewater.

Audience Take Away:

- Co@NC had an excellent PMS activation efficiency with trace cobalt leaching in aqueous solution.
- 2. 1O_2 was the dominant reactive oxygen species for pollutant degradation over Co@NC.
- Co nanoparticles together with N-doping graphene induced the non-radical pathway.
- This study provided a new insights in catalyst design for PMS-based advanced oxidation for organic pollutants degradation in wastewater.

Biography

Qilong Xie, grew up in China and received his master's degree from the Northwest A&F University in 2014. After he obtained his master degree from the Northwest A&F University, he joined Professor D. B. Li's Laboratories at State Key Laboratory of Coal Conversion, Institute of Coal Chemistry as a research assistant in 2014, Mainly engaged in the study of Catalytic material characterization and environmental chemistry.

Immobilization of bisphosphine ligands on nanomagnetite Pd/Fe₃O₄

Ashouri Akram*, Samadi Saadi, Pouriyan Somayeh and Nasiri Behzad

Laboratory of Asymmetric Synthesis, Department of Chemistry, Faculty of Science, University of Kurdistan, Zip Code 66177-15175, Sanandaj, Iran.

A novel magnetically separable Pd/Fe₃O₄ catalyst was synthesized, either through the postgrafting or immobilization of phosphine ligands which is a highly efficient catalyst for the alylation of aldehyde and conversion to alcohol. The prepared catalysts are easily recovered by simple magn etic decantation and reused with the no significant decrease in activity.

- Design of new magnetically separable Pd/Fe₃O₄ catalyst.
- Use of highly high efficient catalyst for organich reactions which are easily recovered by simple magnetic decantation and reused with the no significant decrease in activity.

Biography

Dr. Ashouri studied Chemistry at the Tarbiat Moallem University, graduated as Ms and received her PhD degree in in 2010 at the same university She then joined the research group of Prof. Hayashi at Kyoto University as postdoctoral fellowship at the Asymmetric Synthesis Laboratory. In Iran, she obtained the position of a Professor at University of Kurdistan. She has published more than 15 research articles in SCI(E) journals

A novel design for ammonia production

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¹Chemical Engineering, Oil and Gas Department, Shiraz University of Technology, Shiraz, Iran

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Haber-Bosch is one of the most common petrochemical processes to generate ammonia from synthesis gas. Unfortunately, the process is usually very expensive, because it is run in high pressures (approximately 220 bar). In this work, a novel dense Pd-Ag membrane reactor is proposed to enable methane reforming and ammonia production to be carried out simultaneously. The Ni based and Iron based catalysts are used for methane reforming and ammonia production respectively. The produced hydrogen from methane reforming permeates to react with nitrogen for ammonia generation.

The coupling process is modelled to evaluate the performance of the proposed design. To obtain the mass and the energy balance equations, a differential element was considered along the reactor. The model was considered one-dimensional and steady and all the conditions are in according to operating conditions. In order to solve the governing equations, Modified Rosenbrock method (ode23s) in MATLAB software is used. The results of the modelling show that 15% of nitrogen conversion could be achieved from the proposed design at the pressure of 10 bar. This novel process is an appropriate alternative for avoiding, the extra costs of Haber-Bosch process.

Audience Take Away:

- This paper opens a new point of view for audience to think about the other alternative designs for Haber-Bosch process.
- The new design is more cost effective with using the other catalysts such as Ru. This paper will interest the audience to do more researches about finding the alternative catalysts for Haber-Bosch process.

Biography

Dr. S.M. Jokar is an assistant professor in the department of chemical engineering Oil and Gas in Shiraz University of Technology, Shiraz, Iran. He earned his PhD, master's and bachelor's degrees in chemical engineering at Shiraz University, Shiraz, Iran. He spent his sabbatical in a membrane lab in Italy (ITM-CNR). He has authored 21 papers and 9 conference presentations. Most of his works concerned with Flare systems, environmental problems, process design, reactors, Pd based membrane reactors.

Cobalt aluminate-modified alumina as a carrier for cobalt in Fischer–Tropsch synthesis

Yan Liu*, Litao Jia, Qilong Xie, Dekui Sun, Bo Hou, Debao Li

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Fischer-Tropsch is an important technology for the efficient use of energy such as coal, natural gas and biomass which can convert syngas into high value-added chemicals. Co-based catalysts are promising Fischer-Tropsch synthesis industrial catalysts due to their excellent carbon growth ability and low water vapor shift reaction. In order to improve the performance of Co-based catalysts, it is necessary to conduct a comprehensive and in-depth study and exploration of its Fischer-Tropsch synthesis mechanism. Modified alumina carriers were obtained by pre-coating cobalt aluminate on the surface of common alumina. Next, supported cobalt catalysts were obtained by incipient wetness impregnation, and their FTS performances were evaluated in a fixed-bed reactor. In situ XRD results suggested that HCP Co was obtained after reducing the aluminate-modified alumina-supported cobalt catalysts, as opposed to FCC Co, which was supported on common alumina. H₂-TPR results demonstrated that the modified catalysts possessed lower reduction temperatures. CO-TPD and in situ CO-FTIR characterizations indicated that bridged rather than linear CO adsorption occurred on the modified catalysts.

The evaluation results indicated that the aluminate-modified catalysts possessed higher CO conversion rates, higher C5 selectivity, higher cobalt specific activity, higher C5+ space-time yields (STYs), and lower methane selectivity than conventional catalysts in the FTS process.

Audience Take Away:

- Modified alumina with useful surface features was obtained by pre-coating cobalt aluminate.
- Bridged adsorption and direct dissociation of CO was obtained on HCP Co produced after the reduction of modified alumina-supported cobalt.
- Modified cobalt catalysts showed higher cobalt specific activity and lower methane selectivity.

Biography

Liu Yan, Ph.D., Industrial Catalysis, Assistant Research Fellow, Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, is mainly engaged in the research and development of new Fischer-Tropsch synthesis catalysts and supporting technologies. He has published 21 academic papers and obtained 17 authorized patents.

SiC thin films loaded Cu as a visible light responsive photocathode for the photoelectroreduction of CO₂

Samira Kaci, Yahia Ouadah, Lamia Talbi, Karima Benfadel, Assia Boukezzata, Isma Bozetine, Aissa Keffous, Saida Aachacha, Amar Manseri, Sabrina Belaid

Research Center on Semiconductor Technology for Energetic, CMSI Division, CRTSE, 2 Bd Frantz Fanon, PB 140, 7M, Algeria

In this study, SiC loaded copper particles (Cu-SiC) thin films were elaborated, characterized and studied for photoelectrochemical (PEC) reduction of CO₂ into methanol under visible light ($\lambda > 470$ nm) irradiation. The SiC thin films were deposited via sputtering method followed by a vacuum evaporated of Cu particles on the surface of SiC thin films. photocathode characterization was done by Scanning electron microscopy (SEM), UV-vis absorption spectra, and VMP3 station. Linear sweep voltammetry (LSV) was employed to evaluate the photocatalytic activity of the prepared photocathode under visible light ($\lambda > 420$ nm) irradiation for CO₂ reduction reactions. SEM results indicated that the Cu particles were well dispersed on the SiC thin film surface. The band gap energy of the Cu-SiC catalyst was 1.8 eV. The flat band potential was calculated using the Butler relation and was found at -0.46 V vs Ag/AgCl. During LSV, the onset potential was shifted positively (~100 mV) under the light-on condition than the dark condition in CO₂ saturated solution suggests an increase in photocurrent and occurrence CO₂ photoreduction reaction. The PEC performance of Cu-SiC photocathode showed an increased methanol formation under visible light irradiation.

Audience Take Away:

- Converting CO₂ into useful product using photoelectrochemical process and semiconductor thin films as a photocathode is a meaningful way to reduce the CO₂ in the atmosphere.
- Loading Cu on SiC reduced the band gap and hence increased visible light absorption by shifting the band-gap of commercial SiC into a new band gap of Cu-SiC.
- This study can help researcher and students which work on the catalytic reduction of CO₂. This research once published could serve as a course for those aiming to investigate thin films as a visible light responsive catalyst and expanding their research or teaching.
- This research can bring together researchers, industrialists and policymakers from across disciplines to further the use of CO₂ as feedstock for the manufacture of chemicals, minerals and fuels. Realization of these aims will help society to take a more environmentally sound approach to chemical production.

Biography

Dr. Kaci studied Chemistry at the Faculty of Chemistry, USTHB University, Algeria. She obtained her Magister in 2004. She started to work at CRTSE (ex UDTS) in 2004 until now as researcher in the team of Dr Keffous. She registered to Doctorat in 2009 which was supervised by Prof. Trari. She received her PhD degree in 2014 at the same Faculty. After two years postdoctoral she obtained the position of a Senior Researcher at the CRTSE. She has more than 20 research articles in SCI(E) journals. She is now Director of Thin Films Surface and Interfaces Division at CRTSE.

Fatty acid methyl ester analysis of olive oil degraded by *Pseudomonas fluorescens* and enzymatic characterisation of the lipase

Popoola Bukola Margaret

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Bacteria are very useful in protecting the environment. The lipolytic activities of physiologically diverse bacteria have great potential to degrade oil spills in the environment. Fatty acids are the major components of lipids; and the physical, chemical and physiological properties of a lipid class depend primarily on its fatty acid composition. There is need for extensive characterisation of the bacterium lipase for the treatment of vegetable oil-polluted sites. This work was carried out to preliminarily characterise the lipase of *Pseudomonas fluorescens* and to check the fatty acid composition of olive oil. Gas chromatography method can be used for the identification of microbiological degraded fatty acids in vegetable oils as methyl ester.

Pseudomonas fluorescens was screened for lipase production using standard methods. Temperature, pH, ion concentration (NaNO₃ and MgSO₄), enzyme concentration, nitrogen concentration, substrate concentration, time course and agitation speed were optimised for the lipase activity as well as growth.

Crude enzyme of *Pseudomonas fluorescens* had the highest lipase activity and growth of 0.8 U/mL and 1.418 mg/mL respectively at room temperature, but when production was optimised higher activity 0.9 U/mL was seen in the use of glucose as substrate. Agitation with the speed used did not support lipase production but supported growth (1.998 mg/mL) at agitation speed of 100 rpm. Olive oil degraded by lipase of *Pseudomonas fluorescens* grown in two different Mineral Salt Medium, was studied over 25 days. Olive oil was analyzed for fatty acids commonly present in olive oils which are Myristic, Palmitic, Stearic, Oleic, Linoleic, Linolenic, Behenic and Lignoceric, which have specific carbon number and their values in approximate percentage are C14:0 (0.4), C16:0 (14.0), C18:0 (5.5), C18:1 (76.4), C18:2 (3.4), C18:3 (0.1), C22:0 (0.1) and C24:0 (0.1) respectively. Oleic acid percentage is high in olive oil which contained considerable amount of 76.4%.

The reduction of fatty acid by *Pseudomonas fluorescens* after 20 days was 8.2% in the media used. Lipase from *Pseudomonas fluorescens* had potential for degradation of fatty waste. It could therefore be employed in environmental cleanup of oil spill site.

Audience Take Away:

- The audience will be informed on the existence of microbial lipases.
- They will learn certain conditions in which these lipases best function.
- They will know the potential of these lipases in the clean-up of our polluted environment.
- They should be able to support researchers in enhancing better operational level in the clean-up of the polluted environment.
- They will employ researchers who will work extensively in search of more and capable lipases and help in further detailed molecular characterization of these lipases in order to achieve maximal results.
- It will greatly assist in achieving accuracy and great experimental designs that will be carried out effectively and produce profitable results

Biography

Dr. B. M. Popoola, is presently working at Faculty of Natural Sciences, Department of Biological Sciences Ajayi Crowther University, Oyo, Oyo State, Nigeria. She received her Ph. D in Environment and Industrial Microbiology at the Department of Microbiology in the University of Ibadan. She has taught a variety of courses in Microbiology field such as Microbial Genetics, Microbial Physiology, Microbial Ecology, Virology, Bacteriology, Microbial Techniques and Petroleum Microbiology. She has authored or co-authored for 10 articles in both International and national referred journals and has published a book as well.

Activation of CO on cobalt catalyst supported on Al₂O₃: Promoted by Ru

Dekui Sun*, Qilong Xie, Yan Liu, Litao Jia, Bo Hou, Debao Li

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Fischer-Tropsch is an important technology for the efficient use of energy such as coal, natural gas and biomass which can convert syngas into high value-added chemicals. Co-based catalysts are promising Fischer-Tropsch synthesis industrial catalysts due to their excellent carbon growth ability and low water vapor shift reaction. In order to improve the performance of Co-based catalysts, it is necessary to conduct a comprehensive and in-depth study and exploration of its Fischer-Tropsch synthesis mechanism. In this paper, the adsorption and activation of CO on the surface of cobalt-based catalysts were investigated by in-situ DRIFTS, in-situ Raman, in-situ XPS, XRD and chemical transient, adsorption and desorption methods. It was found that there are three adsorption modes of CO on the surface of the catalyst, such as line type, bridge type and hollow type, and bridge type adsorption is mainly found at room temperature. As the temperature increases, the bridge adsorption CO decreases rapidly, and the catalyst retains only linear adsorption above 200 °C. This shows that linear adsorption of CO has higher thermal stability. During the heating process in H₂ atmosphere, there is a significant transition from the bridge-to-line morphology of the adsorbed CO. Only CO in the linear adsorption was observed on the surface of the catalyst at the reaction temperature, and the formation of C₃H₈ was apparent after the introduction of H₂. Therefore, the linear adsorption was more likely to be an adsorption form having Fischer-Tropsch synthesis activity. This study can provide a reference for the exploration of cobalt-based Fischer-Tropsch synthesis mechanism.

Audience Take Away:

- The linear adsorption was more likely to be an adsorption form having Fischer-Tropsch synthesis activity.
- This study can provide a reference for the exploration of cobalt-based Fischer-Tropsch synthesis mechanism.

Biography

Dr. D. Sun studied Chemistry at the Institute of Coal Chemistry, CAS, and received her PhD degree in 2010. He then joined the research group of Prof. Debao Li at the same institution.

Selective catalysis reduction of NO by NH₃ over Co/Cr-Ce catalysis at mid-low temperature

Gai Zeng^{a,b}, Xiaomei Hua, Daojian Huang, Dingsheng Chen, Jiqiang Daia, Chaoping Cena, Zhiyi Deng^b, Zhihang Chen^a

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The promotional effect of Co on Cr-Ce catalyst for the selective catalytic reduction of NH₃ to N₂ was investigated. The catalytic activity and SO₂ tolerance of Cr-Ce catalyst were greatly enhanced by the addition of 5wt% Co, in the temperature range of 250oC-350oC. And the N₂ selective of Cr-Ce had been highly enhanced from 40 to 98% at 240oC. With addition of Co, Ce⁴⁺ species on surface was led to a better dispersion, as a result the redox properties of the catalysis was enhanced. Moreover, Co carried out the reaction towards the conversion of N₂, the 5wt% Co/Ce-Cr catalyst reduced the formation of NH₄NO₂, and the SCR reaction over Co/Cr-Ce followed the Eley-Rideal mechanism.

E-POSTERS

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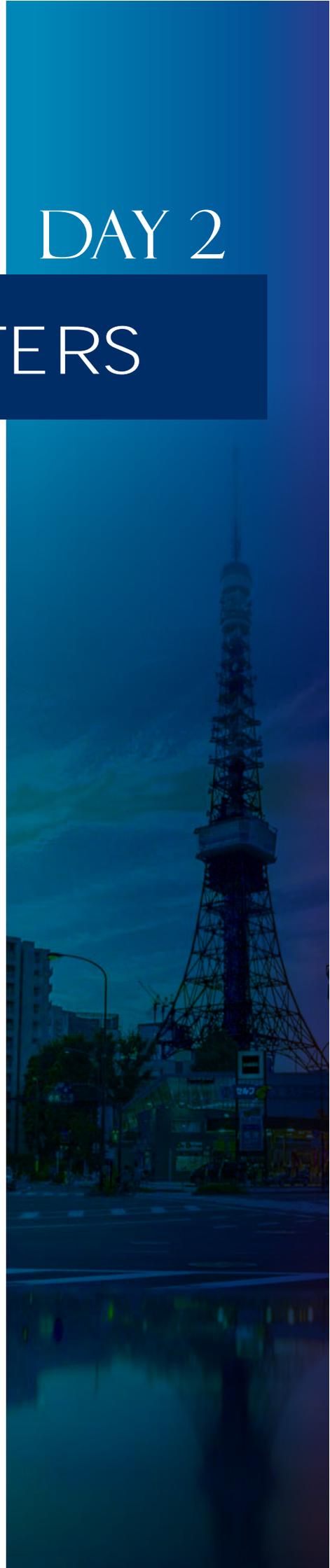
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16-18, 2019

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CFD simulation of crude petroleum boiling process inside reboilers

Dr. Alon Davidy

Tomer/Heat Transfer Researcher, Tel-Aviv, Israel

An advanced coupled simulation has been performed in order to analyze the performance of re-boiling process of crude petroleum flowing inside reboilers. This work includes analysis of fire heater and crude boiling process. The proposed model is composed from Heptane fire heater and a reboiler. The convective and radiative heat flux produced from burner is transferred to the crude oil flowing inside the pipe. The proposed computational model is composed of two phases — Simulation of fire by using Fire Dynamics Simulator software (FDS) version 5.0 and then a Nucleate boiling computation of the crude oil. FDS code is formulated based on CFD of fire-driven fluid flow. The FDS numerical solution carried out using Large Eddy Simulation (LES) method. FDS software calculates simultaneously the temperature, density, pressure, velocity, and chemical composition within each numerical grid cell at each discrete time step. It also calculates the temperature, convective and radiative heat flux. The thermophysical properties (such as: thermal conductivity, heat capacity, surface tension, viscosity) of the crude oil were estimated by using empirical correlations. The thermal heat transfer to evaporating two-phase crude oil mixture occur by bubble generation at the wall (nucleate boiling) has been calculated by using Chen correlation. It has been assumed that overall convective heat transfer coefficient is composed from the nucleate boiling convective coefficient and the forced turbulent convective coefficient. The former is calculated by Forster Zuber empirical equation. The latter is computed from the Dittus-Boelter relationship. This work can be further extended to include also the structural integrity aspects of the reboiler metal pipe by using COMSOL Multiphysics software.

Audience Take Away:

- The audience will be able to apply the physical principals described in this work, in other chemical processing installations such as steam reforming, Fluid Catalytic Cracking unit, or steam cycle thermal power plant based on biomass burning.
- They will gain knowledge regarding empirical correlations applied to estimate the thermo physical properties of petroleum fraction from easily measured properties such as: Temperature,
- Normal boiling point (NBP) and specific gravity (SG).
- The benefits achieved from this proposed work are:
- Accurate CFD tool to estimate the heat produced by the fuel burning.
- Accurate calculation of the convective and radiative heat flux transferred to the pipe.
- Two phase heat transfer
- This work can be extended to include additional aspects concerning safety and structural integrity aspects of the reboiler metal pipe such as: calculation of the Von Mises stresses of the pipe, calculation of the rupture time period of the steel pipes.

Biography

Alon Davidy received the B.Sc. degree in nuclear engineering from the Ben Gurion University in 1995 and the M.Sc. and Ph.D. degrees in the faculty of mechanical engineering from the Technion – Israel Institute of Technology at Haifa in 1998 and 2004, respectively. He worked in Israel prime minister office from 2015-2017 and in Israel Military Industries (IMI) from 2003-2015. His research interests include multi-physics simulations, heat and mass transfer, chemical reactions, CFD and Fire Safety simulations. He is member of American Chemical Society (ACS) and International Association for Fire Safety Science (IAFSS). He has published more than 30 research articles.

The decomposition reaction of hydrogen peroxide by the model catalysts

Nazym Zhunusbekova^{1*}, Nurzhan Chinibayeva², Tynyshtyk Iskakova¹, Gulsara Kussainova¹

¹Institute of Chemical and Biological technologies, Satbayev University, Almaty, Republic of Kazakhstan

The decomposition rate of hydrogen peroxide by polymer catalysts was investigated. As a result of the study of the activity of polymeric catalysts, it was found that the activity of these catalysts is much lower than the activity of catalase. However, these model immobilized biocatalytic systems exhibit sufficient catalase activity for use as enzyme substitutes, are stable during long-term storage, for 6 months, while the native enzyme loses activity within a week.

Our contribution is part of a complex biocatalyst creation project. Creation new polymer hydrogels based on synthetic and natural polymers as potential biocatalysts is an urgent and promising task. Materials for polymeric networks can be classified according to their source as natural or synthetic. Biocompatibility and biodegradability of appropriate materials are essential to their application in different areas. Biomaterials for control swelling systems are used or designed to elicit specific cellular functions. By this reason, natural hydrogels were gradually replaced or modified by synthetic types due to their higher water absorption capacity, long service life, and wide varieties of raw chemical resources, as expected.

The Michael's constants for the created systems as model catalysts are calculated. Method and optimal conditions for determining the catalytic activity of polymer-metal complexes have been chosen as results of this paper. The Michael's type curves are obtained, which are straightened in the Lineweaver – Burke coordinates. For a kinetic description of catalytic processes, one can use a scheme in which the interaction of the active center and the substrate proceeds through the formation of an intermediate complex.

Audience Take Away:

- Obtaining and modifying new polymer hydrogels based on synthetic and natural polymers as potential biocatalysts is an urgent and promising task.
- The study of the decomposition of hydrogen peroxide can be a source for new studies of polymer catalysts with the properties of catalase activity as well as one of the promising areas for the use of polymer catalysts.

Biography

Dr. Nazym Zhunusbekova studied at the Al-Farabi Kazakh National State University, Republic of Kazakhstan and graduated as MS in 2001. She then joined the research group of Prof. E. Bekturov at the Institute of Chemical Sciences, Academy of Sciences Republic of Kazakhstan. She received her PhD degree in 2003 at the same institution. After postdoctoral fellowship at the Institute of Macromolecular Chemistry of the AS CR, UNESCO course, Prague, Czech Republic and summer school, Hamburg, Germany she obtained her Associate Professor in 2011 (Academy of Sciences Republic of Kazakhstan). She won the Bruce Hartman Prize for young scientists for the best report and presentation 2010, Siegen, Germany, World Forum on the Use of Polymeric Materials "POLYCHAR 18". Now she is the scientific supervisor of one of the projects of a large program # BR05236302 (2018-2020) "Scientific and technical substantiation of innovations in the chemical cluster in the field of creating new materials and technologies for increasing the efficiency and environmental sustainability of industrial production". She has published more than 80 research articles.

Acknowledgements

The research for this paper was financially supported by the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan, grant no. BR05236302.

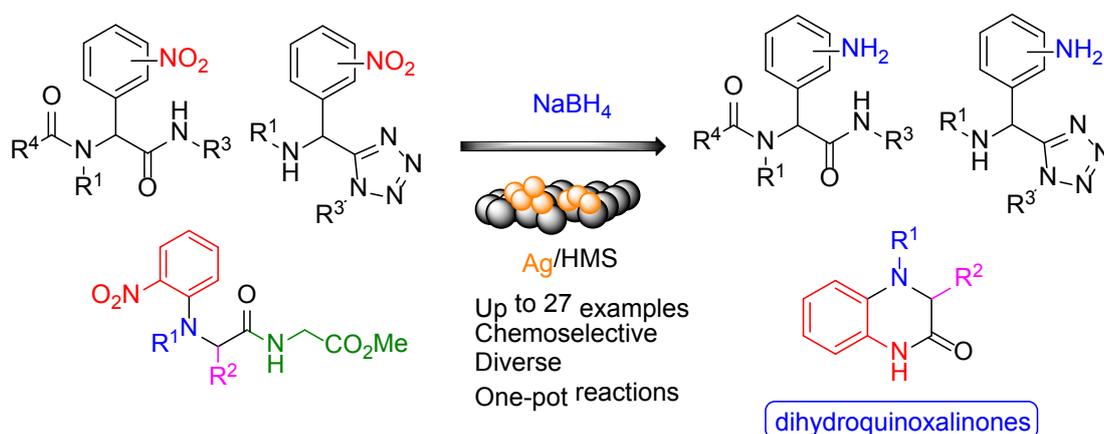
Chemoselective transfer hydrogenation of multifunctional nitro compounds catalyzed by silver nanoparticles: A Facile synthetic methodology towards dihydroquinoxalin-2-ones

Domna Iordanidou,^{1*} Tryfonas Zarganes-Tzitzikas,² Konstantinos Neochoritis,² Alexander Domling² and Ioannis N. Lykakis,¹

¹Department of Chemistry, Aristotle University of Thessaloniki, University Campus 54124, Thessaloniki, Greece; phone/fax: +302310997871;

²Faculty of Science and Engineering, Groningen Research Institute of Pharmacy, Antonius Deusinglaan 1, 9713 AV Groningen, the Netherlands.

The catalytic hydrogenation of nitro compounds is one of the most important chemical reactions as the product amines are forceful intermediates for the synthesis of various natural and industrial products like agrochemicals, pharmaceuticals, dyes, and polymers.¹ Through the Multi-Component Reactions (MCRs), which are an important method since carbon-carbon, carbon-nitrogen and carbon-oxygen bonds are created in a single stage,² the facile mesoporous silica-supported silver and gold nanoparticles catalyzed chemoselective reduction of multifunctional nitro-compounds into the corresponding amines in high isolated yields, employing NaBH₄ or Et₃SiH as reducing agents,³ is reported. The present catalytic system represents an rattling approach towards the production of the heterocyclic bioactive compounds of dihydroquinoxalin-2-ones with high yields, via a catalytic two-step one-pot ring closing pathway based on the reported chemoselective reduction.



Audience Take Away:

- It is the first example of chemoselective reduction by silver or gold nanoparticles applied in multifunctional nitro-compounds at ambient conditions without the use of specific instruments or reactants.
- Nitro- compounds owning amino- acids in their molecules could be reduced conveniently letting intact the part of amino acids. Furthermore, other easily reducing or detaching groups remain inert under the above conditions.
- In one-step, without the handling of toxic or dangerous materials, for the first time, dihydroquinoxalin-2-ones are produced. These molecules are bioactive molecules with anticancer and anti-inflammatory properties, as well as against neurological diseases. The paper with those molecules has been successfully deposited for immediate availability to PubMed Central (PMC). Our synthesis gives an easy access to inhibitors of the soluble epoxide hydrolase (sEH), an important target for therapies against hypertension or inflammation.
- The catalyst, with unique properties, will be removed easily from the reaction's mixture by centrifugation and it could be reused at least 5 times.

Biography

Dr. Iordanidou studied Chemistry at the Department of Chemistry, in Aristotle University of Thessaloniki, Greece and graduated as MS in 2014. She then joined the research group of Prof. Ioannis N. Lykakis in the faculty of Organic Chemistry at the same department. She received her PhD degree in 2019. From September to December in 2016, she joined the research group of Prof. Jean- Luc Renaud in the laboratory of Organic and Thioorganic Molecules in Ecole Nationale Supérieure d'Ingénieurs de Caen (ENSICAEN), in France. She has published 2 research articles in SCI(E) journals and another 5 are to be submitted.

Stereocontrolled biocatalytic reductions of carbonyl compounds

Ioulia Smonou^{*1}, Vasileios Giannopoulos¹, Kamela Mirtollari¹, Apostolos Hatzoudis¹

¹Department of Chemistry, University of Crete, Heraklion, Crete, Greece

The contribution of biocatalysis in asymmetric organic synthesis is of great importance. Biocatalysts show high chemo-, regio- and stereo- selectivity and are active under mild reaction conditions. Asymmetric biocatalytic reduction of ketones is particularly important, since chiral alcohols are present in a wide spectrum of pharmaceuticals or can be used as chiral building blocks in the synthesis of numerous natural products and biologically relevant compounds.

Our continuing interest on stereoselective ketoreductase-catalyzed reductions of various di- and tricarbonyl compounds led us into the synthesis of optically active keto alcohols, diols, hydroxy esters, dihydroxy esters, valuable chiral synthons for the synthesis of high added value compounds.

Recently, we have focused in a new class of structurally interesting carbonyl compounds with substituents bearing different heteroatoms, which are very useful chiral synthons of a large variety of bioactive compounds. We will present here our latest results on the enzymatic asymmetric reduction of these compounds.

Audience Take Away:

- The audience will become familiar with the biocatalytic reduction processes which combine particularly mild reaction conditions with excellent stereoselectivity, benefits that have made them very useful at both laboratory and industrial scale.
- The research results which will be presented can be easily used as useful examples during teaching on how to use enzymes in order to achieve optically pure high added value compounds.
- The chemoenzymatic methodology provides a practical solution in synthetic problems because it simplifies efficiently the whole synthetic process.

Biography

Dr. Smonou studied Chemistry at the University of Athens, Greece; Ph.D. in Organic Chemistry (1985), National Research Institute and University of Athens, Greece; Postdoctoral Research Fellow, University of California Los Angeles with Prof. M. E. Jung. She became Lecturer of Organic Chemistry in 1992 and is now Associate Professor in the Department of Chemistry, University of Crete, Greece. In 2006 she was Visiting Professor at the California Institute of Technology (Caltech) with Prof. Frances Arnold (Nobel 2018). She has published more than 40 research articles in SCI(E) journals.

The 3-axis portable filament winding machine embedded with wireless technology

Ma Quanjin*¹ and Mohd Ruzaimi Bin Mat Rejab¹

¹Faculty of Mechanical and Manufacturing Engineering, Universiti Malaysia Pahang, 26600 Pekan, Pahang, Malaysia

Filament winding process is a traditional composite fabrication technique, which is mainly produced for open or close end structures such as vessels, pipes, tanks and domes. Filament winding technique has three winding patterns: hoop, helical and polar winding. Compared to other fabrication processes, filament winding process offers higher fibre volume fraction, higher degree of automation and low-cost characteristics. It is used in many application fields such as infrastructure, military, aerospace and mass transportation. Nowadays, filament winding machine has developed to advance its application with different axes. For axes perspective, the 6-axis winding machine has the highest axes level, which offers 3 linear and 3 rotation motions. However, several available filament winding machines provide complicated and copyright control system, which is typically used wire method. In order to design a portable winding machine with minimum-axis demand, the 3-axis filament winding machine has developed with wireless method using Bluetooth and WiFi modulus. The 3-axis winding machine has been tested to evaluate the winding performance, which refers to winding circular test and winding angle measurement test. Further, the 3-axis filament winding machine have produced several filament wound composite products such as tubes and vessels. For winding angle scope, it can offer 20° to 90° degree with $\pm 1^\circ$ winding angle standard deviation. The control system of this machine is mainly selected Arduino Uno and CNC v1 shield module, which has an inexpensive and open-source control system features. In conclusion, wireless technology is successfully applied to this laboratory scale 3-axis portable winding machine control system, which makes a significant contribution to control system methods.

Audience Take Away:

- Filament winding technique is a higher automated fabrication method to manufacture filament wound composite products such as tubes, vessels and domes.
- Filament winding technique provides low-cost, high-repeatable and high-flexible strengths compared to other composite fabrication processes.
- Available filament winding machines have large machine structure, sophisticated and copyright control system, which limits its application fields and winding technique development.
- The 3-axis portable winding machine has been successfully designed, fabricated and tested, which broadens the potential composite market in filament winding process or relevant equipment.
- Wireless method is applied in the laboratory scale 3-axis filament winding machine using Bluetooth and WiFi module, which simplifies its structural type and control system.
- The 3-axis portable winding machine is suitable for several industries such as small or medium manufacturing industries, aerospace advanced material industries, polymer manufacturing industries and academic research or teaching prototype.

Biography

Ma Quanjin obtained Bachelor Degree at Ningxia University, China in 2016. He received Master Degree at Universiti Malaysia Pahang, Malaysia in 2018. Now, he is pursuing PhD at Universiti Malaysia Pahang, Malaysia. He is appointed as research assistant in Faculty of Mechanical Engineering. He has published 4 journals, 1 book chapter, and 6 conference papers. He has won 9 medals (3 gold and 6 silver) in different kinds of International Innovation, Technology & Research Exposition. He has obtained 1 Malaysia Patent: PI 2018701785, and 1 Chinese Patent is in progress.

Characterization of polymer-silicate composite materials

Nazym Zhunusbekova¹, Nurzhan Chinibayeva², Tynshtyk Iskakova¹, Gulsara Kussainova¹

¹Institute of Chemical and Biological technologies, Satbayev University, Almaty, Republic of Kazakhstan

This paper's aim is improvement and imparting new properties to polymeric complexes in order to obtain fundamentally new materials based on them - polymer-silicate composite materials. In this case, the polymer-silicate composite has properties that differ from the properties of the individual components. The most promising component as a filler are layered silicates (clay materials), which have useful properties, such as non-toxicity, high plasticity, sorption capacity, and are characterized by low cost and large reserves. The next stage of research was the modification of layered silicates with organic compounds. The synthesis of composite polymer materials containing clay particles was carried out by intercalation polymerization of synthetic 2-hydroxyethyl acrylate monomers, in the presence of a crosslinking agent, at a temperature of 1 hour. The resulting materials were crosslinked three-dimensional structures in the form of gels based on acrylic acid derivatives, where inorganic cations intercalated into the polymer network during the formation of the polymer composite. As a result, inorganic cations were intercalate into the polymer network during the formation of the polymer composite. The composition of the inorganic modifier was studied. For increasing the sorption capacity, layered silicates were activated before being incorporated into the polymer composite. The study of the influence of the filler on the gel properties shows that increasing of the clay content in the sample lead to a variable change in the sorption properties of gel.

It was established that the main component of the material under study is silicon dioxide, amounting to 60.51 wt.%, which is the main component of almost all terrestrial rocks. Common known that the best technological properties are possessed by bentonites with exchangeable sodium cations, in our case sodium cations are contained in the form of sodium oxide (2.41 wt.%). In order to increase the content of exchangeable cations, it was expedient to pre-activate the clay before polymer composite synthesizing, the carbonate of calcium (magnesium) formed during the ion exchange can form inorganic deposits that are precipitated from aqueous compositions of these activated bentonites. Polymeric composite materials modified with activated layered silicates have been synthesized by the intercalation polymerization of synthetic monomers in the presence of a crosslinking compound.

Audience Take Away:

- Obtaining and modifying new polymer hydrogels based on polymer-silicate composite materials is an urgent and promising task.
- This paper's aim is improvement and imparting new properties to polymeric complexes in order to obtain fundamentally new materials based on them - polymer-silicate composite materials. In this case, the polymer-silicate composite has properties that differ from the properties of the individual components. The most promising component as a filler are layered silicates (clay materials), which have useful properties, such as non-toxicity, high plasticity, sorption capacity, and are characterized by low cost and large reserves. This study can be a source for new studies of the promising areas for the use of polymer-silicate composite.

Biography

Dr. Nazym Zhunusbekova studied at the Al-Farabi Kazakh National State University, Republic of Kazakhstan and graduated as MS in 2001. She then joined the research group of Prof. E. Bekturov at the Institute of Chemical Sciences, Academy of Sciences Republic of Kazakhstan. She received her PhD degree in 2003 at the same institution. After postdoctoral fellowship at the Institute of Macromolecular Chemistry of the AS CR, UNESCO course, Prague, Czech Republic and summer school, Hamburg, Germany she obtained her Associate Professor in 2011 (Academy of Sciences Republic of Kazakhstan). She won the Bruce Hartman Prize for young scientists for the best report and presentation 2010, Siegen, Germany, World Forum on the Use of Polymeric Materials "POLYCHAR 18". Now she is the scientific supervisor of one of the projects of a large program # BR05236302 (2018-2020) "Scientific and technical substantiation of innovations in the chemical cluster in the field of creating new materials and technologies for increasing the efficiency and environmental sustainability of industrial production". She has published more than 80 research articles.

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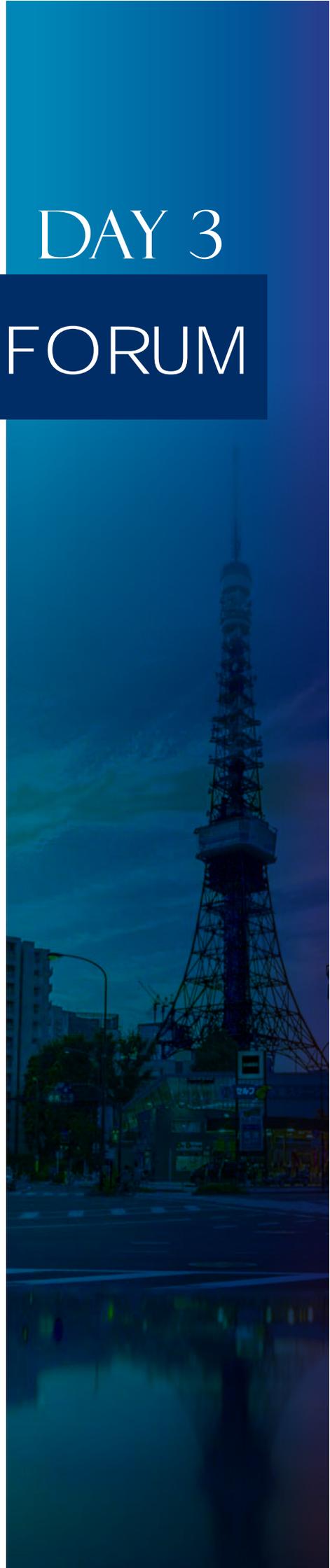
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Biography

Dr. Jian Zhi Hu received his BS degree in Physics from Lanzhou University of China in 1983, his MS degree in 1986, and his Ph.D degree in 1994 from a joint-University of Utah, USA and the Chinese Academy of Sciences Ph.D program. He joined the Pacific Northwest National Laboratory, USA, in year of 2000 as a junior research scientist and is currently a senior staff scientist. Dr. Hu has published more than 200 peer reviewed publications with an h-index of 40. He received 11 USA patents and two R&D 100 awards.

In situ magic angle spinning NMR: A powerful tool for catalyst research

Jian Zhi Hu

Pacific Northwest National Laboratory, Richland, WA 99354, USA

High resolution magic angle spinning (MAS) NMR is a powerful technique for studying structure and dynamics in a heterogeneous system containing a mixture of e.g., solid, semi-solid, liquid, and gaseous phases. Due to its intrinsic advantage of probing local structure at molecular level, MAS NMR is an attractive tool for in situ (operando) investigations of reaction mechanisms, including but not limited to the identification of active centers, intermediates, and the reaction dynamics associated with material synthesis or chemical reactions using solid catalysts. However, the commercially available reusable-MAS rotors are rarely capable of achieving 100% seal while fast spinning even at ambient conditions. In particular, reusable sample cells that can efficiently perform at combined high temperature (> 100 C) and high pressure (> 10 atm) are challenging due to technical complications associated with sealing heterogeneous solid/fluid/gaseous samples at high temperature and pressure while spinning at several kHz or more inside a strong magnetic field. Recently, we have developed a perfectly sealed MAS NMR rotor that is capable of sealing a heterogeneous sample containing solid, semi-solid, gases and liquids or a mixture of them under extreme experimental conditions of combined high pressure and high temperature.¹ Herein, we would like to introduce this powerful operando NMR technique to the catalysis community with new examples of application in material synthesis and catalytic reactions, including but not limited to (a) Mechanisms of phenol-cyclohexanol alkylation in zeolite H-BEA studied by ¹³C and ¹H NMR,²⁻³ (b) The crystallization of AlPO₄-5 by ¹H, ²⁷Al, and ³¹P NMR,⁴ and (c) Genesis and stability of hydronium ions in zeolite channels by ¹H and ¹H-²⁹Si CP NMR, and (d) Zeolite framework stability and degradation in hot water studied by high field and fast spinning ²⁷Al MAS NMR.

Audience Take Away:

- A new analytical tool for in situ (operando) studies of catalyst reaction mechanisms using heterogeneous catalysts (i.e., solid catalysis), including but not limited to characterizing active centers, reaction dynamics and pathways, adsorption and desorption mechanisms on catalyst surface, all at real world reaction conditions.
- We will show that in situ MAS NMR allows reaction intermediate detection that are impossible to capture at room temperature.
- We will show significant re-arrangement of alumina tetrahedral-sites accompanied by the conversion of partially bonded octahedral alumina to tetrahedral alumina sites at high temperature for HBEA with Si/Al=100. The results yield new insight into the high stability and reactivity of this catalyst for biomass conversion that could not be obtained previously.
- We will show that the combined advantages of high field and fast spinning for quadrupolar nuclei will make the in situ MAS NMR a powerful method for catalysis and materials research.
- The methodology can be a general tool for faculties and students in their own research associated with catalyst design, materials synthesis and reaction mechanisms investigations.



Biography

Prof. Zhu's research interests exist in advanced catalysis, gas/liquid adsorption and separation, direct carbon fuel cells and solid oxide fuel cells. His publications include one edited book, 8 book chapters, and over 250 journal papers. He holds 8 patents, 4 patents have been licensed to the industrial sponsor. He has raised a total research funding from government and industries in excess of \$20 million. He is the recipient of a number of awards, including RK Murphy Medal 2013, Freehills Award IChemE 2011, 2nd place Innovator of the Year Award Global IChemE 2011, the University of Queensland (UQ) Foundation Research Excellence Award in 2007.

Ultrathin iron-cobalt oxides nanosheets as highly active electrocatalyst for water splitting

Zhonghua Zhu

School of Chemical Engineering, the University of Queensland, Brisbane, 4072 Australia

Electrochemical water splitting is an effective method for storing electrical energy in the form of H₂ fuel, but hindered by the sluggish anodic oxygen evolution reaction (OER). It is thus important to develop an efficient OER catalyst with large surface area, abundant active sites, and good stability through simple and economical method. Herein, we introduce a facile solution reduction method to prepare the iron-cobalt oxide nanosheets with a large specific surface area, ultrathin thickness (1.2 nm) and, importantly, abundant oxygen vacancies. The activity of the new catalyst was superior to those of commercial RuO₂ and most of reported OER catalysts. The mechanisms for the excellent OER catalytic activity of the new catalyst will also be discussed (Advanced Materials 2017, 29 (17), 1606793).

Audience Take Away:

- Nanostructured metal oxide catalysts are extensively used in chemical industry, clean energy and environment. From this talk, the audience can learn how to synthesize ultrathin metal oxide nanosheets with a facile solution reduction method, and how to significantly improve the surface area and active sites of the catalysts, thus making the catalysts highly active and stable.
- The audience from universities or research institute can use the same method to synthesize novel metal oxide nanosheets in their own areas either as catalysts, adsorbents, membranes or sensors.
- The industry can use similar methods to synthesize highly effective and economical catalysts. Due to the very high activity of the novel nanostructured catalysts, some noble metal catalysts can be replaced by cheap metal catalysts, thus greatly saving the costs.



Biography

Tsodikov, Mark V. was born on August 18, 1945 in Moscow. He studied Degree in organic chemistry, D.I. Mendeleev Russian University Chemical Technology, 1968. Doctor of Philosophy in Chemical Technology, Russian Academy of Sciences, 1975. Doctor of Science in Chemistry, Russian Academy of Sciences, 1992.

He is a Russian chemistry professor, researcher. Achievements include research in synthesis, structure and catalytic properties of multicomponent metal containing systems; research in low-temperature sol-gel synthesis base on colloid organic solutions and single-phase multicomponent metal oxides. Member of Menelev Chemical Society Russia. Mark V. Tsodikov has been listed as a noteworthy chemistry professor, researcher by Marquis.

Structurally - dimensional effects in selective heterogeneous catalysis of renewable biomass into important products of petrochemistry

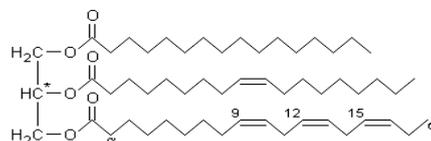
M. V. Tsodikov

A.V. Topchiev Institute of Petrochemical Synthesis RAS

In recent years, much attention has been paid to the use of renewable biomass as an alternative raw material for the production of fuel components, hydrogen and syngas, as well as important monomers. In this direction, a special role is given to catalytic processes using nanoscale catalytic systems that provide highly selective conversion of renewables.

The report presents the results obtained during recent years in the laboratory of Catalytic nanotechnology of A.V. Topchiev Institute of Petrochemical Synthesis RAS concerning with the study of the structural organization of nanoscale metal-containing active components effect on selective conversion of ethanol and fermentation products, fatty acid triglycerides and plasma-catalytic dry reforming of mixed kraft lignin in the main energy carriers and important petrochemical products.

It was found that by increasing the ratio of the active components of Sn/Pt to 5 in Pt-Sn/Al₂O₃ catalysts, the selectivity in the reaction of reducing deoxygenation of a large number of esters, including fatty acid triglycerides, increases in the hydrocarbon components by the number of carbon atoms corresponding to the ether fragments and water:



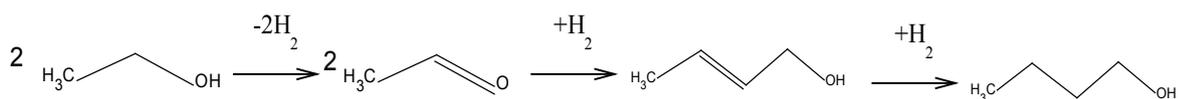
The yield of light hydrocarbons C₁, C₂ and carbon oxides CO₂, CO does not exceed 0.5%. The study of the evolution of the active components structure showed that high selectivity is provided by the formation on the surface of the nanoscale intermetallic particles PtSn_{3±δ} and tin oxides with a size of 2-3 nm.

Using a porous hybrid membrane-catalytic converter obtained by self-propagating high-temperature synthesis of Ni(5% Al)-Co composition, a high conversion is achieved in the process of dry and steam reforming of methane, hydrocarbons, ethanol and fermentation products into synthesis gas, reaching 80-120m³/dm³membr.h. The role of Al on the formation of reforming active components on the inner surface of the converter channels was established. The study evolution structure with use X-Ray and TEMHR showed that in the presence of 5-8% Al, the formation of the converter proceeds by the so-called mechanism of aluminothermal synthesis, as a result of which aluminum atoms reduce cobalt from its oxide, turning into aluminum oxide particles up to 200 nm in size, on the surface of which highly dispersed intermetallic particles of Ni-Co alloy with a size of 5-8 nm are formed:



The methods of nickel-and iron-containing components formation on the surface of mixed lignin of wood origin, having the ability to possessed by high possibility to absorb of microwave irradiation (MWI) with plasma generation. Dry reforming of organic mass of lignin (OML) proceeds in the mode of plasma stimulated by MWI at the average temperature of the reaction zone 700-800C. Conversion to OML reaches 65% at selectivity in producing syngas of H₂/CO – 1 up to 92%. Time of carrying out of process is 15 min. With using vibration and messbauer spectroscopy, TEMHR and magnetic measurements have studied evolution of the structural organization of the active components having high ability to absorption of MWI and catalytic activity in dry reforming process.

High activity (60%) and selectivity (85-90%) in reactions of selfcondensation of supercritical ethanol to n-butanol and -alkylation of isopropanol-2 by ethanol to pentanol-2 were reached in the presence of nanosize



bimetallic catalysts such as Au-Ni; Au-Cu and Au-Fe forming on the surface of γ -Al₂O₃ as nano size particles 2-3 nm. It was shown that the role of gold co- reagents is providing by high activity and selectivity of the catalysis consist of in an obstacle of agglomeration of the gold nanoparticles and formation of Au⁺.

Acknowledgements:

This work was supported by the Russian Science Foundation (agreement no. 17-13-01270).

SPECIAL TALK

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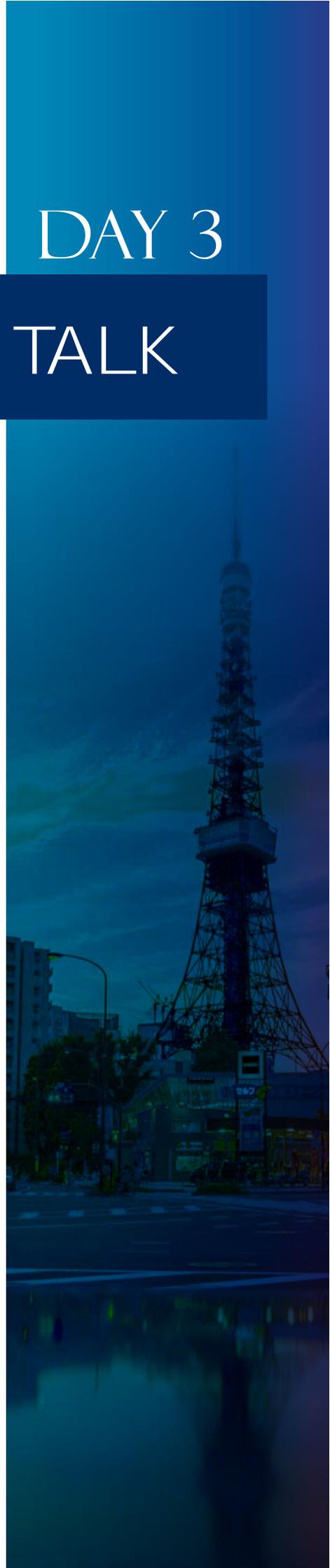
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Textual differences between the engineering research article (RA) and its subsequent poster

Dr. Tharwat M. EL-Sakran

English Department, College of Arts and Sciences, American University of Sharjah Sharjah, United Arab Emirates

Converting a RA into a poster is a highly complex, recursive reading-writing activity involving constraints that can impose an overwhelming cognitive load on academic poster designers, thereby adversely affecting their production. This study contributes to a growing, but still relatively ambiguous, body of research which emphasizes the importance of designing clear and easy to navigate through academic posters. Another contribution of this study is that it proposes practical and user-friendly guidelines for poster design and presentation of research contents. A total of 20 RAs with their subsequent posters were used for this investigation. It probes into how the collected RAs discourse is presented in posters and what elements in the RAs are modified, changed or totally removed. Several software packages were employed to help find answers to the research questions. Comparisons of the RAs with their subsequent posters show that the longer the original RA is, the smaller the matching percentage between them. Yet, further analyses reveal that posters mirrored the same rhetorical structure of the RA. As for the contents, results indicated that the RA contents were copied and pasted onto the poster in 95% of the cases examined. The present researcher, in an attempt to provide clear guidance regarding what research content(s) to display on the poster, proposes that poster contents may reflect the original RA structure with more emphasis allotted to new information in the research. Such a practice will help reduce the limitations that the poster space may impose on the contents, allow the poster presenter more freedom to use a bigger font size, and most importantly; interact and engage actively with the interested audience. The research concludes with limitations and recommendations for further research.

Biography

Dr. Tharwat M. EL-Sakran is a professor of linguistics in the English Department at the American University of Sharjah in the United Arab Emirates. He has published several papers on various issues related to teaching English for specific purposes, cross-cultural communication, translation, interpreting, forensic linguistics and discourse analysis. Dr. EL-Sakran is also an associate member of the Association of Certified Fraud Examiners (ACFE) and a certified fraud examiner (CFE).

SPEAKERS

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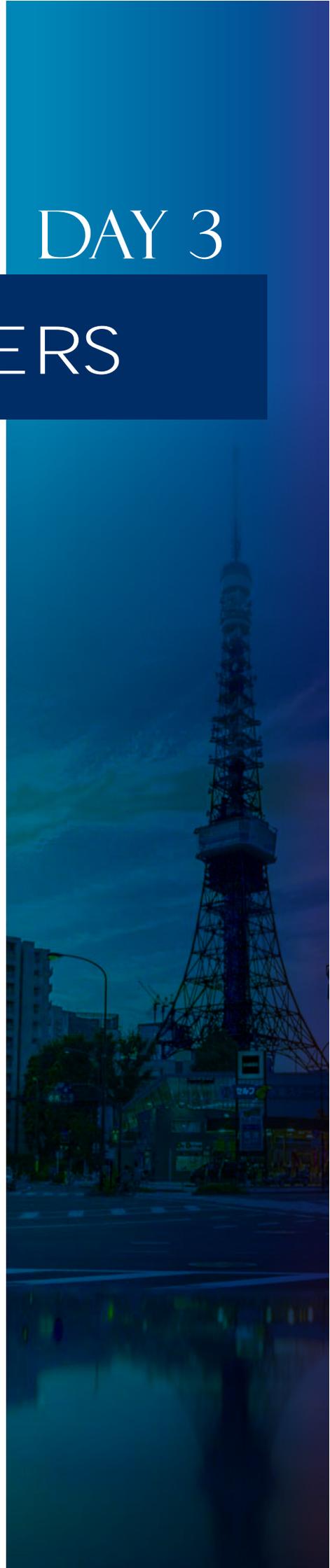
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Dynamics of flow pattern in standard mixing vessel stirred by pitched blade turbine

Tomáš Brůha¹, Václav Uruba¹

¹ Institute of Termomechanics, Academic of Science Prague, Department of fluid mechanics, Praha, Czech Republic

The lecture deals with theoretical and experimental study of flow pattern dynamics and its manifestation on liquid surface in flat bottomed and four baffled cylindrical mixing vessel stirred by down pumping six pitched blade turbine. Mixing vessel with inner diameter $T = 0.29$ m was filled with water to the height $H = T$. Diameter of impeller D was $T/3$, and impeller bottom-of clearance $C = T$. Width of baffles was $b = 0.1 T$ and impeller speed was set to 6.67 s^{-1} (400 rpm). Based on flow visualisation in middle vertical plane passing just front of opposite baffles, quasi periodical behaviour of macro-flow was detected and investigated. It was found, that responding macro-flow pattern can be divided to lower and upper part, with lower part express periodical behaviour of generating, growing and subsequently disintegrating of main circulation loop while upper part is characteristic by presence of so-called flow macro formation which are separated from main circulation loop and moving to liquid surface where some of them caused surface macro-swelling. Visualisation in horizontal plane passing through the vessel at $3/4 H$ showed that mentioned flow macro formations are present just at the baffles with practically equal frequency for each baffle. And anyway so liquid surface macro-swelling. Furthermore was found, that while one cycle of main circulation loop, approx. 2-4 flow macro formation are separated within one quadrant of vessel. Described flow-pattern behaviour is supposed to be manifestation of well-known low frequency phenomena of flow macro-instability in mixing vessel.

Audience Take Away:

- Detail knowledge of flow pattern dynamics in mixing vessel is important mainly from two point of view:
- For purpose of effective mixing (resp. blending) is very important to know position of application (injection) of mixed phase which ensure fastest dispersion (mixing) over whole bulk of vessel, which obviously depend on flow dynamics.
- As was proved and publicized in previous contribution, phenomena of flow macro-instability has non-negligible dynamics force effect on whole body of mixing vessel, including baffles, shaft and impeller.
- Based on this fact is possible to conclude that as practical goal is lowering mixing expanses (which over whole world yearly reach up to several milion dollars) results of this investigation can help to this goal by at first make mixing and blending more effective with lower mixing times and at second to designing mixing systems taking into account minimizing stress on body of mixing vessel and its installation.

Biography

Tomáš Brůha studied on Faculty of Mechanical engineering, Czech Technical University Prague and graduated as MS in 1992. Subsequently he was working as chief technical officer in company ENEX, l.t.d. dealing with complex heating solutions. In 2008 he started post gradual study on Institute of Chemical Engineering Prague, where he joins to research of mixing fluid dynamics. He received PhD degree in 2012 on some institution. After that, he participated on research concerning new diagnostic method of lung cancer on Charles University Hospital, Prague. Currently he is participating on research of flow field in mixing vessel with PIV, take place on Institute of Termomechanics, Prague. He is author (co-author) of 4 articles in SCI (E) journals and 10 oral and poster presentation on international congress.

A prospective life-cycle assessment (LCA) of monomer synthesis: Comparison of biocatalytic and oxidative chemistry

Marie A.F. Delgove,^{1*} Achille-B. Laurent,¹ John M. Woodley,² Stefaan M.A. De Wildeman,¹ Katrien V. Bernaerts,¹ Yvonne van der Meer¹

¹Aachen-Maastricht Institute for Biobased Materials (AMIBM), Maastricht University, Geleen, the Netherlands

²Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby, Denmark

Enzymatic reactions are typically perceived, and sometimes claimed, as being greener than the corresponding chemical conversions. The use of water as reaction medium, the selectivity of enzymes to avoid protection/deprotection steps, and the renewable aspect of enzymes are just a few examples of the presumed benefits of biocatalysis. These assumed environmental benefits are an incentive for the development of such enzymatic processes. They are few methodologies to evaluate the environmental impact of (bio)chemical reactions. Life cycle assessments (LCAs) are being more widely performed by the scientific community in order to obtain an accurate quantification of the environmental impact of reactions or processes. An LCA is a standardized and internationally recognized tool specifically designed to quantify the environmental impact of a product or service, taking into account its entire life cycle (ISO14044:2006). So far, LCAs are considered as “the best framework for assessing the potential environmental impacts of products currently available” by the European Commission because several environmental impacts are considered.

The goal of the current study is to compare the environmental impact of two synthetic routes for the preparation of lactones. A cradle-to-gate LCA was performed to compare the chemical and biochemical synthesis of lactones obtained by Baeyer-Villiger oxidation (Figure 1). This LCA is prospective since the studied process development is still at laboratory scale. The results of the LCA show that the impacts of both routes are similar for all the impact categories evaluated (climate change impact, damage to human health, use of primary energy, and ecosystem quality).

Key process performance metrics affecting the environmental impact were evaluated by performing a sensitivity analysis. Recycling of solvents and enzyme was shown to be crucial and to advantage the enzymatic synthesis. Additionally, the climate change impact was demonstrated to be dramatically affected by the source of electricity used (laboratory scale experimentation). The use of renewable electricity is therefore relevant because it can decrease the carbon emissions by 74 %.

The study shows that the LCA methodology, including the sensitivity and the uncertainty analysis, can be used to usefully support decisions from the early-stage of process development. The environmental impact comparison allows selecting the most promising route for developing a new process. As shown in the sensitivity analysis, the implementation of the recycling of enzyme is relevant from a carbon emission point of view. It is also relevant to identify the key process performance metrics for the improvement of the environmental impact of these reactions.

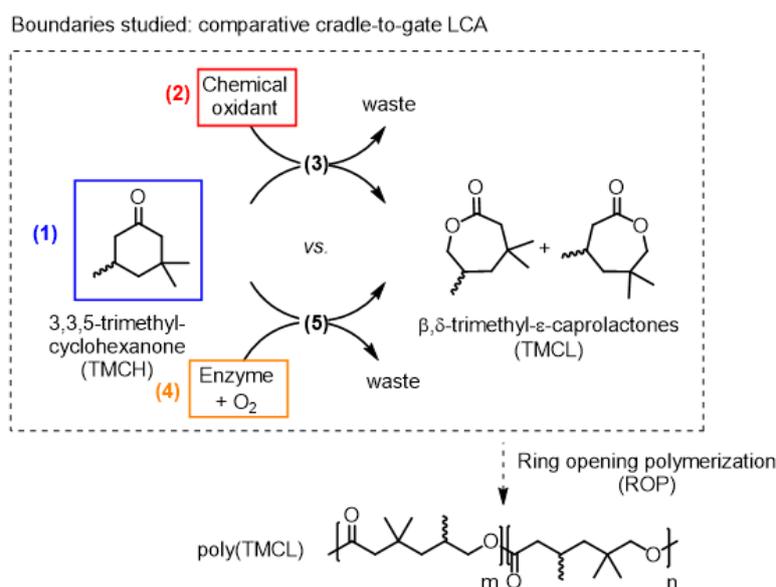


Figure 1. Boundaries studied for the synthesis of the lactones: comparative cradle-to-gate life-cycle assessment

Audience Take Away:

- The talk addresses a common perception in the field of biocatalysis and provides a quantitative answer.
- This talk demonstrates how the fields of sustainable chemistry and biocatalysis can collaborate, and how such environmental studies can be extended to other fields (catalysis, polymer chemistry, materials, ...).
- This talk will inspire the audience to use early-stage life cycle assessment for the development of greener processes.
- The audience will learn the role that the process performance metrics of reactions can play in sustainable chemistry.

Biography

Marie Delgove studied chemistry at the Ecole Nationale Supérieure de Chimie de Mulhouse (France). She obtained her Master degree in 2015, with a specialization in polymer chemistry and material science. She is currently performing her PhD at the Aachen-Maastricht Institute for Biobased Materials AMIBM (the Netherlands). By combining biocatalysis and polymer chemistry, she evaluates the use of oxidative enzymes for the synthesis of monomer building blocks, which are used as precursors for polymers.

Design and application of virus imprinted polymer (VIP) for the rapid and selective detection of Foot-and-Mouth Disease Virus (FMDV)

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¹Nanomaterials Laboratory, Center for Materials Science, Zewail City of Science and Technology, 6th October City, 12578 Giza, Egypt;

²Applied Organic Chemistry Department, National Research Centre (NRC), Dokki, 12622, Giza, Egypt;

³Virology Department, Animal Health Research Institute (AHRI), Agricultural Research Center (ARC), Egypt;

⁴Chemistry Department, Faculty of Science, Cairo University, Giza, 12613, Egypt

⁵Microbiology Department, Faculty of Veterinary Medicine, Alexandria University, Egypt

Foot and mouth disease virus (FMDV), is a highly contagious virus due to its ease of transmission. FMDV has seven genetically distinguished serotypes with many subtypes within each serotype. The traditional diagnostic methods of FMDV have demonstrated many drawbacks related to sensitivity, specificity, and cross-reactivity. In the current study, a new viral imprinted polymer (VIP)-based biosensor was designed and fabricated for the rapid and selective detection of the FMDV. The bio-recognition components were formed via electrochemical polymerization of the oxidized O-aminophenol (O-AP) film imprinted with FMDV serotype O on a gold screen-printed electrode (SPE). The overall changes in the design template have been investigated using cyclic voltammetry (CV), atomic force microscopy (AFM), Field emission-scanning electron microscopy (FE-SEM), and Fourier-transform infrared spectroscopy (FT-IR). Optimal conditions were achieved through investigating the capturing efficiency, binding stability, selectivity and lifetime of the developed biosensor. The results depicted a high selectivity of the biosensor to the serotype O over all other genus serotypes A, SAT2 and Lumpy skin disease virus (LSDV), as well as, the inactivated serotype O. The limits of detection (LOD) and quantification (LOQ) were around 2 ng/mL and 6 ng/mL, respectively, in addition to the tested repeatability and reproducibility values with a variance coefficient of 1.0% and 3.6%, respectively. In comparison with the reference methods (ELISA and PCR), the analysis of saliva real samples using the developed affordable biosensor offered 50 folds lower LOD with the possibility of an on-line monitoring in the field with no prior sample treatment.

Audience Take Away:

- How to design electrochemical VIP sensor for the detection of Virus.
- Highlight the advantages of the sensor in comparison with traditional methods.
- Application of the proposed technique for the production of portable sensor to be used for in field early diagnosis of the virus.

Biography

She is full Professor of Analytical Chemistry, Faculty of Science, Cairo University since 2014; adjunct professor in Zewail City of Science and Technology, Giza. She has got the State incentive award for technological science (basic sciences sector) for the year 2015, besides several travel and research grants from DAAD, TWAS and Center of special studies in Alexandria library. Her research interests include: Molecularly imprinted polymers synthesis and different applications including solid phase extraction, sensors and drug delivery systems, nanoparticles synthesis. She has published more than 45 research articles in SCI(E) journals.

A Novel synthesis of thiolato and phenoxo platinum (II) complexes by using phase transfer catalysis

Jaafar K. Jawad

Dean in the International University of Erbil, Iraq

The synthesis of platinum bipy (bipy = 2, 2' - bipyridyl) complexes containing some anionic Group 16 ligands with kinetic studies of the oxidative – addition reaction of MeI to phenoxo platinum (II) complexes are reported. Complexes of the form [(4- X C₆H₄E) Pt (bipy)] (E = O,S ; X = H,CH₃,Cl,Br) are prepared by the reaction of the chloro complex with substituted phenols or substituted thiophenols and KOH in a two-phase system of water and chloroform in the presence of triphenyl phosphonium chloride . Platinum (IV) complexes are formed by oxidative – addition of MeI to the platinum (II) complexes obtained. The complexes were characterized by elemental analysis, uv – visible, i. r, nmr spectroscopy. The x-ray crystal structure of square planar[(bipy)Pt(OC₆H₄-4-OMe)₂] is reported. The reaction of methyl iodide with di(4-ClC₆H₄O)(2, 2' - bipyridyl) platinum(II) to give iodo (methyl) di(4-ClC₆H₄O)(2, 2' - bipyridyl) platinum(IV) follows the rate law, rate = K₂[Pt(4-ClC₆H₄O)₂(2, 2' - bipyridyl)] [MeI] . The values of K₂ increase with increasing polarity of the solvent, suggesting a polar transition state for the reaction.

Biography

Educational Qualifications:

- B.Sc, Baghdad University, Iraq.
- M.Sc, University of Wales, Aberystwyth, U.K.
- Ph.D, University of Liverpool U.K.

Teaching Experience:

- Teacher of Chemistry in various secondary schools in Iraq.
- Lecturer and Assistant Professor, Head of the Department of Chemistry, and Vice Dean, College of Education, University of Salahaddin, Iraq.
- Associate Professor, Faculty of Education, Hodeidah, University of Sana'a, Republic of Yemen.
- Associate Professor, Faculty of Science, and Faculty of Medicine, University of Sana'a, Sana'a, Republic of Yemen.
- Assistant Professor, Chemistry Department, College of Science, Sultan Qaboos University, Muscat, Oman.
- Assistant Professor, Biological Sciences & Chemistry Department, College of Arts & Science, University of Nizwa, Oman.
- Associate Professor , Dean, Education College, SABIS University, Erbil (2013 – 2015)
- President's Academic Advisor, International University of Erbil, Erbil – Kurdistan(2015 – 2016)
- President's Assistant for Administrative Affairs, International University of Erbil, Erbil, Kurdistan(2016 – onwards)
- Dean, College of Engineering, International University of Erbil, Erbil, Kurdistan, Iraq.

Supervision of postgraduate students:

Supervision of M.Sc. Student:

- I have so far supervised a few students at the M.Sc. level on various aspects of Chemistry.

Supervision of Ph.D. Students:

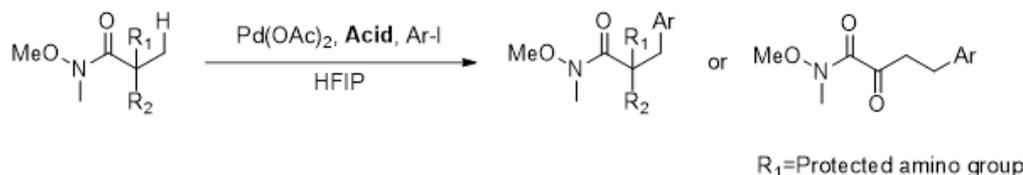
- I have supervised two Ph.D. students, their research titles:
- Thermodynamic and Kinetic Studies of some Transition Metal Complexes.
- Study of new complexes containing ligands with biological effects.

Palladium-catalyzed β -C(sp³)-H arylation of Weinreb amides via acidic ligands

Liming Yang,¹ Yaohang Cheng,¹ Guanghui An^{*1,2}

¹Key Laboratory of Functional Inorganic Material Chemistry (MOE), School of Chemistry and Materials Science, Heilongjiang University, No. 74, Xuefu Road, Nangang District, Harbin 150080 (P.R. China)

²College of Materials Science and Chemical Engineering, Harbin Engineering University, Harbin, 150001



Scheme 1 Palladium-Catalyzed β -C(sp³)-H Arylation of Weinreb Amides via Acidic Ligands

Pd-catalyzed C-H functionalization of weak-coordinating substrates remained challenging and limited.¹ Traditionally, nitrogen-based, strong coordinating groups have been most widely used as directing groups for C(sp³)-H activation, presumably because of the facile cyclometalation process that forms stable palladacycle intermediates. On the other hand, utilizing oxygen-based neutral-coordinating groups such as Weinreb amides to direct C(sp³)-H activation remains a significant challenge. Recently, Yu and coworkers reported the discovery of 3-pyridinesulfonic acid as a uniquely enabling ligand for Pd catalyzed β -C(sp³)-H arylation of Weinreb amide.² In the course of our investigation in regioselective arylation of arenes, we disclosed that such a process can also be promoted by other inexpensive acidic commercially available ligands in a highly efficient mode. These acidic ligands would provide a suitable cationic Pd (II) center without binding nitrogen, in some cases even active Pd(I) species, for the efficient Csp³-H activation. It also enables rapid domino synthesis of ketoamide. Remarkably, such process allows late stage functionalization of peptides.

Audience Take Away:

- They will find this chemistry useful for developing their own catalytic domino reactions.
- In the presentation, a novel catalytic mode for C-H activation will be disclosed. Such as process would change the previous auxiliary view for chelation assisted C-H activation. This presentation will help others to better design their own C-H activation process in a more efficient way.

Biography

A/Prof Guanghui An has received his B.S. (2005) and Ph.D. in Chemistry (2010) both at Nanjing University. He has also received his Postdoctoral Associate in Chemistry (2014) at Texas Tech University. He is an Associate Professor in School of Chemistry and Materials Science at Heilongjiang University (2014) and in College of Materials Science and Chemical Engineering at Harbin Engineering University (2015). Additionally, he has a membership in the Chinese Chemical Society (CCS). He has published more than 40 research articles in SCI (E) journals.

Furthermore, A/Prof An has received the Outstanding Reviewers for Chemical Communications in 2016 and has reviewed more than 200 papers for: Chem Communications, Organic Letters, Rsc Advances, Organic & Biomolecular Chemistry, New Journal of Chemistry, Journal of Materials Chemistry, Dalton Transactions, CrystEngComm, etc.

Energy flux from the sun and the greenhouse gases in the infrared to the earth harvested as boson-supply in platinum-fullerene compound material and as source of electrons for electrical applications

Hans Wilfried Peter Koops

CEO and Chief Scientist HaWilKo GmbH, Ober-Ramstadt, Hessen, Germany

A Novel and revolutionary way of Energy harvesting from the IR-Emission by Greenhouse gases to the earth is presented. On Earth a detector layer is used having sub-micro-meter thickness from a Nano-granular deposit from Platinum crystals with 800 atoms, which are totally embedded in at least 2 layers of Fullerene-crystals (C60). These can absorb during day and at night up to 10^{28} photons/m², and store and deliver at room temperature the energy to the user. Using a 2 metal compound wire helps with its potential to release electrons from the detector as a supply for work.

Audience Take Away:

- The paper presents a better, cheaper and simpler way how to collect and use the energy of the sun and of the greenhouse gas emissions from the atmosphere at day and at night for applications of electrical energy without additional expensive storage. Up to 10^{28} photons/m² stored in the Platinum-Fullerenes compound can be used at the earth, and this stored energy can be delivered to electrical machines. The storage stores Bosons in compound materials from Platinum and Fullerenes using electron and hole having parallel spin. Using a 2 materials extractor layer in parallel to the Boson layer having a higher potential at its positive end releases electrons from the Bosons with a few volts, which can be delivered to the electrical machines for work.
- This new knowledge started to be understood at Deutsche Telekom Research (FTZ) in the Year 1994 by examinations of nanometre thick layers of such compound materials (Pt/Fullerene). The material converts white light into phonons in the Pt/C compound, which looked totally black. This meant that the incoming white light in the optical microscope was totally absorbed by the deposited layer and converted into current.
- Additional understanding was obtained from the paper: Energy budget of the Earth by NASA, Leob et. al., J.Clim, 2009, Treuberth et. al. BAMS 2009, NP 2010-05-265-LARC. The radiative Balance from Calspace Courses. There the high advantage was explained in using green-house gas emissions DAY and NIGHT compared to solar energy emissions.
- In 2014 at HaWilKo GmbH the author learned that by using organometallic compounds from Pt having a Carbon attachment by electron beam induced deposition it was possible to deposit from the organometallic compound Pt-cyclopentadienyl-tri-methyl-methyl with a conventional electron beam with a hot cathode Nanocrystals built from Pt atoms with 800 atoms which condensate at 450 °C on a Carbon foil sample, and are totally embedded during the ongoing cooling of the sample from Carbon-fullerene nanocrystals. This structure has two materials with different work function: Pt: -5,4 V, and Fullerene +4,8 V. This material was defined in its potential: Pt: 5,4 eV, whereas C was emptied from electrons and had holes from 4,8 eV to 5,1 eV. This structure could absorb electrons, which were freed by incoming IR radiation in case this material was hit by photons having an energy above 5, 1 eV. These released electrons could be collected and could be used to perform work, after they were set free at the border of the material and were fed into normal materials energy levels.

The high advantage was explained in using green-house gas emissions DAY and NIGHT compared to solar energy emissions.

- Explain how the audience will be able to use what they learn? The first step is to understand, that electrons and holes in the same environment can form Bosons at Room temperature. They follow no longer the Fermi Dirac Statistics, but "speak Bose-Einstein language"- Electron and Hole but with parallel spin! This means 10^{28} electron-hole pairs /m². The release of electron and hole must be done with care, not to melt the wires. It can be controlled with the voltage
- Explain how the audience will be able to use what they learn? The second thing to learn is, to control the electron current, when it is released for use. There is no better power source around. Use the flat detectors with a size that you get enough current for your problem. Such sources can be very small, meaning only a few cm². Be a revolutionist to find the right detector size for your applications. Convince your colleagues to understand that the novel detector is the right choice to save energy. Develop new teaching courses with experiments to prove the concept. The solution

is applicable to all energy questions.

Biography

Dr. Koops studied electron-optics with Prof. Möllenstedt for PhD at University Tübingen, DE in 1971. He changed to Prof. Scherzer at TU Darmstadt for chromatically and spherically correction of aberrations in the TEM. He worked at IBM T.J. Watson Research Center in State of New York for 1,5 Years (1985-87) on single beam material deposition. 1989: Deutsche Telekom Res. Ctr. Darmstadt, high resolution electron beams. In 2000 he founded NaWoTec GmbH for E-Beam mask-repair, now as ZEISS world market leader. 2006 retired. 2009 to 2015 Consultant at Hitachi High Technology, Japan. Chief of HaWilKo GmbH. 165 Papers, including 60 patents.

⁵¹V-NMR chemical shifts and analyses of vanadium complex catalysts: A Cooperation of QC calculation and MLR analysis

Jun Yi and Masahiko Hada*

Department of Chemistry, Tokyo Metropolitan University, Hachioji, Tokyo, Japan

In recent studies, Nomura and his coworkers found a good relationship between the catalytic activity and the vanadium chemical shift (⁵¹V-NMR) for the (imido) vanadium complex in ethylene polymerization. They deduced that the high catalytic reactivity originates from stabilization of the active site by electron-donating substituents. The trend of observed ⁵¹V-NMR chemical shifts was well reproduced by the quantum-chemical calculations (LC-BLYP/cc-pVTZ). Calculated ⁵¹V NMR chemical shifts were analyzed by the multiple linear regression analysis (MLRA) method with a series of calculated molecular properties. We obtained a reasonable correlation ($R^2=0.95$) between ⁵¹V-NMR chemical shifts and natural charge (Q), HOMO-LUMO energy gap ($\Delta\epsilon$), and Wiberg bond index of V=N bond (ω).

Audience Take Away:

- I will explain shortly how to use the quantum-chemical method, especially an accurate calculations of metal NMR chemical shifts of metal complexes.
- I will explain mainly about the interplay between experiments and quantum-chemical calculations. The combination between observed and calculated metal NMR chemical shifts gives useful information to analyze various catalytic reactions and design new high-performance metal-complex catalysts.

Biography

Masahiko Hada studied Quantum Chemistry (QC) in Kyoto University. Recently he has his interests centered around accurate QC calculations including the electron-correlation and the relativistic effects, and computational approaches for analyses of chemical reactions, spectroscopies and molecular properties. Recently his expertise is extended to 2c-relativistic quantum-chemical theories and its applications to NMR, electronic excited states and spectroscopies (UV, CD, MCD, CPL), and chemical reactions on metal and metal-oxide surfaces, and chemical reaction mechanisms of enzyme containing transition metals.

Towards a transient multi-site kinetic model of Cu-chabazite for NH₃-SCR linked to the active site hydrothermal aging kinetics

Selmi Erim Bozbağ¹, Gülden Hazal Karadağ¹, Deniz Şanlı², Onur Demir², Barkın Ozener², Gokhan Hisar², Can Erkey^{1*}

¹Department of Chemical and Biological Engineering, Koç University, Sarıyer, Istanbul, Turkey,

²Ford Otosan R&D Center, Sancaktepe, 34885, Istanbul, Turkey

Cu-chabazites (CHA) are widely used as catalysts for NO_x abatement using NH₃-SCR (Selective Catalytic Reduction) technology within the aftertreatment systems (ATS) of the diesel engines. The design and calibration of ATS are usually accomplished with the help of engine dynamometer and vehicle tests that span a large operation region of the engine. However, such tests are very long, labor intensive and expensive. An alternative is to utilize mathematical models based on the physico-chemical phenomena occurring in the reactors which make up the ATS. In order to describe the hydrothermal aging effects of a multi-active site containing Cu-CHA catalysts on the NH₃-SCR performance, a multi-site transient kinetic model is required. For this, one needs to describe the hydrothermal aging kinetics effects on the active site concentrations and link these with the multi-site kinetic model. However, there is no such model in the literature for the Cu-CHA. For this purpose, a multi-site kinetic model on a commercial Cu-Chabazite washcoated monolith was developed using laboratory scale data and the model was validated using engine dynamometer tests. The hydrothermal aging effects on the active sites were measured using an aging protocol consisting of aging the catalyst for certain time at a certain temperature followed by the measurement of NH₃ adsorption, desorption and TPD. NH₃-TPD curves were deconvoluted into three sites consisting of Cu1, Cu2 and Brønsted sites with peak centres at 317, 456 and 526, °C, respectively along with sites associated with weakly bound NH₃ desorbed during the isothermal desorption at 110 °C before the TPD for the degreened catalyst. The changes in the concentration of these sites were modelled using first order kinetics after hydrothermal aging at 650-800 °C upto 45h. The total NH₃ storage and release did not change with hydrothermal aging at 650 °C after 45h but decreased after aging at higher temperatures. The concentration of Cu1 sites decreased by 6% after aging at 650 °C for 0.7h then started increasing after an aging time of 3h and after 45h it reached to a value 28% higher as compared to its concentration after degreening. The concentration of the Cu2 sites, on the contrary, initially increased with aging time upto 0.7h reaching a value 12% higher than the degreened concentration, then decreased with aging time resulting in a drop of 23% as compared to the degreened value. The concentration of the Brønsted sites exponentially decreased with aging time reaching a plateau of 85% lower than the degreened concentration at 36h. Hydrothermal aging kinetics of the active sites were linked to the multi-site kinetic model through the addition of site migration reactions for each active site. The effects of both aging time and temperature on the NH₃ adsorption, desorption, oxidation and NH₃ to NO reaction were successfully simulated in the 150-600 °C range. This study is the first step towards the development of a multi-site, multi-reaction, kinetic model of the NH₃-SCR process for NO_x reduction which is able to simulate the effects of hydrothermal aging according to both aging time and temperature.

Audience Take Away:

- NH₃-SCR Mechanism on Cu-Chabazites
- Aging protocols and kinetics associated with the active sites of the Cu-CHA catalyst
- Incorporation of active site aging kinetics into a multi-site, multi-reaction based kinetic model

Biography

Professor Can Erkey started his academic career in the Chemical Engineering Department at the University of Connecticut in 1995 as an Assistant Professor. He was promoted to Associate Professor in 2001 and to Full Professor in 2006. He then joined the Chemical and Biological Engineering Department at Koç University in Istanbul, Turkey in 2006. He is serving as the director of the newly established Koç University Tüpraş Energy Center. His research interests are in nanostructured materials, catalysis, supercritical fluids and energy. Prof. Erkey has 110 refereed journal publications with 4210 citations and a h-factor of 39.

Noble and base-metal nanoparticles supported on mesoporous metal oxides: Efficient catalysts for the selective hydrogenation of levulinic acid to γ -valerolactone

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¹Department of Chemistry, University of Johannesburg, Johannesburg, South Africa

²Department of Chemistry, University of Johannesburg, Johannesburg, South Africa

The selective hydrogenation of levulinic acid, LA to γ -valerolactone, GVL in water and solvent-free systems using metal oxides supported noble and base-metal nanoparticles was investigated. Highly stable and meso-structured TiO₂, NiO and MnO₂ were synthesized using an inverse surfactant micelle method, and the mesoporous metal oxides supported Ru, Pd, Cu and Cr nanoparticles were synthesized by homogeneous deposition precipitation. The N₂-physisorption study showed that all the synthesized materials were mesoporous with type IV isotherms and type I hysteresis loops. The materials have a narrow pore size distribution of uniform size, with the pore diameters of 3.2, 3.7 and 13.3 nm for TiO₂, NiO and MnO₂, respectively. The diffraction peaks observed in the low angle region of the p-XRD patterns confirm the successful formation of the meso-structured materials, whereas the wide-angle diffraction patterns show that the crystalline structure of the pure nanocatalysts is maintained upon deposition of the metal. The Temperature-Programmed Reduction study showed that the reduced supported nanocatalysts consist of metallic Ru, Pd, Cu and Cr, and the average particle sizes obtained from the high-resolution transmission electron microscopy study were found to be of 2 to 6 nm in diameter. The mesoporous supported noble and base-metal nanocatalysts as synthesized in this study were revealed to be highly stable and efficient for the conversion of biomass-derived LA to GVL, an ideal sustainable liquid fuel. The best performance with complete conversion of LA and >95% GVL selectivity was obtained from the TiO₂ and MnO₂-based nanocatalysts when water was used as a solvent. The order of reactivity of the supported metal nanoparticles was established as: Pd \approx Ru > Cu > Cr. With a TOF of up to 277273 the low cost copper-based nanocatalysts as synthesized in this study could be an alternative to the high cost noble metal-based catalysts. The catalysts could be reused several times without substantial loss of activity and selectivity.

Audience Take Away:

Over the last decades, consumption and substantial depletion of fossil resources together with its impact on the environment have raised concerns on the utilization of renewable and green energy resources. To achieve sustainable development, renewable biomass is regarded as a potential carbon-neutral energy resource for the production of biofuels and many value-added chemicals. Thus, the catalytic hydrogenation of levulinic acid, LA a typical renewable biosourced material to γ -valerolactone, GVL a low-toxic potential fuel component is of inherent interest.

Nowadays, a number of supported transition metals-catalyzed hydrogenation of LA to GVL with improved performances has been reported, of which noble-metals led to the best results. The most widespread catalysts for the synthesis of GVL from LA are 5%-Ru/C and 10%-Pd/C; with the 5%-Ru/C being the most conventional one. Although good performances obtained, the catalysts used are mostly based on precious-metals and their high cost is a real issue and can therefore reduce their applications to certain extent. Therefore, activity of catalysts based on base-metal which are cheaper can be improved and there is potential for such catalysts. The low cost copper-based nanocatalysts as synthesized in this study (1%-Cu/TiO₂ or MnO₂) could be an alternative to the high cost noble metal-based catalysts.

Biography

Dr Matumuene Joe Ndolomingo obtained his Ph.D. in Chemistry from the University of Johannesburg (UJ) in South Africa in 2016. Presently, he is a Post-Doctoral Researcher at Prof. Meijboom's Research Center for Synthesis and Catalysis, in the Department of Chemistry, Faculty of Science at UJ. His current research interests include the synthesis, characterization and development of heterogeneous catalysts for industrial reactions. His research outputs have been published in high impact factor journals such as Journal of Applied Catalysis B: Environmental, and one of his published papers was featured in Advances in Engineering, an online engineering newspaper

Cobalt ion species in water as an active homogeneous catalyst for oxidative decomposition of ammonium ion with ozone

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Treatment of accumulated radioactive liquid waste in laboratories is urgent task not only for the storage space but also for safety management of the facilities. Liquid wastes generated by R&D activities often contain various reactive reagents. Since the liquid waste has to be treated inside shielded devices such as concrete cell or glove box due to its radioactivity, easy operations for the treatment are preferred.

In order to develop new technologies for the treatment of radioactive liquid waste containing various reactive chemicals, Japan Atomic Energy Agency launched a project named STRAD (Systematic Treatment of RAdioactive liquid waste for Decommissioning). One of the targeted chemicals in this project is ammonium ion and now we are investigating oxidative decomposition with ozone as a promising method. Decomposition of ammonium ion under mild reaction conditions has been successfully achieved in the presence of Co_3O_4 , which acts as a heterogeneous catalyst. In addition, we also have demonstrated that cobalt nitrate acted as a homogeneous catalyst for the reaction and chloride ion in water was indispensable for the catalyst to effectively promote the reaction. Homogeneous catalyst is rather desirable than heterogeneous one for the operation in the shielded area due to its simple procedure and high efficiency for the reaction. Since treatment methodology of radioactive solution containing only nitric acid and metallic ions has already been established, the addition of nitrate salts to the solution are acceptable for the treatment. In the present study, chemical state of cobalt ion in the solution under the reaction conditions was evaluated through in-situ XAFS measurement on Co in order to gain insight into the reaction mechanism involving cobalt ion as a homogeneous catalyst for the decomposition of ammonium ion.

Test solutions were prepared by dissolving ammonium chloride and cobalt nitrate in water. pH of the solution was parametrically changed from 4 to 12. Mixture of ozone and oxygen (ozone concentration about 5%) was supplied into 80 mL of the solution with 100 mL/min. Co K edge XAFS measurement with fluorescence mode was performed at BL5S1 beamline of AichiSR, Japan. During the measurements, temperature of the solution was precisely controlled at 333 K. No energy shift in the XANES spectrum was observed during the measurement, demonstrating that cobalt ion was stably present as divalent cobalt. Whereas, intensity of the white line slightly increased as operation time with keeping intensity of the pre-edge. These results suggest that the divalent cobalt species coordinated with chloride ions was formed in the solution, which might be an active catalytic species for the reaction. EXAFS analysis on the X-ray absorption spectra is currently underway to give further information on the catalytic reactions.

Audience Take Away:

- Necessity of developing treatment for radioactive liquid waste.
- Benefit of homogeneous catalyst for mild condition and simple operation.
- New decomposition mechanism of ammonium ion.

Biography

Ms. Aihara studied chemistry at Tokyo Metropolitan University, Japan and graduated as MS in 2011. She joined in Japan Atomic Energy Agency in 2011 and was assigned to aqueous reprocessing group. Studied about fast reactor reprocessing process and Fukushima radioactive waste. She entered Hokkaido University, Japan in 2016 and now PH.D. Student. She is studying catalytic oxidation under Professor Kamiya.

Palladium/carbon nanotubes/charcoal hybrid composite and its catalytic behavior in the hydrogenation of trans-cinnamaldehyde

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In the present study, we addressed the palladium (Pd) decoration of multiwalled carbon nanotube (CNT)/activated carbon (AC) hybrid composites (MWCNT/AC), and examined the catalytic behavior of the composites in the hydrogenation of trans-cinnamaldehyde. The MWCNT/AC composites were prepared by growing CNT network on the surface of AC granules, using the chemical vapor deposition method. XPS analysis revealed that the MWCNT/AC and COOH-MWCNT/AC composites and isolated AC adsorbed Pd at different oxidation states when dipped into a Pd microemulsion: isolated AC and the COOH-MWCNT/AC composite adsorbed Pd nanoparticles at di- and tetravalent states (Pd²⁺/Pd⁴⁺), while the MWCNT/AC composite adsorbed Pd nanoparticles at zero and tetravalent states (Pd⁰/Pd⁴⁺). The MWCNT/AC composite may thereby have hierarchical Pd adsorption properties dependent on the MWCNT network type grown onto the AC surface. Regarding the catalytic performance, the (Pd⁰/Pd⁴⁺)-MWCNT/AC catalyst displayed higher selectivity to hydro-cinnamaldehyde formation (95.9%) when compared with the (Pd²⁺/Pd⁴⁺)-AC and (Pd²⁺/Pd⁴⁺)-COOH-MWCNT/AC catalysts (72.1% and 91.4% selectivity, respectively). The catalytic performance of the (Pd⁰/Pd⁴⁺)-MWCNT/AC catalyst with 2.8 wt% of Pd loading was also superior than the catalytic performance of commercial catalysts with 5 and 10 wt% of Pd loading and other Pd/CNTs catalysts reported in the literature.

Audience Take Away:

- Exploration of the hybrid properties of metallic nanoparticles on CNTs due to the electronic transfer between them;
- How the use of a hybrid carbon nanocomposite (CNTs/AC) can avoid the harmful effects of CNTs as nanomaterials are linked on the surface of micrometric material as CNTs were synthesized directly onto the activated carbon surface;
- How CNTs could improve Pd catalytic behavior, minimizing its use, cheapening the reaction and making it more selective.

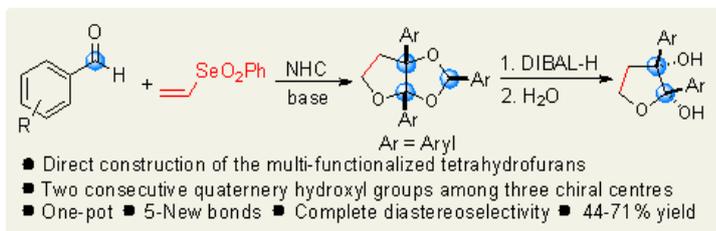
Biography

Elaine Matsubara holds a BA (2002) in Chemistry, PhD (2010) in Science from the University of São Paulo (USP), a part of her PhD studies from the Instituto de Ciencias de Los Materiales de Madrid - Spain, Italian National Agency for New Technologies Energy and Sustainable Economic Development, and University of Rome La Sapienza - Italy. She is presently PhD researcher at University of São Paulo (USP), Brazil. Her work focuses on synthesis of doped carbon nanotubes, 3D hybrid hierarchical carbon nanomaterials and graphene for energy devices applications. Her experience is focused on energy devices and nanocomposites to filtration, catalysis, environmental remediation and polymer reinforcement.

Organocatalyzed domino reactions for asymmetric organic synthesis

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A concise and catalytic preparation of multi-functionalized scaffolds in a stereoselective manner is highly desired in organic synthesis. This can be achieved via one-pot multicomponent reactions or domino reactions. The most of the success in this arena has come using toxic and highly expensive transition metal catalysts. Over the last decade or so, organocatalysis has emerged as an alternate and often better mode of activation due to their inherent properties. Among different organocatalysts, N-Heterocyclic Carbenes (NHC) and Hypervalent Iodine-based catalysts have received increasing attention due to their unique mode of activation. For example, NHCs generate three different reactive intermediates from enals namely, enolates, homoenolates and acylanions. These all three intermediates allow for an access to completely three different class of products from the same substrate, which is unparalleled for any other mode of catalysis. The diversity of these catalysts further multiplies in combination with co-catalysts like Bronsted acids, Lewis acids, etc. Similarly, hypervalent iodine-based catalysts lead to exclusive rearrangements through migration of substituents, expansion or contraction of rings to produce new stereocentres selectively. These properties of NHCs and hypervalent iodines have enabled the discovery of a wide range of new and novel reactions.

On the other hand, the preparation of organo-selenides/selenones has been revisited in the recent past because of their biological properties as well as unique reactivity. The organoselenide/selenones often undergoes a self-induced interesting, transformations like vicinal group functionalization, and the formation of rings/stereocentres via rearrangement because of a weaker C-Se σ -bond. Despite these attractive properties, metal-free catalytic asymmetric synthesis of organoselenones has remained less explored.

With organocatalysis as the guiding principle of our research, we have reported several new and novel asymmetric transformations using NHCs and Hypervalent Iodine organocatalysts. These include a one-pot stereoselective construction of 2,3-dihydroxy-2,3-diaryl tetrahydrofurans via NHC-catalysed domino reactions of aldehydes and vinyl selenone (Figure), first NHC-catalyzed phospho-Brook rearrangement, first NHC-catalyzed synthesis of 3-phosphonate-derived heterocycles, first NHC-catalysed preparation of chiral organoselenones, etc. In addition, we have developed method for the asymmetric dihydroxylation of chalcones using hypervalent reagent.

Audience Take Away:

- A one-pot stereoselective construction of 2,3-dihydroxy-2,3-diaryl tetrahydrofurans via NHC-catalysed domino reactions of aldehydes and vinyl selenone
- First NHC-catalysed phospho-Brook rearrangement
- First NHC-catalysed synthesis of 3-phosphonate-derived heterocycles
- First NHC-catalysed enantioselective preparation of organoselenones
- First asymmetric dihydroxylation of chalcones using hypervalent iodine reagent
- Explain how the audience will be able to use what they learn?

This oral presentation will discuss about one-pot preparation of dihydroxy-diaryl tetrahydrofurans via NHC-catalysed domino reactions of aldehydes and vinyl selenone. This methodology gives an easy access to complex tetrahydrofuran scaffolds which is very common in bioactive compounds. A library of these challenging compounds can be prepared for bioactivity evaluation.

- How will this help the audience in their job? Is this research that other faculty could use to expand their research or teaching? Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient? Will it improve the accuracy of a design, or provide new information to assist in a design problem? List all

other benefits.

- A number of NHC and hypervalent iodine catalyzed methods for the preparation of potentially useful materials will be discussed. This presentation includes the first study on using selenones under NHC-catalysis. Our initial breakthrough will encourage the chemist to further explore and expand this area. Most of the protocols provide practical method for the preparation of potentially useful molecules. Therefore, makes the designer's job more efficient.

Biography

Dr. Bhoopendra Tiwari received his M.Sc. degree in Chemistry from Tripura University, India in 2002. He then joined the group of Dr. S. Chandrasekhar at Indian Institute of Chemical Technology, Hyderabad, India for Ph.D. After a short stint at Sai Advantium Pharma LTD, India, he joined the group of Prof. Robin Chi at Nanyang Technological University, Singapore for his postdoctoral studies. He moved back to India to join Centre of Biomedical Research, Lucknow as an Assistant Professor in 2014, and subsequently got promoted to Associate Professor in 2017. His group is actively pursuing research in the area of asymmetric organocatalysis.

Chemical engineering and the new generation of multi-purpose catalyst test setup with investigation of the catalytic process of MeOH to light olefin

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The multi-purpose catalyst test Setup can be employed as a live-maquette of industrial design that allows for the possibility of thermodynamic research (System PVT) and the extraction of basic data for simulation. Parallel form of fixed bed, CSTR and Moving Bed reactors in this plan contribute to understanding and training how to select a reactor, compare performances, determine the impact of different mass transfer resistances and provide a highly efficient kinetics model. Due to the fact that in long-term testing, the researcher may not be available, the system operator may be alone and nobody may have enough mastery to work with the device, online access is needed. On the other hand, the operator's actions and results including ESD, process data change and others will be saved with the details of the hour and user name for higher access level. When a human error occurs, the control system will be alert and gives alarm. Meanwhile, the related routine procedure of problem-solving will be revealed by smart PLC system and managed by it. In case of negligence and ignoring of the red lines, the ESD will be automatically activated. The type and level of danger possibility may activate the third layer of safety. This last layer of safety is programmed by manufacturer and even works without main power and guarantees the safety of working with the system. For example, if for any reason temperature exceeds the allowed range of furnace temperature, Nitrogen flow will be injected to cool the system in the preheated form in an attempt to prevent thermal shock. Then, the temperature will be reduced with a suitable slope to reach the allowed temperature. The control system is custom-made and includes the following defaults:

- The possibility of changing the reactor size, and volume of catalyst in each test as well as the creation of extremely accurate isothermal, isobar or adiabatic conditions for each reactor.
- Control and display of level, flow rate, pressure, temperature and composition at different points of the system (even the temperature of pipelines).
Dilution of the feed with an inert gas to reduce the partial pressure with high precision, activating the catalyst with controlled gas flow and studying catalyst regeneration
- Dilution of the feed with pure and controlled steam, if necessary, in order to reduce the coke formation at high process temperatures
- Using intermediate product as a feed for the next part and changing the reactor layout in parallel, series or combination.
GC Online was used to control the composition of feed, mid and end products.
- Finally, DME production as intermediate with methanol dehydration on parallel fixed-bed reactors by gamma-alumina catalyst and light olefins as final production via DME dehydration by Laboratory SAPO catalyst with fixed-bed and series reactors was studied at adiabatic state by recent catalyst test setup.

Audience Take Away:

- Using parallel flow in the Catalyst Test Setup, it is possible to perform and complete experiments under different process conditions, based on experimental design by reducing the required time.
- The suitable safety system, perfect design and existence of online gas chromatograph make it easier to conduct research and view the results.
- It is possible to change the arrangement of the reactors in parallel, series and combination or to use a part of the system. It is therefore fully applicable to various academic and industrial researches and training.
- In addition, due to the observation possibility of online reports for process conditions, either in numeric or graphical, less sampling and almost no human errors will be observed.

Biography

Arash-Goshtasbi-Asl was employed as an elite senior researcher at the Iranian Petrochemical Research Center (in 2001) and was selected as the project manager of the methanol demo plant in 2003. Then, he was accepted for basic engineering of first commercial MTP-plant in the world by Lurgi Company, Frankfurt am Main, Germany in 2007. He obtained an invention certificate for the design of a micro-reactor with DFK team in 2010. The experience of collaborating with the HAZOP team, mastering simulation software, publishing a book titled "An Overview on Process Control in Chemical Engineering" and presenting different papers are among his honors.

Synthesis and characterization of catalysts based on Pd-Ni bimetallic nanoparticles

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The development of nanomaterials and nanotechnology makes it possible to create new catalysts, which in turn can be successfully used to solve various problems, in particular, for the reductive dechlorination of persistent organic pollutants (POPs) and the production of valuable chemical products from recycled wastes. The currently accumulated stocks of excessively produced halogen-containing by-products and POPs require environmentally friendly disposal, which necessitates the development of methods for the disposal of halogen-containing organic substances and their transformation into less hazardous compounds.

In recent years, the share of studies of the processes of reductive and substitution dechlorination of POPs has sharply increased. In addition, the catalytic reduction method allows you to regenerate the hydrocarbon component of halogenated molecules for reuse, which meets the objectives of resource conservation and the principles of “green” chemistry. The most common catalytic systems used for the reductive dehydrochlorination of organohalogen substances are palladium-containing catalysts on inert supports. The palladium content in such catalysts reaches up to 10%. Therefore, studies to reduce the cost of palladium catalysts due to the “dilution” of the noble metal with other metals with low cost characteristics are a trend in recent years. We carried out work on the development of bimetallic catalysts based on noble nanoparticles (palladium) and transition metals (nickel deposited on birch activated carbon of BAU-Agrade). To identify the features of the formation of active centers of the developed catalysts, various physicochemical studies (SEM, TEM, X-ray diffraction) were carried out. We studied the characteristics and properties of the obtained catalysts using the methods of dynamic laser light scattering, UV spectroscopy, X-ray diffraction, scanning electron microscopy (SEM), and transmission electron microscopy (TEM).

The catalysts were black powders consisting of a carbon matrix with Pd-Ni nanoparticles dispersed in it on a carbon support. The microstructure of the support and catalyst were investigated by X-ray diffraction and SEM. According to the results of transmission electron microscopy, the synthesized catalysts consist of isolated Pd-Ni nanoparticles, which are selectively formed on a surface layer up to 200 nm thick. The catalytic systems developed by us were tested for hydrodechlorination of chlorobenzene in ethanol. Preliminary tests established the effectiveness of the catalysts obtained by the method of reducing activated carbon Pd-Cu in the pore volume in the process of chlorobenzene dechlorination, with a yield of conversion products equal to 94.46%.

Audience Take Away:

- A study was conducted on the use of a cheaper carrier - birch activated carbon for applying bimetallic nanoparticles of Pd-Ni metals with the aim of hydrodechlorination of organohalogen substances, including chlorobenzene.
- The obtained data may well be used by chemists in teaching students colloid chemistry, physical and chemical research methods, etc. established data can be used by young researchers in studying the problems of the disposal of organohalogen substances.

Biography

Dr. Sana Kabdrakhmanova studied Chemistry at the East Kazakhstan State University, Kazakhstan and graduated as PhD in 2007. In 2017, she joined the research group of Professor B. Selenova and S. Kudaibergenov at the Laboratory of Engineering Profile of Kazakh National Research Technical University named after K. Satbayev. She was a leader and executive in charge of 4 grant research projects. Within the scientific group Kabdrakhmanova S.K. took part in the development of gel-immobilized and polymer-protected metal nanoparticles on various carriers. She has published more than 90 research articles.

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