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ICG
2019

4th Edition of International Conference on

Catalysis and Green Chemistry

May 13-14, 2019 - Tokyo, Japan

Collaboration & Publishing partner

Springer

Theme: *Catalyzing Inventive Technologies and Estimating Methodologies to Modernize the approaches in Catalysis and Green Chemistry*

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BOOK OF ABSTRACTS

4th Edition of International Conference on

CATALYSIS AND GREEN CHEMISTRY

Theme:

Catalyzing Inventive Technologies and Estimating Methodologies to Modernize the approaches in Catalysis and Green Chemistry

MAY 13-14, 2019
TOKYO, JAPAN

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United Kingdom

Ziyi Zhong
Guangdong Technion
Israel Institute of Technology,
China

Suleiman Bifari
Jubail Research & Innovation
ClusterHUB, Saudi Arabia

Thank You
All...

Welcome Message

Ladies and Gentlemen “welcome on board” of the 4th International Conference on Catalysis and Green Chemistry (ICG 2019). It is an honor and a pleasure to send you a short welcome address, just to underline how Catalysis and Green Chemistry represent a very promising marriage to develop novel economic and environmentally friendly industrial processes. Thus, the adjective sustainable appears more appropriate for novel industrial processes, for which both economic and environmental aspects has to be considered (doing, for example, the difference between fine and organic chemistry) if we want to remove relevant drawbacks of some current processes, preserving the added value and having real application perspectives. To achieve this goal, a multidisciplinary approach is necessary to be able to revised critically the existing literature and develop new idea and collaborations focused to open new scientific courses. From this point of view ICG 2019 represent an exciting opportunity to meet different competences and establish contacts focused to develop new research collaborations, Thus, welcome and enjoy the Meeting!

PROF ANGELO VACCARI,
Alma Mater Studiorum – University of Bologna,Italy

Welcome Message

Dear Colleagues,

One of the critical challenges facing modern society is conversion of wastes to renewable, eco-friendly, socially acceptable, economically competitive, sustainable and fungible liquid fuels and chemicals to replace fossil feedstocks. Novel catalytic materials combined with advanced catalytic processes based on extensive fundamental research and developed by state-of-the-art scientific tools hold the key to the conversion of carbon dioxide and waste biomass to green products. The use of abundant and low-cost renewable materials are essential for a sustainable future. Although some progress in the production of renewable chemicals and fuels has been made over the past decade, more intense scientific efforts are needed to accelerate development. ICG-2019 provides the platform for excellent scientific exchange in the key issues of catalysis and green chemistry.

M.Herskowitz
Blechner Center, Ben Gurion University at Negev,
Israel

Welcome Message

On behalf of the organizing committee, it is with great enthusiasm that I am addressing to all of you my warmest welcome to this Conference on catalysis and Green chemistry.

The adoption and use of the term “Green” by nearly all fields of the human activities is relatively recent. Although the term was already used to indicate a more environmentally-friendly way to do things as a consequence of the sustainable development imperative, its generalized utilization comes in the nineties. Thus, all scientific and technical/technological endeavours towards sustainability are nowadays qualified as “Green”. Green chemistry and engineering are playing a role of paramount importance in this direction.

We are convinced that the importance of the topics covered by this conference will attract a high number of important “players’ in this area who will guarantee the successful presentation and future adoption of new paradigms towards the targeted sustainability.

Being myself a humble contributor in this field, I an eager to meet you and exchange with all participants on these matters of great importance for our future.

Prof. Nicolas Abatzoglou, Eng.
Université de Sherbrooke, Canada

keynote speakers

Lutz F. Tietze
Georg-August-University
Göttingen, Germany

Nicolas Abatzoglou
Université de Sherbrooke
Canada

Leszek Moscicki
Lublin University of Life
Sciences, Poland

Moti Herskowitz
Ben Gurion University
Israel

Victor Kogan
Russian Academy of
Sciences, Russia

Giang Vo-Thanh
Institute of Molecular
Chemistry and Materials in
Orsay, France

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 ICG 2019

Magnus group takes enormous inclination & feel privileged in inviting the prominent researchers, scientists, and scholars across the world to the 4th Edition of International Conference on Catalysis and Green Chemistry during May 13-14, 2019 in Tokyo, Japan with the theme "Catalyzing Inventive Technologies and Estimating Methodologies to Modernize the approaches in Catalysis and Green Chemistry."

This conference is an unique worldwide platform that is a conversion of all partners of the Global chemical Academia, Researchers, Industries, Innovators – meeting up to display and examine flow Topics in Rejuvenating development and difficulties in sustenance science which will explore the advances in Catalysis and Green Chemistry. It will be a foremost event that joins an exciting and International mix of experts and pioneers both from the academic and industry world to exchange their knowledge, experience and research advancements to develop a world Catalysis and Green Chemistry meet.

We have not just expanded the quantity of chances for you to connect with colleagues from over the world yet additionally presented more engaged sessions that will include cutting edge introductions, unique board exchanges, and livelier cooperation with industry pioneers and specialists.

PUBLISHING PARTNER

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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 NOx 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.

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DAY 1

KEYNOTE FORUM

4th Edition of

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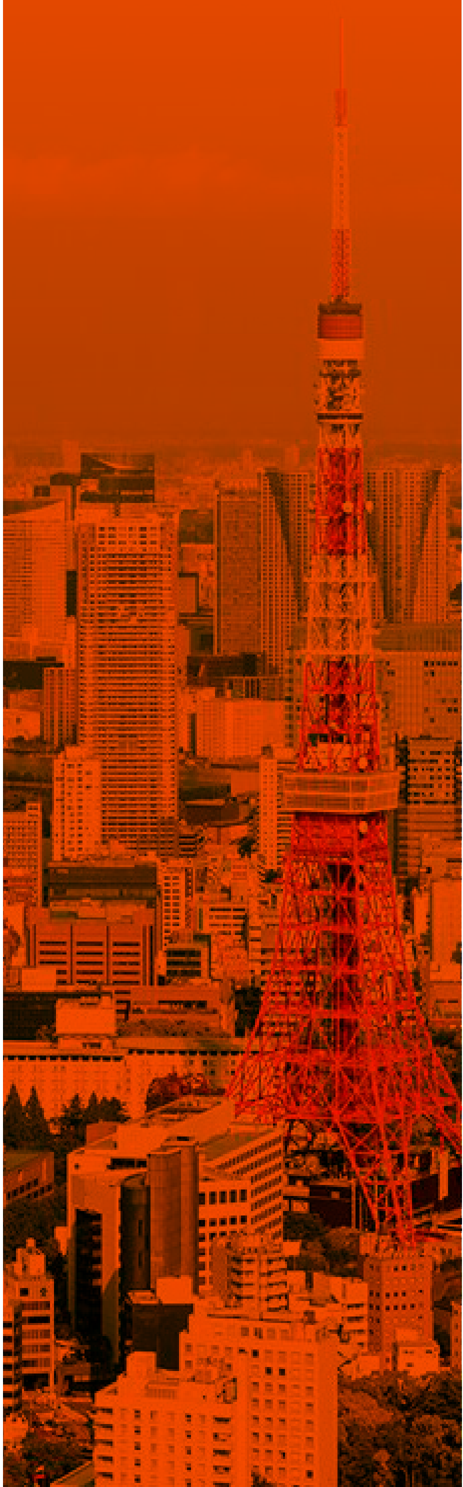
ICG 2019



Biography

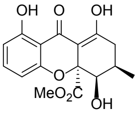
Lutz F. Tietze studied chemistry at the universities of Freiburg and Kiel, Germany and obtained his doctorate in 1968 in Kiel. He then worked as a research associate with Prof. G. Büchi at MIT, Cambridge, USA for two years and got his habilitation at the University of Münster in 1975. He got several calls as professor to different universities and has been professor and director of the Institute of Organic and Biomolecular Chemistry at the Georg-August-University in Göttingen since 1978. He has received many awards as the very prestigious Emil Fischer Gold medal of the German Chemical Society. He is member of several academies and got the title of doctor honoris causa of the University of Szeged and Goettingen. He was head of a Collaborative Research Centre (Sonderforschungsbereich), has served as a member of the DFG-Panel (Fachforum) for eight years and was dean and vice dean of the faculty of chemistry in Göttingen again for eight years and he is President of the German Stirring Committee of the German Chemical Societies (DZfCh).He has almost 500 scientific papers, 38 patents and six books to his name. His research focuses on the development of efficient and selective synthetic methods using domino reactions and the development of new selective anticancer agents employing monoclonal antibodies. He has educated 180 PhD-students and a multitude of postdoctoral fellows have worked with him.

Domino reactions. The green and economical art of chemical synthesis

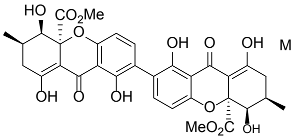
Lutz F. Tietze, Ph.D.

Institute of Organic and Biomolecular Chemistry, Georg-August-University Göttingen,Tammannstr. 2, D-37077 Göttingen, Germany

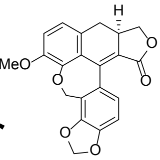
The efficient synthesis of natural products, drugs, agrochemicals and materials is a very important aspect in academia and industry. To allow an ecologically and economically favourable approach in a green fashion the former stepwise procedures must be replaced by domino reactions which allow the preparation of complex molecules starting from simple substrates in a straight forward way. Domino reactions[1] allow the reduction of the amount of waste being formed and the preservation of our resources. Moreover, they are also favourable in an economical way since they consume less time and less material.



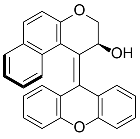
(-)-Blenolide A



Secalonic Acid E



Linoxepin



Molecular Switches

The usefulness of the domino concept[1] is demonstrated with the syntheses of some fungal metabolites as blennolide A[2] and secalonic acid E[3] with a dimeric tetrahydroxanthenone skeleton using an enantioselective domino-Wacker/carbonylation/methoxylation reaction and of the natural aryldihydronaphthalene lignan linoxepine[4] employing a domino-carbopalladation/Heck reaction. The approach has also been applied for the synthesis of novel materials such as molecular switches[5a-e] and fluorescence dyes[6a,b] using a domino-Sonogashira/carbopalladation/CH-activation reaction.

Biography

Giang Vo-Thanh obtained his Ms in 1994 and his Ph.D in 1997 from the University 'Pierre et Marie Curie' (Paris VI, France). After three year postdoctoral fellowships, he took up, in 2000, an academic position as an assistant professor at the University Paris-Sud. In 2006, he obtained his Habilitation diploma and in 2007, he was pointed Full Professor at the University Paris-Sud. His research interests include all aspects of synthetic methodology, including the design and synthesis of chiral ionic liquids and their uses as chiral reaction media (solvent and/or catalyst) in asymmetric synthesis and catalysis, the synthesis of new chiral molecules (amino alcohols, diamines, phosphines, thioureas, thiourea-phosphines, NHC,…) derived from biomass products and their applications as ligands or organocatalysts for asymmetric catalysis, and the preparation of molecules or molecular scaffolds of biological interest.

Chiral catalysts derived from biomass: Design, synthesis and applications in asymmetric catalysis

Prof. Dr. Giang Vo-Thanh

Institute of Molecular Chemistry and Materials in Orsay (ICMMO)
University Paris-Sud / University Paris Saclay, France

The development of new and more efficient catalytic systems is the subject of increasing attention from both academic and industrial research. Moreover, biomass is an endless supply of hydrocarbon materials that can be used as renewable raw materials for the development of new organic compounds. In this context, many research groups have devoted their works to products with a natural chirality source, non-toxic, biodegradable and usually inexpensive for the development of new chiral catalysts. Some new chiral molecules derived from biomass such as carbohydrates, natural aminoacids acid have been synthesized and used as chiral ligands or organocatalysts for asymmetric catalysis leading to the formation of expected products with good yields and high enantiomeric excess. The results of these studies will be presented and discussed in this communication.

Catalysts and catalytic processes for converting waste to fungible liquid fuels and chemicals

M. Herskowitz, Ph.D

Ben Gurion University at Negev, Israel

Fungible liquid fuels and chemicals produced from renewable and alternative feedstocks are essential components of the future transportation and commodities outlook. The abundant and low-cost raw materials are carbon dioxide (GHG) as carbon source and water as hydrogen source. Fatty acids and triglycerides mixtures separated from low-cost waste are also renewable feedstock.

The Blechner Center has developed proprietary technologies for production of fuels and chemicals from renewable feedstocks based on fundamental research and development of catalytic processes. The presentation will focus on the scientific aspects of the novel Fe-based and SAPO-11 catalysts and catalytic processes studied and developed at the Blechner Center. The effects of the nature of catalysts precursors, especially their structure and chemical state of iron ions in different Fe-oxide matrices were studied. Solid mono-, bi- and tri-metallic oxide matrices where Fe(2+,3+) ions are distributed in different chemical/spatial environments. All matrices were basified with K-promoter. The optimal activation conditions for every material were selected based on TPR/TPC/XRD data. The Fe-matrices were characterized by N2-adsorption, temperature-programmed reduction (TPR), temperature-programmed carburization (TPC), X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM, HRTEM-EELS), XPS. The SAPO-11 catalysts display relatively low hydrothermal stability in hydrotreating of vegetable oils. Application of XRD, HRTEM, NH3 TPD, TPO, H2 pulse chemisorptions and Si MAS NMR revealed that the reason for the hydrothermal deactivation of SAPO-11 is partially the reversible desilication of its framework.

Biography

Moti Herskowitz (https://en.wikipedia.org/wiki/Moti_Herskowitz) is professor of chemical engineering and researcher in the fields of advanced materials, heterogeneous catalysis, and reaction engineering and renewable fuels. He served, among other positions, as Vice-President for R&D at the Ben-Gurion University from 2003 to 2014. Moti established the Blechner Center for Industrial Catalysis and Process Development in 1995 and has led scientific programs and technology development work ever since. Applications developed at the Blechner Center (http://in.bgu.ac.il/en/indcat/Pages/default.aspx) have been commercialized.

Moti has published over 145 papers and 26 patents based on basic and applied research. Many publications are related to advanced catalytic materials and processes in general and their application in the production of novel renewable and sustainable fuels and chemicals in particular.

DAY 1

SPEAKERS

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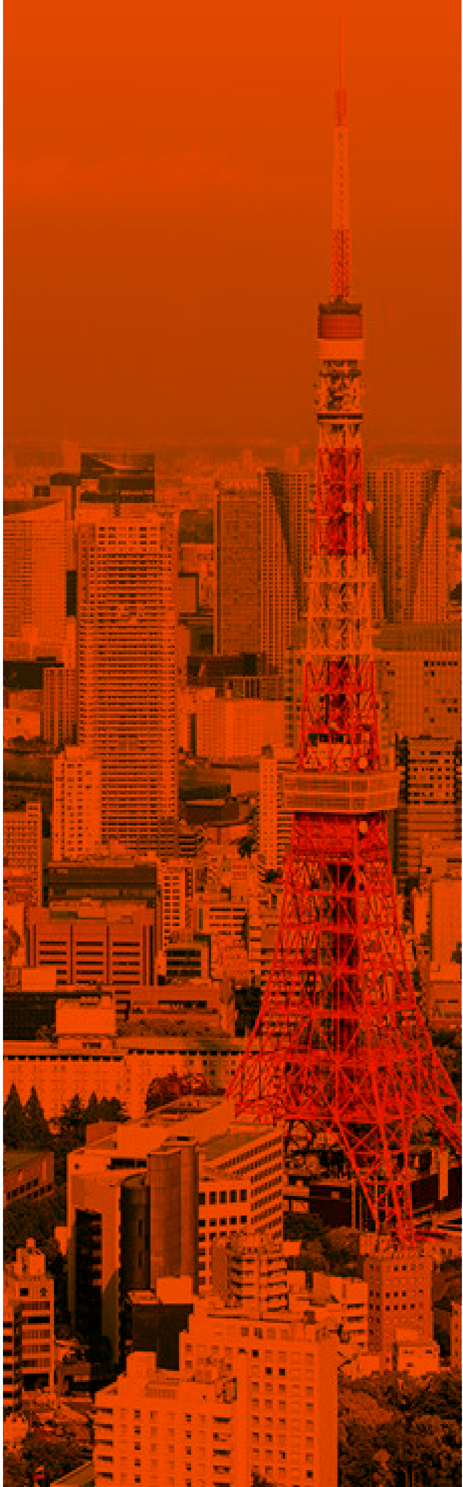

ICG 2019

Green synthesis and the photothermal effect of transparent chlorophyll thin-films

Donglu Shi[1,2*] and Lucas Zhao[2]
[1]Tongji University School of Medicine, Tongji University, Shanghai, China
[2]Department Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio, USA

In nature, most of the metallic conducting materials are known to be transparent, and photo-activated to create heat, therefore acting as a photon-to-heat converter. The photothermal effect has been extensively studied for gold and other metallic materials and attributed the energy conversion to the localized surface plasmon resonance (LSPR). A localized plasmon is the result of the confinement of a surface plasmon in a nanoparticle smaller than the wavelength of the incident light. However, for many energy-related applications, it is required to have the base materials highly transparent for efficient collection of photos, for instance, natural sunlight. But the LSPR effect has been previously demonstrated for both noble metals and conducting metal oxides (CMOs) with significant charge carrier densities ($n \approx 10^{21} - 10^{23}$ electrons/cm^3). As is also well-known, most of the transparent materials (such as silica) are neither conducting nor photo-thermal active. It is, therefore, important to seek for highly transparent photothermal materials for the energy applications that rely on photon source. Chlorophyll has been found to be a highly transparent material that exhibits strong photothermal effect. The molecular structure of chlorophyll (chlorophyll a) consists of a chlorin ring, whose four nitrogen atoms surround a central magnesium atom, and has several other attached side chains and a hydrocarbon tail. Chlorophyll features a saddle-like spectrum with two peaks respectively at 400 nm (blue-violet) and 700 nm (NIR), which is responsible for its transparency. In this study, we report the synthesis and processing of chlorophyll-based thin films. The as-processed chlorophyll thin films can be made in multi-layers and exhibiting high transparency and the photothermal effects for both energy and medical applications. The fundamental operating mechanism of photothermal heating of chlorophyll is identified.

Audience Take Away:

- Explain how the audience will be able to use what they learn?
  The audience will learn a new "green material" for energy and medical applications. A new photothermal mechanism will be identified for chlorophyll.
- The green materials synthesis will have profound impact in materials science and enginerring for a wide spectrum of applications. The knowledge learned from this presentation will provide them with new information for frontier technology jobs. Once presented, there will be expected many research groups to be following the new synthesis routs developed by our group. The transparent thin films will have direct applications for energy efficiency and photothermal cancer therapy. The photothermal thin film will provide new information to assist in a design problem. For instance, the thin film will be deposited with multi-layers that can control the heat conversion and light transmittance, those are key design parameters.

Biography

Prof. Donglu Shi is currently the Chair of the Materials Science and Engineering program at College of Engineering and Applied Science, University of Cincinnati. Donglu Shi's research focuses on nano medicine and energy materials, which involve designs of unique Hybrid material structures that not only interface with biological systems but also offer new bio-chemical-physical properties at nano-scale for fundamental studies. Donglu Shi has so far published 280 refereed SCI journal publications including *Nature, Physical Review Letters, Advanced Materials*. He is currently the Editor-in-Chief of Nano LIFE, and Associate Editor of *Materials Science & Engineering*:C, and J. of Nanomaterials.

Carbon deposits in a single catalyst particle as studied by correlated 3D X-ray microscopy and pore network modeling

Roozbeh Valadian[1*], Martin Veselý[1], Mareike Toepperwien[2], Kathryn Spiers[3], Jan Garrevoet[3], Eelco T. C. Vogt[1,4], Tim Salditt[2], Bert M. Weckhuysen[1] and Florian Meirer[1]

[1]Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Universiteitsweg 99, 3584 CG, Utrecht (The Netherlands)

[2]Institute for X-ray Physics, University of Göttingen, 37077 Göttingen (Germany)

[3]Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg (Germany)

[4]Albemarle Catalysts Company BV, Research Center Amsterdam, PO box 37650, 1030 BE Amsterdam, The Netherlands

Catalyst deactivation is one of the major problems in heterogeneous catalysis. Solid catalysts can be deactivated both reversibly and irreversibly by a reduction of accessibility or by destruction/deactivation of the catalyst's active sites. An example for (typically) reversible deactivation is carbon deposition in the pore structure of a catalyst. Here various carbon species (also called 'coke') are deposited in the pore structure of the catalyst and can cover the active sites of the catalyst or block pores causing diffusion limitations for both products and reaction species. Mapping and modeling of the catalyst pore system can help to understand the coking process and its effects by studying the changes in a catalyst's pore structure and interconnectivity related to carbon deposition. In this context pore network (PN) modeling was shown to be a powerful tool to obtain quantitative morphological and topological information about individual catalyst particles.

In this study, a spent industrial fluid catalytic cracking (FCC) catalyst particle was used as an example for a coked hierarchically complex porous catalyst body. X-ray holotomography on the same catalyst particle before and after coke removal via extensive calcination was used to map changes in the macro-porosity of the catalyst. Next, two pore networks were generated from these two correlated data sets (before and after calcination) to quantify changes of the macropore structure such as pore clogging and a decrease of connectivity caused by carbon deposits. We observed a clear increase of porosity, pore size, total volume, and the number of nodes (branching points of the pore network) being accessible from the particle surface when comparing these pore networks, evidencing the presence of coke in the macro-pore structure of the spent FCC catalyst.

An example of pore narrowing and blockage is displayed in Figure 1 highlighting the effects of carbon deposition in a sub-volume of the catalyst particle. Figure 1d displays how after calcination, i.e. coke removal, the path connecting the yellow and green nodes (blue) is shorter than before calcination (red path), providing direct, visual evidence for the pore clogging effect of carbon deposits.

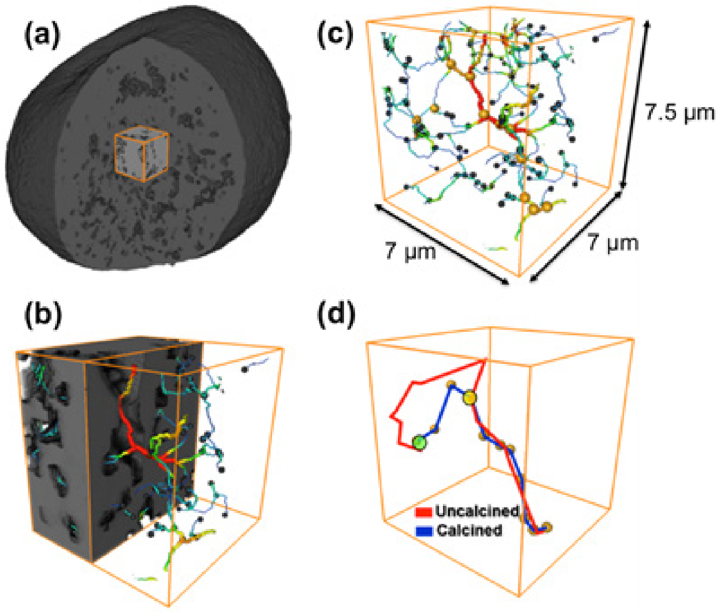

Figure 1. *(a) The catalyst particle as imaged by X-ray holotomography; in (b) and (c) the sub-volume of the particle indicated in (a) and the corresponding PN is shown. In (d) the change in the shortest path between two nodes (yellow to green) cause by coke removal is visualized.*

Key Points:

- By combining three separate state-of-the-art X-ray microscopy measurements we obtained correlated 3-D maps of carbon deposits, macro-pore space, zeolite domains, and poisoning metals present in the catalyst. This correlated information allowed deepening our understanding of the coking process and its deactivating effects during fluid catalytic cracking.
- By correlating the 3-D maps of carbon deposits and metals we were also able to pinpoint the effect of coke promotion by poisoning metals such as Ni and identify regions that are most active in coke formation.
- This developed approach also allowed us to distinguish two types of carbon deposits based on their density and location, i.e. i) surface carbon deposited during the FCC process, which is denser and mainly aromatic in nature, ii) non-surface carbon formed by cracking and dehydrogenation reactions during FCC, which was found to have a lower density.

Biography

Roozbeh Valadian studied Chemical Engineering - Process Design at the Tehran University, Iran and graduated as BSc in 2012. He then did his master study in chemical and energy engineering in the research group of Prof. Dr.-Ing. habil. Evangelos Tsotsas at the Institute of Thermal Process Engineering, Otto-von-Guericke-University in Magdeburg, Germany. He started his PhD in 2017 at the Inorganic Chemistry and Catalysis group of Utrecht University under the supervision of Dr. Florian Meirer and Prof. Dr. Ir. Bert Weckhuysen.

Techno-economic analysis of coal to liquids based on direct coal liquefaction technology

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Direct coal liquefaction (DCL) is the conversion of coal in which coal is transformed into liquid hydrocarbon-based fuels through chemical reactions at elevated pressures and temperatures without being gasified to form syngas. The main objective of this paper is to carry out a comprehensive thermodynamic and economic evaluation for the DCL process based on the two primary conversion options under consideration: (a) Catalytic Coal Liquefaction (CCL) - the use of non-donor solvents with added hydrogen pressure; (b) Thermal Coal Liquefaction (TCL) - the use of solvents with some H-donor properties without hydrogen pressure and catalysts in the coal liquefaction reactor. For this purpose, steady-state process models for the DCL process are developed. The process modules address only the primary DCL processes and do not include any upgrading to transport fuels and chemicals as this will be conducted at refinery facilities by co-processing with petroleum fractions. To better understand the technical parameters and benefits of each scenario, a technical analysis has been conducted using the ECLIPSE modelling software. The overall cost estimation is carried out based on the cost of individual modules. The economic viability of catalytic and thermal direct coal liquefactions is also analysed in the paper.

Technical results showed that the oil yields (light and middle distillates) were around 1045 barrels per day from the CCL process and 745 barrels per day from the TCL process. Based on economic assumptions the light and middle distillate price would be €47.5/barrel with the CCL technology and €51.5/barrel with the TCL technology.

Audience Take Away:

- Help audiences for understanding a clean and efficient Syncrude oil production technology.
- Provide industries with new information and assistance to tackle the oil crisis.
- Provide practical solutions which will benefit not only the coal industry but also a number of sectors encompassing the oil, water and waste industries.

Biography

Prof. Ye Huang is a professor of Energy Engineering at Ulster University. He is a Member of the Energy Institute, a Chartered Engineer and a Fellow of the Higher Education Academy. He was awarded a PhD in Clean Coal Technologies in 1998 from Ulster University. He has specific technical expertise in carbon capture and storage, energy system modelling and fossil fuel power plant optimisation. He has 30 years' experience with scenario analyses of fossil fuel combustion. He has wide experience in establishing multi-partner collaborative projects to develop and exploit fossil fuel and biomass/waste technologies, covering all aspects of techno-economic analysis and life cycle assessment studies. He has published more than 80 peer reviewed journal and conference papers.

Cellular automata based simulations for the autocatalytic mechanism in pitting corrosion

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[2]Institute of Chemistry, Phaculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszynski University, Warsaw, Poland

A review of my and my collaborators' work on corroding and passivating systems is presented. We focus on the autocatalytic mechanism in the pitting corrosion that leads to a peculiar scenario of corrosion processes in a corroding cavity initiated by a single punctual damage of the protecting cover at the surface in contact with an aggressive environment. In our simulations we observe an initial period of rather slow corrosion till the incubation time when the system crosses over to a regime of fast corrosion. The crossover transition is marked by the unstable cavity shape with funny, symmetry breaking forms caused by the appearance of cathodic and anodic reaction zones – a microcell structure accompanied by formation of basic and acidic solution zones in the solution adjacent to cathodic and anodic surface regions. There is a critical size of the cavity for the transition related to the competition between reaction and diffusion. Below this size diffusion neutralizes the solution within cavity and impedes the microcell formation. Then the development of cavity is isotropic. At the transition size the cathodic and anodic zones break this isotropic growth. For sizes much larger than the transition one we arrive at isotropic growth again with decorations on the cavity periphery of the order of the transition length. In this case the transition size is directly related to the ratio of diffusion rate to inhomogeneous reaction rate. We present more examples of passivating and corroding systems where there is such a characteristic length. In certain cases the characteristic length or characteristic time appears fairly explicitly. The examples are regular nanopore network formation and oscillatory phenomena in passivation.

Audience Take Away:

- Cellular automata can be used to simulate complex phenomena in inhomogeneous systems with autocatalytic mechanism.
- There are characteristic lengths in such systems that govern the system behavior.
- Such systems can be used for a useful pattern generation at electrodes or elsewhere.

When designing a reaction-diffusion system for a pattern generation it is useful to be aware of the characteristic lengths that can be involved in the problem. It is fairly pedagogical and idea to relate the pattern of microcells on a corroding surface to a competition between anodic-cathodic zone separation and restoring neutrality diffusion. It gives a nice basis for common corrosion knowledge that the steel pipes corrode faster in still water rather than in the flow or agitation because of destroying inhomogeneities created by autocatalytic corrosion process.

Biography

Dr J. Stafiej graduated from the Department of Physics, Warsaw University, 1980. In 1991 he defended PhD thesis supervised by prof. Zofia Borkowska, Institute of Physical Chemistry, Warsaw, (ICHF). He collaborated with JP. Badiali in Paris for over 20 years on statistical field theory for interfacial electrolytes. His habilitation thesis concerns branching pattern of differential capacitance caused by ionic profile depletion (ICHF 2002). Since 2014, as a professor in the Institute of Chemistry, Cardinal Stefan Wyszynski University, Warsaw, he works on corrosion, passivation, nanopore formation and oscillatory phenomena within cellular automata approch. He authors 59 SCI papers.

An efficient way of producing fuel hydrocarbon from CO_2 and activated water

Tadayuki Imanaka*, **Tadashi Takemoto**
The Research Organization of Science and Technology, Ritsumeikan University, Kusatsu, Shiga, Japan

Here we show that petroleum can be formed efficiently at normal temperatures and pressures from carbon dioxide and activated water. The CO_2 nano-bubble containing water was treated with photocatalyst in the presence of oxygen under UV irradiation. The activated water was mixed vigorously with kerosene or light oil and carbon dioxide to form an emulsion. The emulsion gradually separated into a two-phase solution. After phase separation, the volume of kerosene or light oil, depending on which oil was utilized, increased by 5 to 10%.When n-tetradecane was used, n-tetradecane was only produced. These results suggest template-dependent synthesis. It is also shown that commercial light was purified by removing organic and inorganic impurities, resulting in premium oil. The industrial machine for continuous production of oil was constructed.

Biography

Tadayuki Imanaka, graduated from Osaka University, receiving the degree of Bachelor of Engineering in 1967, finished the post-graduate course at the same university, receiving the degree of Master of Engineering in 1969, and awarded the degree of Doctor of Engineering from Osaka University in 1973. Postdoctoral research associate at Massachusetts Institute of Technology (USA) from 1973 to 1974, associate Professor of Biotechnology at Osaka University since 1981, and Professor of Biotechnology at Osaka University since 1989. Professor at Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University since 1996, and Professor at Department of Biotechnology , Ritsumeikan University since April, 2008. He was awarded Biotechnology award of the Society for Bioscience and Bioengineering, Japan, in 2001, Arima Prize of Japanese Biotechnology Association, in 2001, Fellow in American Academy of Microbiology, in 2003, The Chemical Society of Japan Award, in 2005, and Japan Society for Environmental Biotechnology Award, in 2008. He was selected as a member, Science Council of Japan, since 2005. He received the Purple Ribbon Medal in 2010, and The Order of the Sacred Treasure, Gold Rays with Neck Ribbon from Japanese Emperor in 2018.

“Bio-based solvent”: New solvent for the synthesis of heterocycles containing oxygen, sulfur and nitrogen

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The search for alternatives with less environmental impact and the study focused on the selection of solvents used in the chemical laboratories has been increasing in recent years. There are already several articles that have been reporting bio-based solvents as effective alternatives to conventional solvents derived from petroleum for the synthesis of O, S, N-Heterocyclic compounds. Continuing the field of our team with a view to the development of new methodologies and greener approaches in the synthesis of heterocycles containing oxygen, sulfur and nitrogen, we explored the potentialities of a new solvent. The synthesis process started by the identification of two unusual solvents and later the study of its application in several reactions to show the potential and efficacy as a greener alternative in the synthesis of O, S, N-Heterocyclic compounds via some Pd-catalysed methodologies. Pd-catalysed processes have become an approach of choice in modern organic synthesis. In this work, we described the successfully application of a “new bio-based solvent” in several Pd-catalysed methodologies (CH activation, Suzuki-Miyaura coupling, Sonogashira-Hagihara coupling and Migita Kosugi Stille coupling). It was showed the potential and efficacy as a greener alternative in the synthesis of O, S, N-Heterocyclic compounds. As our article is in the submission process, the name of the bio-based solvent was not mentioned yet.

Audience Take Away:

The use of greener routes are well-appreciated approaches in the fields of green chemistry and synthesis of N-heterocyclic, due to the remarkable importance that these compounds represent in the area of medicinal chemistry. Solvents play an important role in the chemical industry and their effectiveness in acting with the reagents and products in reaction processes is a crucial factor. The choice of solvent is going to influence chemical reactivity, selectivity and yield of the process of synthesis. One way to try to minimize safety, toxicity, and emissions problems is to find or develop replacement solvents commonly used. In recent years, valid proposals have been reported as green solvents used in the synthetic processes. With all this results in the search for safer solvents, the concepts of green chemistry have achieved remarkable progress in developing greener approaches in organic synthesis. We believe this oral presentation will provide information to further advance the applications of “bio-based solvent” in Pd-catalysed methodologies. Additionally, the sharing and discussion of this work would be helpful to a broad community of scientists working in medicinal chemistry.

Biography

Joana Filomena Campos, born in Trofa, Portugal, in 1989. She completed her BSc degree (Pharmacy) in 2011 from CESPU, and MSc degree (Medicinal Chemistry) in 2013 from the University of Minho. Currently, she is in 3rd and last year of PhD at the Institut of Organic and Analytical Chemistry (ICOA) of the University of Orléans (France) under the supervision of Professor Sabine Berteina-Raboin. Her research interests focus on the study of new and greener approaches for the synthesis of O,S,N-heterocyclic compounds. Since the beginning of her PhD, she has published with her team 6 articles and others are in preparation for submission soon.

DOZN™- A quantitative green chemistry evaluator

Samy Ponnusamy
MilliporeSigma, United States

MilliporeSigma created a unique web-based greener alternative scoring matrix, also known as DOZN™- A Quantitative Green Chemistry Evaluator based on the 12 principles of green chemistry. The 12 principles of green chemistry provide a framework for learning about green chemistry and designing or improving materials, products, processes and systems. DOZN™ scores products based on metrics for each principle and aggregates the principle scores to derive a final aggregate score. The system calculates scores based on manufacturing inputs, Globally Harmonized System (GHS) and Safety Data Sheet (SDS) information which provide a green score for each substance and is flexible enough to encompass a diverse portfolio of products ranging from chemistry to biology based products. The DOZN™ system has also been verified and validated by a third party to ensure best practices are applied. This new Greener Chemistry initiative offer customers' an increased breadth of Greener Alternative products with confirmatory documentations to validate greener characteristics.

Biography

As a founder of Sigma-Aldrich's Green Chemistry team in 2007, developing MilliporeSigma's Corporate Green Chemistry initiatives, managing/expanding new Green Business Opportunities, Greener Alternatives R&D and greener product developments. Developed a unique and state of the art Quantitative Green Chemistry Evaluator, DOZN system based on the Twelve Green Chemistry Principles. Also have extensive experiences in applying concepts of Polymer/Organic Chemistry and process technology skills for developing new and innovative bio-polymers for drug delivery applications. I have managed product developments to successfully introduce new products that have recorded sustained growth (>$100 million cumulatively). Have extensive knowledge (over 30 years) in managing product developments from bench scale through product launch.

How the design of nanomaterials allows to control their properties

Sophie Cassaignon*, Corinne Chanéac, Olivier Durupthy, David Portehault
Sorbonne Université, CNRS, Collège de France, Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP), Paris, France

Emergence of nanotechnology increasingly shows examples of the material potentiality which has, at least one dimension less than 100 nm. The preparation of nano-objects by soft chemistry in aqueous solution with crystal structure, size and morphology perfectly controlled is based on the use of molecular precursors and adjustment of physico-chemical parameters (acidity, ionic strength, temperature…) during the precipitation of the solid. The growth of nano-crystals can be limited or favoured in some crystallographic directions. It is also possible to involve redox processes in addition to the acido-basic reactions. That can significantly enhance the potentiality of this chemistry in the design of particles. Furthermore, the synthesis of hierarchical materials with multiple scales of organization and often formed from the assembly of nanoparticles, raises a growing interest, mainly thanks to their ability to combine the functions of the various elementary units. This allows to consider interesting applications of these systems in various fields and especially in the field of Energy, either for conversion or storage and (photo)catalysis.

Audience Take Away:

- Show the versatility of soft chemistry to control the formation of functional nanoparticles
- Show how the design of materials can control their properties
- Present some examples of application in energy and (photo)catalysis

Biography

Sophie Cassaignon is Professor in Materials Chemistry at Sorbonne University (Paris, France). She received his B.Sc and M.Sc, in Chemistry from UPMC (Now Sorbonne University). She received her PhD degree in 1998 at the same institution. Currently, she is working in the Laboratory of the Condensed Matter of Paris and her research interests are nanomaterials synthesis, conversion/storage of Energy and (photo)catalysis. She has published more than 60 research articles in peer-reviewed journals.

CO oxidation over Au catalysts supported on CuO/Cu_2O both in O_2-rich and H_2-rich streams: Necessity of copper oxide

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In this work we prepared nanometer copper oxide and cuprous oxide with different morphologies followed by the deposition of Au nanoparticles. The reaction of CO oxidation in both hydrogen-rich and oxygen-rich streams was investigated over as-prepared CuO/Cu_2O materials and the corresponding supported Au catalysts. A comprehensive analysis of the catalytic results demonstrates that CuO species not Cu_2O play much more critical role as the active sites for the oxidation of CO and the synergistic enhancement in catalytic activity can be realized via its strong interaction with nanogold particles.

Audience Take Away:

- The audience will see why and how our catalytic system reveals the high catalytic performance by using the appropriate catalyst physicochemical characteristics.
- The audience will know why and how the cooperation effect between CuO and nanogold were confirmed and played an important role for the high performance of present catalytic system.
- Our work may help the audience who work in the same topic to design a better catalyst for CO-PROX reaction.
- This research can be used by others to expand their research.

Biography

Dr. Caixia Qi, 52 years old, is the Director / Professor at Shandong Applied Research Centre of Gold Nanotechnology (Au-SDARC), Yantai University, China and engaged in the research of gold catalysis and populating industrial applications of gold nanotechnology. She received her Ph. D degree from Lanzhou Institute of Chemical Physics of Chinese Academy of Sciences in 1996 and served as a STA postdoctoral fellow, an associated researcher and a guest researcher in Osaka National Research Institute of Japan (Kansai AIST), Royal Military College of Canada and Tokyo Metropolitan University, respectively. She was awarded Shandong Taishan Scholar in 2011 and promoted and organized the Shandong Applied Research Centre of Gold Nanotechnology (Au-SDARC), an open-end industry-academia- research platform for speeding up industrial applications of gold which features regional advantages and compliance of international standards.

Catalytic options for methane valorization catalyst performance evaluation using parallel fixed bed reactor systems and data driven catalyst development

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Avantium, Zernikestraat 29, 1014 BV, Amsterdam, Netherlands

The abundance of shale gas has increased the interest in methane valorization via catalytic conversion. Methane can be used as a feedstock to produce valuable chemicals, mostly by first producing syngas via reforming, followed by one or more catalytic conversion steps. Well-known examples are the methanol-to-olefins (MTO), methanol-to-gasoline (MTG) and the Fischer-Tropsch (FT) processes. Other routes for the valorization of shale gas exist, e.g. the catalytic oxidative coupling of methane (OCM) to produce ethylene.

For the development of new catalyst formulations for these processes, it is crucial to perform well-defined catalyst performance tests. The catalyst tests should provide information on the intrinsic activity of the materials, which facilitates improvement developments between generations of catalysts.

Avantium has used its parallel miniature fixed bed catalyst-testing platform (Flowrence) in many areas of catalysis. This platform has been successfully used to develop and optimize a large variety of catalytic processes, ranging from refining applications, gas-to-liquids, chemicals and biomass conversion. This miniaturized technology has demonstrated to achieve scalable results, even in the presence of highly exothermic reactions, which could hinder catalytic performance. In addition, the our high throughput technology (HTT) allows us to simultaneously evaluate up to 64 catalyst / process conditions, reducing significantly the time required to screen new materials or evaluate process parameters.

In this talk, we will show the design considerations taken to evaluate materials in a miniaturized parallel system, under kinetically control and near ideal conditions. These design considerations include, among others, precise and accurate control of the feed flow rate using glass chips and our proprietary active liquid distributors based on microfluidics technology, improved reactor-to-reactor pressure control by means of an active pressure controller, which can reduce the pressure difference in parallel reactors well below 5% of the operational pressure and accurate temperature control that guarantee quasi-isothermal operation.

Several applications will be used to explain the capabilities and design considerations. These include Fischer-Tropsch, OCM and MTO. Each of these applications have challenges to achieve proper control of the test conditions. For the MTO process, temperature and pressure were shown to have a critical effect. In addition, the fast deactivating behavior of SAPO-34 materials used in MTO represented an analytical challenge that was overcome by the use of a 16-loop sampling valve coupled with a gas chromatograph.

A well-defined Fe catalyst system bearing a tetradentate pnnp ligand: Selective synthesis of hydrosiloxanes via dehydronegative coupling of silanols with hydrosilanes

Tomohiro Takeshita[1,2] **,Yumiko Nakajima***[1,2]**, Kazuhiko Sato**[2]
[1]Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki, Japan
[2]Interdisciplinary Research Centre for Catalytic Chemistry (IRC3), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan

Iron complexes with low toxicity and high terrestrial abundance have recently drawn increasing attention as a new class of catalyst precursors in an attempt to develop environmentally benign and sustainable methods for organic synthesis. Intensive studies on Fe complexes have been conducted to date; however, examples of well-defined reactions remain scarce compared with those of 4d or 5d metal complexes. In this study, a well-defined iron complex system was established using PNNP-R (R = Ph and Cy) as a strong σ-donating ligand with a rigid meridional tetradentate structure. Reactive Fe(0) complexes [{Fe(PNNP-R)}2(*μ*-N$_2$)] were synthesized by the reaction of the corresponding iron diharide with NaBEt$_3$H and structurally fully characterized. The reaction proceeded via the iron dihydride intermediate [Fe(H)$_2$(PNNP-R)], which underwent H$_2$ reductive elimination, supporting the hemilabile behavior of PNNP-R. [{Fe(PNNP-R)}$_2$(*μ*-N$_2$)] catalyzed dehydrogenative coupling of silanols with silanes to selectively form various hydrosiloxanes, which are important building blocks for the synthesis of a range of siloxane compounds. The system exhibited the highest catalytic efficiency among the previously reported transition-metal-catalyzed systems.

Audience Take Away:

- One method to precisely design of Fe complexes using a strong -donating ligand
- Synthetic procedures of reactive Fe(0) complexes bearing labile N$_2$ or silane ligands
- Importance of hydosiloxanes as a raw materials for the silicone production

Biography

She received her Ph.D. from Tokyo Institute of Technology in 2005. She then worked as a Posdoc (sponsored by a Humboldt Research Fellowship) at RWTH Aachen University (2005-2007) and at RIKEN (2007-2008). She joined Kyoto University as an Assistant Professor in 2008. She spent the year 2009-2013 as a JST PRESTO project researcher. She moved National Institute of Advanced Industrial Science and Technology (AIST) as a senior researcher in 2013 and then become a team leader. Her research interests are in organometallic chemistry and coordination chemistry.

Palladium-Catalyzed β-C(sp3)−H Arylation of weinreb amides via acidic ligands

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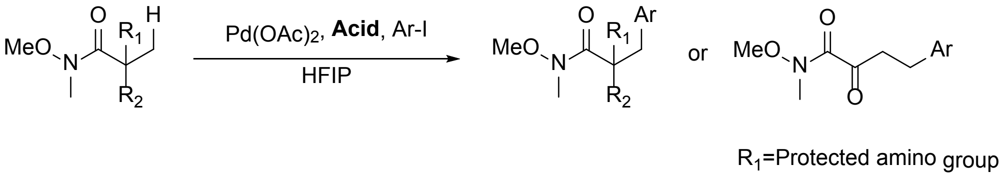
[2]College of Materials Science and Chemical Engineering, Harbin Engineering University, Harbin, 150001



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 catalysed 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.

Role and significance of molybdenum disulfide (MoS_2) as a cocatalyst for photocatalytic hydrogen production

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Modern advancement in design of the efficient visible driven photocatalyst for solar-to-hydrogen generation has been expanded much consideration due to fossil fuels crisis, which convert and store solar energy into chemical fuels. In view point of economic and large-scale application, semiconductor photocatalyst with high stability and efficiency should be required. However, a numerous number of materials have been discovered, challenges still remain for the commercialization. Among the enormous number of materials, layered structured transition metal dichalcogenides (TMDs) based photocatalyst have been shown attractive performance in photocatalytic process owing to their suitable narrow bandgaps, high absorption capacity and fast carrier transport properties. This review to be covered the physicochemical features and recent advancements of various layered structured TMDs based photocatalysts, especially MoS_2 and various approaches to improve the photocatalytic reaction and stability by coupling active carbon materials including graphene, carbon nanotubes (CNTs), active carbon, precious metals and other metal oxides, etc. We rely on this review can reveal some insights of fundamental concepts of role of active chemical species during the solar-to hydrogen conversion processes and their influences in enhanced performance on PEC water splitting

Audience Take Away:

- To understand the important of 2D materials in catalysis
- To understand the latest advancements in development of photocatalysts for water splitting
- To educate the possible mechanism involved in photocatalytic reactions
- To understand the modern techniques to enhance the photocatalytic efficiency and stability of MoS_2 photocatalyst

Biography

Dr. Vattikuti has completed his PhD degree in Nanomaterials and Coatings from Chung Hua University, Taiwan in the year 2010. He received one year postdoctoral fellowship from Yeungnam University (2014-2015). Currently he is International assistant professor in School of mechanical Engineering, Yeungnam University, South Korea. He has published more than 60 papers in reputed journals and has been serving as a reviewer of repute journals. He received three years fund from National Research foundation of Korea (NRF-Korea) (2017-2020). His research focuses on transition metal Chalcogenide materials for energy and photocatalytic applications.

Low temperature catalytic oxidations on bimetallic catalysts employing molecular oxygen

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About 30% of the total production in the chemical industry and many emissions control catalytic reactions use catalytic oxidation processes/technologies. In these oxidation reactions, employing molecular oxygen (O_2) as the oxidant is the most environmentally benign approach, in which, activation of O_2 by catalysts to obtain the desired active oxygen species is crucial. And furthermore, how to develop catalysts workable under mild reaction conditions is a big challenge.

In this work, we report preparation of various supported mono- and bi-metallic catalysts and their applications in several oxidation reactions: (i) the photo-degradation of methyl orange (MO) in water under visible light(ii) the catalytic wet air oxidation (CWAO) of dyes in wastewaters, and (iii) preferential oxidation (PROX) of CO in H_2-rich gas mixtures. It was found that some bimetallic catalysts showed better capability for oxygen activation and for catalytic oxidations than the corresponding monometallic catalysts. For example, the prepared AuPd(3:1)/TiO_2 catalyst with formation of AuPd alloy particles showed high activity towards MO degradation under visible light; Similarly, AuCu and AuPd bimetallic nanoparticles deposited on some other catalyst supports also showed high catalytic activities towards PROX of CO and CWAO of dyes (Safranine O (SO), Methylene Blue (MB) and Brilliant Green (BG)) at reaction temperatures close to 0^{o}C. The effects of calcination temperature, Au/Pd and Au/Cu ratios, catalyst dosage, dye concentration and reaction efficiency were investigated for the hybrid bimetallic catalyst systems. The supported AuPd(1:1) catalyst with an Au/Pd mass ratio of 1:1 calcined at 400 °C possessed the highest catalytic activity for the dye degradation through CWAO. It could be workable for dye degradation with high concentration even at the reaction temperature lower than room temperature, e.g., 5 °C, and exhibited a good chemical stability. In addition, high dye removal efficiency still could be achieved after five times reuse. The mechanism for the improved catalytic activity was investigated, e.g., by indirectly using quenchers for various reactive oxygen species (ROSs). It revealed that superoxide radical ($\bullet O_2$-) and singlet oxygen ($^1O_2$) are the main active oxidative species during CWAO of dyes.

These results show some supported bimetallic catalysts are workable for a number of oxidation reactions at quite low temperatures with high catalytic efficiencies.

Biography

Ziyi Zhong received his Ph.D from Nanjing University in China, then did 5-year postdoc research in Israel, USA and Singapore, and followed with 1-year employment in BRI in Montreal holding a Visiting Fellowship. During the period of 2013-2018, he worked in the Institute of Chemical and Engineering Sciences under A*star in Singapore, and also held an adjunct associate professorship in Nanyang Technological University (2013-2017). In Oct 2018, he joined College of Engineering, Guangdong Technion Israel Institute of Technology (GTIIT) in China as a full professor. His research areas include heterogeneous catalysis, clean energy, waste water treatment, surface chemistry and nanosized materials.

High-Frequency and -Field EPR and Far-Infrared magnetic spectroscopy of transition metal complexes with catalytic properties

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High-Frequency and -Field Electron Paramagnetic Resonance (HFEPR) and Far-Infrared Magnetic Spectroscopy (FIRMS) are relatively new versions of electron spin resonance, the former being performed in magnetic field domain; the latter – in frequency domain. Both are particularly useful to characterize paramagnetic coordination complexes of transition metal ions that are "EPR-silent" in standard conditions because of their large zero-field splitting (ZFS). The HFEPR observables such as ZFS parameters and spectroscopic *g*-values can be directly related to the electronic structure of investigated complexes, and those in turn are linked to their catalytic properties.

Some examples of applying HFEPR and FIRMS to such complexes will be presented. In one example, both techniques were applied to investigate a series of oxoiron(IV) complexes in the spin triplet ($S = 1$) and quintet ($S = 2$) ground states. This type of complexes has been identified as intermediates in the catalytic cycles of many non-heme iron oxygenases. The Que group has synthesized and characterized a number of stable analogs to these enzymatic intermediates and investigated their ability to activate very strong C—H bonds. In order to explain the C—H bond activation ability of spin triplet and quintet $[Fe^{IV}(O)]^{2+}$ complexes, the two-state reactivity model is often invoked, which requires measurement of ZFS parameters enabled by instrumentation at NHFML. Given sufficient time, other examples of applying HFEPR and FIRMS to catalytically-active systems may also be included in this presentation.

Audience Take Away:

- The audience may learn about relatively new and not widely known spectroscopic techniques;
- These techniques are useful for characterizing new metal complexes of catalytic properties;
- Some examples of the applications will be presented;
- The audience will be encouraged to apply the techniques to suitable catalytic systems to better characterize and understand the catalytic mechanisms.

Biography

Jurek Krzystek, Research Scientist at the National High Magnetic Field Laboratory (NHMFL) in Tallahassee, Florida, received a Ph.D. in chemical physics at the Institute of Physics, Polish Academy of Sciences. His postdoctoral appointments were at the University of Stuttgart in Germany and the University of Washington in the USA. Since 1995 Dr. Krzystek has been with the NHMFL. He has specialized in spectroscopy of molecular systems, including Electron Paramagnetic Resonance (EPR), and in particular, High-Frequency and -Field EPR as a characterization method of transition metal coordination complexes. He has published 150+ peer-reviewed articles in this, and other scientific areas.

Multi-walled carbon nanotubes decorated with Cu(II) triazole Schiff base complex and its catalytic performance for adsorptive removal of synthetic dyes

Rehab El-Sharkawy [1,2], **Hoda A. El-Ghamry** [1,3*]
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[2]Chemistry Department, College of science, Jouf University, Aljouf 2014, Sakaka, Saudi Arabia
[3]Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Makka, Saudi Arabia

Hydroxyl functionalized Cu(II) Schiff base named N,N-bis(4 hydroxysalicylidene)-4-H-1,2,4-triazole-3,5-diamine-diaminedicopper (II) has been synthesized. Analysis of the obtained net complex supported the formation the compound in the molar ratio 1:2 [L:M] and it has the structure of $[LCu_2(OAc)_2(H_2O)_2]$.MeOH (Cu_2-L); where L N,N-bis(4 hydroxysalicylidene)-4-H-1,2,4-triazole-3,5-diamine ligand while the spectral results confirmed the geometry around the Cu(II) centers to be tetrahedral. The obtained complex has been supported on modified MWCNT *via* covalent bonds. The obtained MWCNT anchored copper complex ([Cu_2-L]@MWCNT) has been characterized by different tools including elemental analysis, fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmittance electron microscopy (TEM), thermal analysis, UV–Vis spectra and X-ray diffraction which confirmed the loading of bimetallic complex on CNT. The efficiency of ([Cu¬2-L]@MWCNT) for the adsorptive removal of Sunset yellow (SY), Direct red 81 (DR-81), and acid blue 92 (AB-92) dyes from aqueous solutions has been studied under alternative experimental conditions. The experimental results have been analyzed by the Langmuir and Freundlich isotherm models. The equilibrium adsorption data fits Langmuir adsorption isotherm very well owing to the homogeneous distribution of active sites onto ([Cu_2-L]@MWCNT) surface. The experimental kinetics of the data were analyzed using pseudo-first-order, pseudo-second-order and Weber-Morris intra-particle kinetics. The adsorption process follows the second-order kinetics. The adsorption method found to be endothermic and spontaneous as appeared from thermodynamic data.

Audience Take Away:

- Synthesis of MWCNT anchored with different metal complexes
- The characterization and structure identification of the synthesized catalyst
- To what extent the synthesized compound is efficient in different catalytic reactions such as removal of the color from waste water.
- The kinetics of the catalytic reaction will also be analyzed and discussed to assert to assert the type of the kinetic reaction.

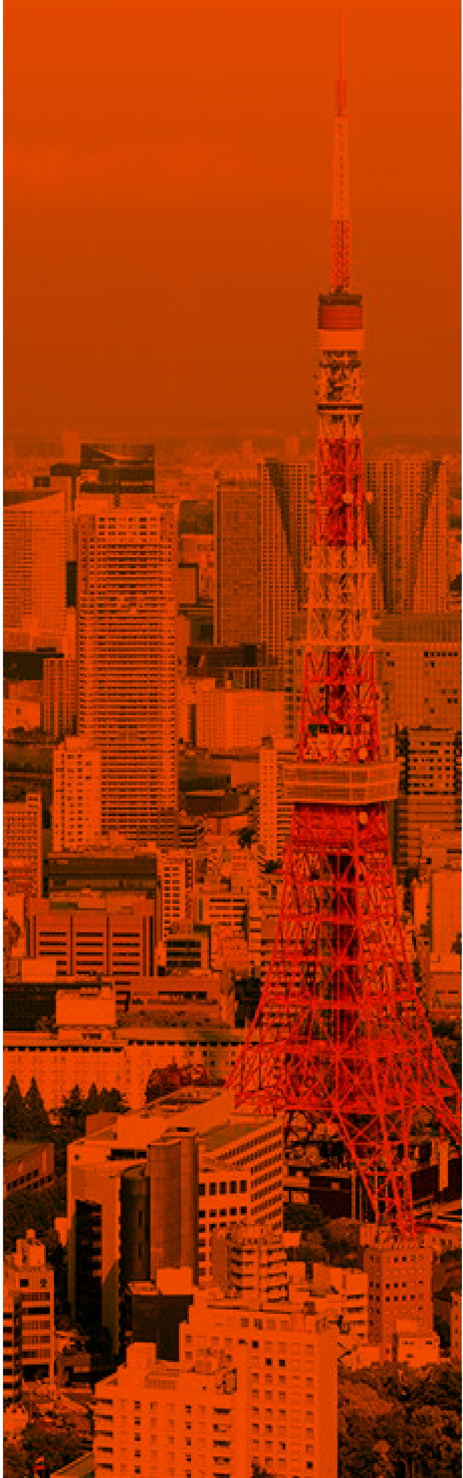
Biography

Dr. Hoda studied chemistry in Tanta University, Egypt and graduated as MS in 2005. She then joined the research group of Prof. Ken sakai in Kyushu University, Japan, in 2008 as visiting researcher for two years. She received her PhD degree in 2010 from Tanta University after which she obtained the position of assistant professor of Inorganic Chemistry at the same university and became associate professor in 2015. She transferred to Umm-Al-Qura university and working as associate professor from 2015 till now. She has published more than 30 research articles in peer reviewed international journals.

magnus
Group

DAY 1

SPEAKERS (HALL 2)



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MAY
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TOKYO, JAPAN

ICG 2019

R&D of new catalysts for the water gas shift processes

N. Schiaroli[1], P. Benito[1], R. Faure[2], G. Fornasari[1], D. Gary[2], C. Lucarelli[3], C. Molinari[1] and A. Vaccari[1*]
[1]Department of Industrial Chemistry "Toso Montanari", ALMA MATER STUDIORUM – University of Bologna, Via Risorgimento 4, 40136 BOLOGNA (Italy)
[2]CRCD Air Liquide, 1 Chemin de la Porte des Loges, 78354 Jouy-en-Josas (France)
[3]Department of Science and High Technology, University of Insubria, Via Valleggio 9, 22100 COMO (Italy)

H_2 is a key raw material in chemical and petrochemical industries, with further increasing interest as promising energy vector. The water gas shift (WGS) reaction is an industrially relevant reaction, which takes place in large scale plants and represents a key upgrading step allowing to adjust different syngas ($CO + H_2$) compositions. The WGS is an exothermic reaction, thermodynamically favored at low temperature, while higher reaction rates are favored at higher temperature, which is why it is currently carried out in 2 steps: i) immediately after the steam reforming reactor (SRr) operating at about 350°C with Cr-rich Fe-based catalysts (HTS); ii) in the subsequent converter at about 220 °C using highly active Cu-based catalysts (LTS). Although on account of its high industrial relevance, the WGS reaction has been widely investigated, in the last years new subjects arose, with an increasing interest for new formulations able to operate in one step at middle temperature (MTS) or to replace the Cr-rich catalysts for HTS step. The former formulations operate at about 300°C with high activity, selectivity and stability with time-on-stream (TOS) reducing capital and operational expenditures (CAPEX and OPEX, respectively). The CO conversion may be increased expanding the PROX step, already present when the application of the H_2 stream is low temperature fuel cells. In the second case, the main drawbacks of current Cr-promoted Fe-based HTS catalysts are the toxicity of Cr (VI) ions and the requirement to use high inlet steam flow to avoid the formation of metallic Fe, able to catalyze hydrocarbons formation. Thus, new formulations have to be Cr- and Fe-free and to operate with low steam/dry gas ratios, allowing to work more efficiently in the previous SR step, with catalytic performances better than those of commercial catalysts. In this contribution, the R&D from the laboratory to the pilot plant of new formulations for MTS and HTS applications are presented, to evidence how also widely investigated reactions such as the WGS may offer interesting opportunities of new research lines and applications of both academic and industrial interest. To obtain active catalysts and avoid interferences due to structure dishomogeneity or phase segregation, hydrotalcite-type (HT) anionic clays were selected as catalyst precursors, which are characterized by homogeneous cation distribution and are simple and relatively inexpensive to prepare on laboratory or industrial scale. The catalysts were fully characterized before and after reaction and the activity determined as a function of the reaction parameters, allowing to determine best compositions for each temperature range. Tests performed in a lab-scale pilot plant for more than 450 h of time-on-stream do not evidence any significant deactivation both in MTS and HTS conditions. These novel catalysts have been jointly patented by the University of Bologna and Air Liquide.

Audience Take Away:

- Also in well-known industrial processes there are margins for significant improvements
- Key role of the literature to design further improvements
- In MTS economic advantages of one step process, with reduction of capital and operative costs.
- In HTS removal of the main drawbacks of the current commercial catalysts.
- Advantages of the catalyst preparation from hydrotalcite-type precursors.

Biography

In 1972, Prof Vaccari graduated in Industrial Chemistry with honors at ALMA MATER STUDIORUM – University of Bologna, were 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 Universitad 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, 265 Congress Communications and 20 Patents (16 EU or WO), with H-index = 43 and 10934 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.

A green approach for the recovery of proteins from meat industries

Zead Elzoeiry, Jesus Hernandez, Md S. Islam, Abel E. Navarro*
Science Department, Borough of Manhattan Community College, CUNY, New York, NY, USA

The adsorption of bovine serum albumin (BSA) and human hemoglobin (Hb) on naturally-occurring adsorbents was studied to evaluate the potential recovery of proteins from meat industry residues. Spent peppermint tea (PM), powdered purple corn cob (PC), natural clay (NC) and chemically-modified clay (MC) were investigated to elucidate the effects of pH, adsorbent dose, initial protein concentration, presence of salts and heavy metals. Equilibrium data was fitted according to isotherm models, reporting a maximum adsorption capacity at pH 8 of 318 and 344 mg BSA/g of PM and NC, respectively. Moreover, Hb displayed maximum adsorption capacity at pH 5 of 125 and 143 mg/g of PM and PC, respectively. Hofmeister salt effect was only observed for PM/Hb system. Salts tend to decrease protein adsorption, and the presence of Cu(II) ions had negligible impacts on the adsorption onto NC and PC. Desorption experiments confirmed that more than 85% of both proteins can be recovered with diluted acids and bases. SEM, EDX and TGA analyses demonstrated that the adsorbents have favorable morphological and mechanical properties. The long-term goal of this study aims to recover soluble proteins from industrial wastewaters to produce animal food or any protein-based product.

Audience Take Away:

- Audience will learn about the alternative use of biowastes, especially lignocellulosic materials.
- This presentation will incentivize collaboration with meat industries to generate a secondary profit, such as animal food industries.
- The use of biowastes can be applied in different Green Chemistry scenarios, including the classroom and industries. These biowastes have low cost and are easy to manipulate.
- Additional collaborations are welcome, mostly in the scaling of the process by using continuous-flow experiment and testing this technique with real industrial wastewaters from meat factories.

Biography

Dr. Abel Navarro studied Chemistry at the Cayetano Heredia Peruvian University in Lima, Peru and then moved to the USA to earn his MS in Organic Chemistry in 2007. Then, he continued with his Ph.D. in Biomolecular Chemistry, with emphasis in protein chemistry, graduating in 2011. Next, Dr. Navarro was appointed as an Assistant Professor at the Borough of Manhattan Community College, part of the CUNY network in New York City. Now as an Associate Professor, he continue conducting research with highly motivated and talented students, coauthoring around 40 peer-reviewed articles since his appointment. The authors would like to acknowledge BMCC and CUNY for the travel funds for Faculty members and PSC-CUNY for funding this research.

Catalytic hydrogenation of stearic acid to stearyl alcohol over cobalt silica catalysts

Zeni Rahmawati[*1] **, James Anderson**[2]
[1] Department of Chemistry, University of Aberdeen, Aberdeen, United Kingdom
[2] Formerly Chemical and Materials Engineering, University of Aberdeen, Aberdeen, United Kingdom

Conversion of basic oleo chemicals to fatty alcohols is a very important transformation as fatty alcohols are widely used in fragrances, detergents, emulsifiers, lubricants, health supplements and pharmaceuticals. In addition, fatty alcohol from petrochemicals is facing several challenges including depleting of the finite source of oil and gas, and many environmental problems such as climate change, air and water pollution that are associated with production, use and disposal of petrochemicals products. Fatty alcohol is commercially produced through the hydrogenation reaction using chromite-based catalysts. However, this process requires elevated temperatures (200-300°C) and pressures (100-300 bar). Additionally, the use of chromite is associated with environmental problems.

In this study, Co/SiO_2 catalysts with varied cobalt loading have been applied in the hydrogenation of stearic acid to produce stearyl alcohol. The influence of cobalt loading and catalytic properties on the activity and selectivity was studied by performing the reactions in a batch reactor at 300°C and 50 bar. Co/SiO_2 was found to convert stearic acid to stearyl alcohol with high selectivity along with octadecanal, octadecane and heptadecane. Experiment results revealed that the cobalt loading influenced the activity of catalysts including the conversion, stearyl alcohol selectivity and reaction rate. The available metal area was observed to be the main reason for the increase of conversion and reaction rate enhancement. While the selectivity to stearyl alcohol was able to be maintained above 93% over cobalt loadings between 4-8 wt%. In addition, the study of turn over frequency over varied cobalt dispersion generated from different cobalt loading confirmed that hydrogenation of stearic acid over cobalt silica is structure insensitive.

Audience Take Away:

- Cobalt silica as an alternative catalyst for fatty alcohol production which successfully converted the stearic acid as a model compound to stearyl alcohol. This catalyst has addressed the challenge of current industrial catalyst in terms of mild reaction condition, economic point of view, and environmentally friendly.
- The preparation and the characterization of catalyst as well as the description of catalyst properties related to the result of stearic acid hydrogenation.
- The highlight of hydrogenation of stearic acid process including the conversion, product selectivity and other significant information linked to the reaction such as reaction order, turn over frequency, and catalyst structure independency.

Biography

Zeni Rahmawati graduated her master in Sepuluh Nopember Institute of Technology, Indonesia in 2013. At the moment, She is pursuing a PhD in Chemistry at University of Aberdeen. She has joined the surface chemistry and catalysis under Prof James Anderson supervision from 2015-2018, and is currently working under Prof. Russell Howe and Dr. Alan McCue. Her PhD is focused on the catalytic upgrade of oleochemicals for fatty alcohol production with the research funding and studentship from Indonesia Endowment of Education, Ministry of Finance Republik Indonesia.

Adsorption of Zinc Acetate (aqueous solutions) on modified activated carbon

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Zinc Acetate catalyst for Vinyl Acetate synthesis (VA) was prepared by the immobilization of Zinc Acetate from aqueous solutions on the surface of oxidized by HNO_3 (15% solution) activated carbon (AC). AGH-2 the characteristics of AC: S_{sp} - 690 m^2/g, pores volume: V_{mac}=1,425 cm^3/g, V_{mes}=0,065 cm^3/g, V_{mic}=0,27 cm^3/g, and total volume - 0,76 cm^3/g. Total concentration of acid groups in g - equivalent NaOH - 1,2.

Study of Zinc Acetate (ZnA) adsorption on oxidated and nonoxidated activated carbons in the conditions of intensive circulation of solution through support bed showed that ZnA adsorption rate on oxidized AC increases 2,5-3 times and the total ZnA amount increases 1,7 times . The catalyst surface on oxidized AC is approximately 100 m^2/g lower, while the amount of supported salt is the same.

When temperature of immobilization is changed in the interval of 0-80^{0}C (T_{max}=50^{0}C) initial adsorption rates and the amount of supported salt (in 1, 2, 3 hours) become sharply dependent upon it (Fig. 1) Catalyst activity in Vinyl Acetate synthesis passes through maximum values at 50^{0}C too. There`s observed an extreame change of S_{sp} at 20-80^{0}C (49 m^2 at 20^{0}C, 90 m^2 at 50^{0}C and 37 m^2 at 80^{0}C) as well.

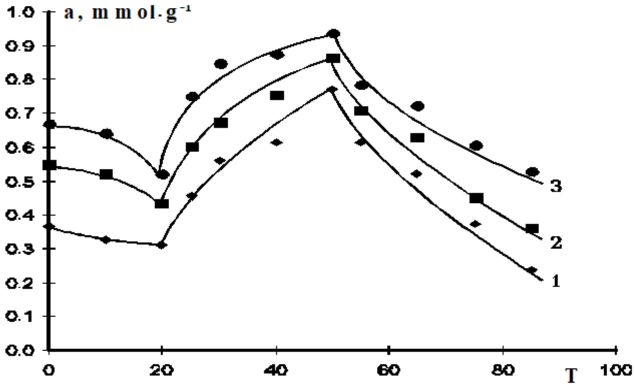

Fig. 1 Dependence sorption amount of zinc acetate sorbed on activated carbon treated with nitric acid vs. temperature T (°C). Sorption duration (min): (1) 60, (2) 120, and (3) 180.

In accardance with these dependences is evident that the process of ZnA immobilization is complex enclosing ZnA adsorption and ion exchange of different forms of Zinc salts (exsothermic and endothermic steps, changing of pH during adsorption) on oxidated AC surface. Dependence of S_{sp} and amount of adsorbed salt (a) upon initial salt concentration in the interval 3-33% (mass) looks unusual as well (Fig. 2).

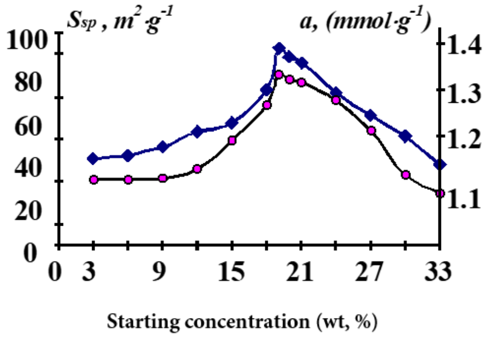

Fig. 2, Dependence of the catalyst characteristics $Zn(OAc)_2/C$ on starting salt concentration in aqueous solution.

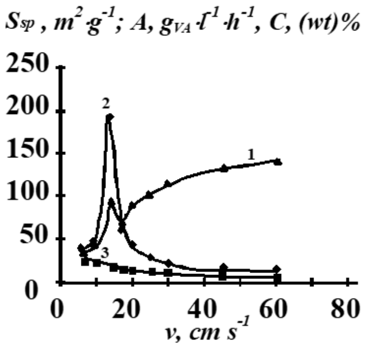

Fig. 3 Dependence of the catalysts characteristics from circulation flow velocity. (1)-Surface (S), (2)-Catalytic activity(A),(3) -amount of $Zn(OAc)_2$ in catalyst, (C).

Circulation rate of the solution in the interval V=7-60 cm/sec has a very noticiable influence upon catalyst. The maximum activity was reached at V=15-18 cm/sec (195 g. $l^{-1}.h^{-1}$ at 230^0C) (Fig. 3). Extremes are observed on the curve S_{sp}-V too. Circulation velocity influences distribution of pores volume on radiuses and the value of pores volumes.

Thus catalytic activity of ZnA on AC is determined by Zn concentration (C), S_{sp} value and the conditious T of immobilization, initial concentration and circulation rate) under which these values namely of S_{sp} and C, have been obtained.

Biography

Hoang Kim Bong - Professor, academician of Russian academy of science and IEA, head of Scientific-research center. He began his higher education in Kishinev State University. Since 1973 to 1985 Hoang Kim Bong read lectures and at the same time held the position of head of laboratory at Hanoi polytechnic university being as well superior technologist and designer of activated carbon production. In 1986-250 tons of these carbons were used in fighting fire at Chernobyl disaster. In 1991-1994 he developed a new technology of production new generation of carbon sorbents and catalysts with superior characteristics, and collaboration with Ukrainian scientist a new technology for production carbon hemosorbent was introduced. In 2002-2003; 2005-2010 he took part in the International Moldo-Ukrainian commission on quality control of carbon sorbent of medical destination. He has read lectures on at France. Turkey, Swiss, Byelorussia universities and the Academy of Ukraine. He has been scientific advisor for 9 PHD, 70 engineers, master and baccalaureates science degree holders. He has published 200 papers and scientific reports. Got 14 patents in Russia and abroad and edited 5 scientific manuals and a book of problems in physical chemistry (coauthor Pusniak A.N. in 1987, Kishinev). In 1998-2009 Hoang Kim Bong took part in International scientific conferences on catalysis and adsorption in USA, UK, Canada, Germany, Bulgaria, Poland, Switzerland, France, Italy, Spain, Belgium, Japan, South Korea, Thailand. Since 2002 he has held the position of head leader and reposition executor of the State scientific-engineering programs of Ministry of industry and technologies of Russian Federation Investigation and development of prior direction of civil destination and Innovative projects Echosorbent launched by Russian Fund of Technological Development. The work has been carried out aiming at ecologic security of Russian Federation. He was awarded gold medal at VI International exposition-congress High Technologies.

The importance of NOx and CO2 on grain and fish production, protection of global warming

Shoichiro Ozaki
The Institute of Physical and Chemical Research 2-1 Hirosawa, Japan

In order to study the reason why global warming is happening. Amounts of CO2 emission, CO2 concentration NOx emission, grain production, fish production , population and CO2 fix from 1900 to 2016 were studied.

Since the industrial revolution, burning of fossil and production of CO2 and NOx increased greatly. Increased CO2 and NOx promoted the CO2 assimilation . Production of grain and fish increased. About 360 billion tone CO2 is produced by burning of much fossil . About 14.4 billion tone NOx is produced in 2015. Most of emitted CO2 is fixed by CO2 assimilation. But since developed country started NOx elimination and NP elimination at around 1975 , half of produced NOx is eliminated. Therefore emitted 360 billion tone CO2 is not fixed completely. Concentration of CO2 increased about 2 ppm . In 2016, 142 billion tone CO2 is remaining to give global warming. 142 billion tone CO2 must be reduced. We must promote CO2 assimilation by complete use of emitting NOx and NP in wast water.

Fossil fuel is burning out soon. We should not spend precious fossil fuel for the elimination of NOx and NP. We must increase CO2 assimilation as much as possible.

Biography

Shoichiro Ozaki has served as the Professor at Ehime University, Department of Chemical Industry and as the Visiting Professor at various reputed universities of the world including University of Konstanz, New York State University and Shangdong University. He had also been a Research Chemist at the Institute of Physical and Chemical Research, Tokyo, Japan. Currently he is the Professor Emeritus at the Ehime University, Japan. He has been the Recipient of Hatsumeishou (Invention Prize) for the invention of Carmofur (antitumor agent), Gakujutsusho (Academic Prize) from the Japan Chemical Society for the synthesis of biologically active compounds (Carmofur, IP3) and Fulbright Award.

Beneficial effect of glycols on the activity of NiMoP/Al_2O_3 hydrotreating catalysts

E.N. Vlasova[1,2*], A. L. Nuzhdin[1], G.A. Bukhtiyarova[1,2], A.A. Porsin[1], I.P. Prosvirin[1], I.V. Deliy[1,2,] V.A. Volodin[2,3], E.Yu. Gerasimov[1,2], and V.I. Bukhtiyarov[1,2]
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The sulfided Co(Ni)Mo/Al_2O_3 catalysts are widely used in the refineries for hydrotreating process of petroleum distillates. To improve the catalytic activity of the sulfide catalysts in hydrodesulfurization (HDS) reaction different approaches are used. Addition of ethylene glycol (EG), diethylene glycol (DEG) or triethylene glycol (TEG), in particular, to aqueous impregnation solution of the active component precursors of the catalysts on preparation step allows synthesizing more active HDS catalysts. It was supposed that the presence of glycols prevents the interaction between supported active component and alumina, which contributes to the formation of an oxide precursor with a high ratio of Co(Ni)/Mo. In current work the effect of EG, DEG and TEG on the catalytic properties of phosphate-doped NiMo/Al_2O_3 catalysts in the hydrotreating of the straight-run gas oil (SRGO) was compared. The NiMo(P)/Al_2O_3 catalysts were prepared using ethylene glycol, diethylene glycol and triethylene glycol as additive. The organic agent was introduced into the aqueous impregnation solution obtained by the dissolving of MoO_3 in H_3PO_4 solution, followed by $Ni(OH)_2$ addition. The support was γ-Al_2O_3 in the form of granules with a trefoil-shaped cross section and a size of 1.2 mm (BET surface area 235 $m^2\ g^{-1}$, pore volume 0.79 $cm^3\ g^{-1}$, average pore diameter 13.4 nm). The Raman and UV–Vis studies show that the impregnation solution contains diphosphopentamolybdate $H_xP_2Mo_5O_{23}^{(6-x)-}$ and $Ni(H_2O)_6^{2+}$ and that these ions are not affected by the presence of glycols. When the impregnation solution comes into contact with the γ-Al_2O_3 surface $H_xP_2Mo_5O_{23}^{(6-x)-}$ is decomposed completely.

The catalysts were characterized by Raman spectroscopy, low-temperature N_2 adsorption, X-ray photoelectron spectroscopy and transmission electron microscopy. The catalysts contained approximately the same amount of Mo (13.1-13.4 wt.%) with the Ni/Mo molar ratios of 0.4. According to the XPS data Mo dispersion in the terms of Mo/Al ratio is increased after glycol addition in the following order: NiMoP/Al_2O_3 < NiMoP-TEG/Al_2O_3 < NiMoP-EG/Al_2O_3 < NiMoP-DEG/Al_2O_3. The catalytic properties of the NiMoP/Al_2O_3, NiMoP-EG/Al_2O_3, NiMoP-DEG/Al_2O_3 and NiMoP-TEG/Al_2O_3 catalysts were investigated in the hydrotreating of SRGO (from Urals crude oil) in a trickle-bed down-flow reactor at temperature of 330-340°C under hydrogen pressure of 3.5 MPa, H_2/feedstock ratio of 300 Nm^3/m^3 with liquid hourly space velocity of 2 h^{-1} after in-situ sulfidation procedure. The sulfur content in the feedstock and hydrogenated products was measured on a Lab-X 3500SCl energy dispersive X-ray fluorescence analyzer (Oxford Instruments) and on an ANTEK 9000NS analyzer (for products containing less than 100 ppm S). It is shown that the sulfide catalysts prepared with glycols display higher activity in the hydrotreating of SRGO than the NiMoP/Al_2O_3 catalyst prepared without the additive. The hydrodesulfurization and hydrodenitrogenation activities depend on the glycol type and are decreased in the following order: NiMoP-DEG/Al_2O_3 > NiMoP-EG/Al_2O_3 > NiMoP-TEG/Al_2O_3 > NiMoP/Al_2O_3. The higher activity of NiMoP-DEG/Al_2O_3 can be explained with the higher dispersion of molybdenum on the surface of the catalyst in the sulfided state.

The work was supported by the Ministry of Education and Science of the Russian Federation, project № 14.575.21.0128, unique identification number RFMEFI57517X0128.

Audience Take Away:

- Addition of glycols to impregnation solution allows creating more active NiMoP/Al_2O_3 catalyst in hydrodesulfurization and hydrodenitrogenation reactions due to the improved dispersion of Mo on the surface of sulfide catalysts;
- Both Mo dispersion in the terms of Mo/Al ratio and HDS and HDN activity of catalysts in SRGO hydrotreating are decreased in the following order: NiMoP-DEG/Al_2O_3 > NiMoP-EG/Al_2O_3 > NiMoP-TEG/Al_2O_3 > NiMoP/Al_2O_3;
- Preparation of NiMoP/Al_2O_3 catalyst using molybdenum (VI) trioxide and nickel (II) hydroxide as precursors of active phase is more environmentally friendly due to the absence of any emissions during heat treatment of the catalyst (for example, using of nickel (II) nitrate as precursor results in NO_2 emissions).

Biography

Dr. Evgeniya Vlasova studied Chemistry at the Novosibirsk State University, Novosibirsk, Russia and graduated as the Specialist in 2009. She then joined the research group of Dr. Bukhtiyarova G.A. at the Boreskov Institute of Catalysis, Siberian Branch of the Russian Academy of Sciences (SB RAS). She received her PhD degree in 2018 at the same institution. The main field of research is co-processing of petroleum distillates and vegetable oils over sulfide Co(Ni)Mo/Al_2O_3 catalysts.

Reactants-induced dynamic responses of the surface of heterogeneous catalysts monitored by microcalorimetry beyond adsorption

S. Wrabetz*, Th. Lunkenbein, P. Kube, V. Streibel, A. Knop-Gericke, A. Trunschke, R. Schlögl
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. of Inorganic Chemistry, Berlin, 14195, Germany

For a detailed understanding of complex reaction networks we need thermodynamic data of high accuracy and information about the nature of the catalyst surface during reaction. Therefore, we quantitatively study the adsorption, activation, and reaction phenomena close to the reaction parameters. Furthermore, we simulate reactants-induced responses of the surface via adsorption/desorption cycles in order to stepwise create an active surface, and thus can get new insights into the dynamic behaviour of the surface. Since perhaps only a minor fraction of all surface atoms form active sites, the quantification requires a very sensitive analytical method. We focus on microcalorimetry beyond adsorption. This is a direct method to determine the number, strengths and energy distribution of adsorption sites, as well as adsorption constants and the active surface area. To facilitate the correlation of microcalorimetric results with the catalytic performance, a molecule similar to the reactant is used. $T_{ads.}$ is chosen lower than $T_{react.}$ to try to separate the adsorption and activation process from the catalytic reactions.

In this work, we present i) i) CO chemisorption cycles on a Ni/MgAl oxide catalyst for dry reforming of methane (DRM) ii) propane and ethane adsorption/desorption cycles on a MoV oxide catalyst for oxidative dehydrogenation of alkanes and iii) CO chemisorption on Ir based catalysts for oxygen evolution reaction (OER)

We impressively show how experiment and theory can be in harmony. For example, apparent activation energy from kinetic experiment, differential heat of adsorption and amount of propane adsorption sites from microcalorimetry in combination with DFT calculations resolves different degrees of V_xO_y oligomerization. Furthermore, Ir-based catalysts are promising materials to electrocatalyze the oxygen evolution reaction in acidic media. To investigate the electronic structure of iridium metal, rutile-type IrO_2 and an amorphous IrOx, synchrotron-based X-ray photoemission and absorption spectroscopies were combined with theoretical calculations. Furthermore, we applied CO chemisorption experiments at 40°C using microcalorimetry under reaction conditions to identify surface differences between active amorphous IrOx and inactive crystalline IrO_2 materials. Only the active amorphous Ir oxide shows average differential heats of 125 $kJmol^{-1}$ due to the CO oxidation. The measured differential heats of reaction agree nicely with those calculated for the reaction enthalpies of CO(g) with electrophilic O^{I-} species.

Audience Take Away:

- Many of the reaction networks are extremely complex and hence are very difficult to dissolve.
- For a better understanding of the complex microkinetics we need quantitative data of high accuracy. Moreover, quantitative data provide a basis for theoretical modeling.
- It is very important to characterize the fresh and post reaction state of the catalysts in order to observe changes, and thus can get new insights into the dynamic behaviour of the surface.
- For the main task, to facilitate a structure reactivity relationship we have to combine the results from the catalytic test with qualitative/quantitative analytical data close to the used reaction parameters.
- The aim should be to obtain experimental and theoretical data to better understand the process. It also serves to validate data and improve the applied models.

Biography

S. Wrabetz was born in Berlin. After high school training as laboratory assistant, she studied process engineering and chemistry. At present, she is working in industry (oil filter recycling company). She received her PhD theses at Fritz Haber Institute of the Max Planck Society (FHI), Department of Inorganic Chemistry (Ruthenium-doped zeolites, Synthesis, Haber-Bosch-Process, Spectroscopy). Since 1999, she is Senior Scientist at FHI (Surface characterization of heterogeneous catalysts with microcalorimetry and spectroscopy, in situ and operando), administrative deputy to the Department Director.

Unraveling the controversy over the catalytic reaction mechanism using a new theoretical methodology: One probe and non-equilibrium green's function surface

Chi Ho Lee, Sang Uck Lee*
Department of Bionano Technology, Hanyang University, Ansan, Korea

We shed light on the longstanding controversial issues on the iodine reduction reaction (IRR) mechanism using a new proposed methodology called "One Probe and Non-Equilibrium Green's Function Surface (OPNS)". The OPNS approach completely alleviates the limitations of traditional slab approach for the electrocatalytic reactions by coupling the surface to an infinite reservoir of electrons at a fixed chemical potential and implements an external electric field environment through a semi-infinite one probe model. With aid of OPNS and in-depth structural analysis under the external electric field, we re-evaluated the previously proposed IRR mechanisms on the Pt(111) surface, consecutive and concerted mechanisms. Our results reveal that the configurational preference of approaching I_2 molecules depending on the external electric field governs the IRR mechanism. Under the reductive potential, I_2 molecules prefer vertical (I_2V) configuration rather than parallel (I_2P) configuration, which leads to the consecutive mechanism where the I atoms are sequentially reduced due to asymmetric charge accumulation on a single I atom to be initially desorbed. Consequently, we can clarify that the IRR follows the consecutive mechanism and we believe that this work can inspire the study of electrocatalytic reaction mechanisms for various catalysts.

Audience Take Away:

- This work clearly explains the controversial mechanism of Iodine reduction reaction.
- We propose new methodology which solves the limitations of current theoretical approach.
- In this work, we emphasize accurate modeling of surface structure for catalytic reaction study by combining semi-infinite electrode and surface structure, named by one-probe model.
- In addition, this work shows the external electric field dependency of catalytic reactions.

Biography

Dr. Sang Uck Lee studied Chemistry at the Hanyang University, Korea and graduated as MS in 2001. He then joined the computational research center of LG Chemical Company, from 2001 to 2012. In 2008, he received his PhD degree in computational materials science supervised by Dr. Yoshiyuki Kawazoe at the Tohoku University, Japan. In 2012, he obtained a position of Assistant Professor at the University of Ulsan, Korea, then he moved to the Hanyang University, Korea, as Associate Professor at 2014. He has published more than 70 research articles in SCI(E) journals.

Description of mass transport through an asymmetric, bio-catalytic membrane reactors

Endre Nagy*, **Imre Hegedüs**
Chemical and Biochemical Procedures Laboratory, Institute of Biomolecular and Chemical Engineering, University of Pannonia, Veszprem, Hungary

The substrate transport accompanied by biochemical reaction has some special transport and operational properties, which can strongly affect the reaction efficiency of a bio-catalytic process. The biocatalyst is mostly immobilized in a porous, relatively thick support layer in an asymmetric membrane. It is assumed that the biocatalysts, which can be native enzyme or pre-treated, e.g. it is bound to nanoparticle for increasing its stability, is uniformly and densely distributed in the membrane and the reaction can be considered as a pseudo-homogeneous process. Membrane can be flat-sheet or capillary one. In this latter case the transport through the membrane is occurring in changing space and depending on the inlet feed side, it may be on the lumen and shell, as it can strongly affect the substrate concentration distribution and consequently the biochemical reaction rate. Operation of the process maybe a so-called one-pass process or the feed solution can be recirculated. The kinetics of the transport or reaction is not basically affected by these operation modes. Both operation modes will be discussed in this presentation, assuming steady state or quasi steady state processes.

The differential substrate balance equation for this process should contain diffusion-, convection-, due to transmembrane pressure if it exists, and reaction terms. The first two terms can have constant or concentration/space coordinate dependent, namely diffusion coefficient, convective velocity, parameters. This description methodology can easily be extended for chemical reaction using e.g. inhomogeneous and/or intrinsically catalytic membranes. Main points of this presentation are as follows: i) presenting the inlet and the outlet mass transfer rates and concentration distribution by constant parameters (diffusion coefficient, convective velocity, reaction rate constant) using flat-sheet and capillary membrane with skin layer either on the shell or lumen; the reaction kinetics used is the general Michaelis-Menten kinetics, as well as first and zero-order reactions as its limiting cases; it is also discussed how the convective velocity and/or the place of inlet feed side can improve the reaction rate, and thus the reaction efficiency

ii) discussion of the effect of concentration dependent diffusion coefficient (linear or exponential dependency) as well as linear space coordinate dependency (increasing or decreasing one); a general approach solution of the differential balance equation will be shown [1], which can be used in case of the nonlinear Michaelis-Menten kinetics, or second order reactions, as well

iii) superior of the membrane reactor is demonstrated, as practical examples, by hydrolysis of oleuropein, and pectin, at which the reaction rate was measured in both the mixed tank reactor as well as by membrane bioreactor.

[1] E. Nagy, Basic equations of mass transport through a membrane layer, Elsevier, Amsterdam, 2019

Acknowledgments: In this The National Development Agency grant OTKA 116727 and GINOP-2.3.2-15-2016-00017 greatly acknowledged for the financial support.

Audience Take Away:

Predicting the efficiency of a membrane reactor or planning its scale up, the correct description of the mass transport is crucially important. This presentation will show:

- The mass transfer rate equations for cases, when the differential mass balance equations can analytically be solved;
- It will also be shown an approach solution in closed mathematical forms for nonlinear cases of the transport process, namely e.g. variable parameters and/or nonlinear reaction rate as e.g. for the Michaelis-Menten kinetics;
- It is also shown how the process efficiency can be increased by the convective flow or by the transport direction in a capillary membrane, in presence of biochemical/chemical reactions;
- Generally, this presentation gives general summary on the description of a bio-catalytic/catalytic membrane reactor and prediction of the process efficiency, which can then be useful in investigation, realization of both laboratory and industrial membrane catalytic processes.

Biography

Prof. E. Nagy studied Chemical Engineering at the University of Pannonia (previously Veszprem University), Hungary and graduated as MS in 1969. He joined in 1971 the Research Institute of Chemical and Process Engineering of Hungarian Academy of Sciences (today Research Institute of Biomolecular and Chemical Engineering at University of Pannonia). He received his PhD degree in 1973 on mass transfer processes. As postdoctoral fellowship and as frame of joint research project has spent more years in Germany and Austria ‘s universities. He became professor in 2000. She has published more than 242 research articles in SCI(E) journals and two books.

Efficient nano-regional photocatalytic heterostructure design via the manipulation of reaction site self-quenching effect

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Heterostructural photocatalysts with rationally aligned energy bands have been proved effective in diminishing the recombination of photo-induced excitons, thus leading to enhanced photocatalytic performance. Besides the enhanced photocatalytic performance with these heterostructures, most of these heterostructures observed a performance decrease when the amount of cocatalysts exceed a critical value. Although some researchers inferred that excessive nano-decorators would lead to an increased light penetration depth in the space charge layer or reaction site blocking in these heterostructures, these explanations are left unverified by experimental result, and the mechanism behind the concentration vanishment of photocatalytic performance is still in controversy. The critical role of charge carrier behaviors and their quenching pathway in determining the overall photocatalytic performance are still not fully explored, which severely hindered the development for efficient photocatalysts. As a result, there may be some omitted channels for the annihilation of photocatalytic performance in the nano-regional heterostructures, which should be further explored.

Herein, to further explore the essential principles of photocatalysis with heterostructures, a representative nano-regional photocatalytic heterostructure was constructed through uniform decoration of visible light activable BiOI nanodots on TiO_2 nanorod assembled microflowers. With which as a well-known prototype of conventional heterostructures, a possible photocatalytic performance annihilation channel via reaction site self-quenching effect in photocatalytic heterostructures was experimentally evidenced for the first time. Based on our experimental results, we evidenced that excessive decoration with BiOI nanodots would result in severe self-quenching of their photocatalytic sites through highly probable charge carrier recombination between migrating electrons along TiO_2 nanorods and reactive holes in adjacent BiOI nanodots. Such fundamental and experimental discovery is not limited to the current model and would shed light on the development of novel nano-regional heterostructures with high photocatalysis performance.

Audience Take Away:

- Reaction site self-quenching effect caused by excessive nano-decorators in photocatalytic heterostructures is discovered and proved by photoluminescent decay curve.
- Ultra-small BiOI nanodots (<3 nm) were synthesized via a reactant prefixing strategy, which could be used in other nano-material synthesis with uniform sizes.
- The p-n junction composed of BiOI mediated TiO_2 heterostructure can significantly enhance the photocatalytic performance.
- It is expected that this work could offer guidance for the rational design of high-performance functional heterostructures in the field of photocatalysis or even photovoltaics field.

Biography

Ms Feng Han studied Environmental engineering at the Nankai University and graduated as BS in 2011 and MS in 2014. She joined the Nanyang Environmental and Water Research Institute in Nanyang Technological University under Interdisciplinary Graduate Programme as a Ph.D candidate in 2016. She now is a fourth year Ph.D student and her research interest is photoelectrochemical methods for organic wastewater treatment.

Ru/TiO_2 CO_2 methanation catalysts: The decisive role of support crystallinity and stability

Capucine Sassoye[1*], Ara Kim[1], Damien Debecker[2], Clément Sanchez[1]
[1]Sorbonne Université, CNRS, Collège de France, Laboratoire de Chimie de la Matière Condensée de Paris, France,
[2]Institute of Condensed Matter and Nanoscience - Molecules, Solids and Reactivity, (IMCN/MOST), Université catholique de Louvain

Effective catalysts that could assess multiple environmental issues are nowadays needed, in a context of growing societal awareness and newly appeared environmental legislations. Challenges for these catalysts are numerous: Their production has to be as green as possible, fast and easy to handle; their use conditions have to be mild without compromising the requirements for high selectivity and high activity; they have to be nearly indefinitely reusable. These drastic requisites have oriented research toward soft preparation methods leading to nanostructured heterogeneous catalysts in which very active species are designed at the nanoscale.

Our work aims at developing innovative nanostructured ruthenium based catalysts with, as chosen fields of investigation, the methanation of CO_2. Ru/TiO_2 catalyst is widely recognized as one of the most attractive formulation, allowing to obtain ~100% selectivity to methane when operating under mild reaction conditions (e.g. at atmospheric pressure and ~200 °C or lower).

Pre-synthesized, monodispersed 2 nm-RuO_2 nanoparticles were used to serve as precursors, deposited on TiO_2 supports annealed in air and then reduced with hydrogen. Such catalysts demonstrated superior catalytic performance in CO_2 methanation to that prepared by Incipient Impregnation (IM) method.

Pure TiO_2 supports with different crystallinity (anatase and rutile) were either prepared in the laboratory (calibrated, specific shape nanoparticles) or obtained from commercial providers (more dispersed in size, ill-defined), mixed, and used as supports in different ratios.

Our studies show the presence of a clear structure-process-performance relationship: the crystal structure of TiO_2 support, as well as its ability to sinter dictate the morphology and dispersion of Ru species, thereby the catalytic performance in CO_2 methanation. Indeed, this is the strong interaction between the RuO_2 nanoparticles and rutile TiO_2 phase that stabilize the system through epitaxial lattice matching during annealing step. Moreover, supported RuO_2 nanoparticles have clearly showed the ability to migrate (from anatase to rutile) over the support surface upon thermic treatment. This migration phenomena is thoughtfully documented with in situ TEM.

This epitaxially-driven migration provokes decisive modifications in the catalyst and can be further exploited to tune the catalyst active phase morphology, localization and thus activity.

Audience Take Away:

- Catalysts prepared from pre-synthesized, monodispersed 2 nm-RuO_2 nanoparticles are more efficient than using the IM method
- In supported catalysis, although the primary role of the support is often thought to be limited to physical dispersant for intact metal active nanoparticles, it is now recognized that the metal-support interactions clearly influence the catalytic activities and/or selectivity.
- State of the art in situ TEM to understand the RuO_2 migration process
- The understanding of the stabilization and migration process allows to further tune more efficient catalysts.

Biography

Capucine Sassoye received her PhD degree in 2001 at the University of Versailles Saint Quentin (UVSQ, France) in 2001. After postdoctoral fellowships at Notre Dame University (USA) and the University of California Los Angeles (UCLA, USA), she is currently assistant professor at Sorbonne Université (France). Her research deals with inorganic nanomaterials, coupling the sol-gel chemistry with advanced process to tune both macroscopic shape and texture, with sustainability in mind, concerning both material synthesis and its further applications. She is particularly interested in relationship between the atomic structure and properties and has recently developed PDF analysis in her laboratory. She has so far authored/co-authored 32 peer-reviewed journal articles.

The most eco-friendly precious metal mining & e-waste processing in the world
- A case study of Green Chemistry, and a better altenative for 2020 Tokyo Olympics medals from e-Waste

Gordon Yu
Managing Director, Taiwan Hsinchu Green Industry Association, Hsinchu, Taiwan

E-waste is now the fastest-growing waste stream in the world. It is estimated this waste stream reached 48.5 million tons in 2018. This figure is expected to almost triple if nothing changes. Yet e-waste is worth at least US$62.5 billion annually, which is more than the GDP of most countries; according to a recent report at Davos 2019 WEF "A New Circular Vision for Electronics: Time for a Global Reboot" by PACE & WEF in support of the UN E-waste Coalition.

Traditionally labor-intensive manual dismantling of e-waste achieves higher liberation rates without breaking the original form of components and materials, which is easier to sort and improves re-usability, and the economically attractive precious metals (PMs) such as gold content recovery can be higher than automatic mechanical method due to better dismantling depth caused by higher separation efficiency; such informal e-waste processing are prevailing in developing countries, yet rudimentary recycling techniques to burn the plastic from electronic goods leaving the valuable metals (melting down lead in open pots, or dissolving circuit boards in acid) lead to workers exposed to many toxic substances, groundwater contaminated, air and soil polluted. The low gold leaching rate further weakened the incentive of such low performing informal e-waste processing.

So far the only lower environmental impact with higher PMs recovery rate alternative mainly implemented in developed countries by using automatic mechanical size reduction based integrated smelter-refinery, which requires substantial investment capital (Umico >500 million Euros) and sufficient economic scale (a typical aluminium smelter in Europe requires a minimum input of 50,000 tons of aluminum scrap per year to run a plant); there are only a few companies in the world equipped with sophisticated capabilities to fulfill the technical and environmental requirements. UWIN, an eco-friendly & innovative e-waste processing technology combines the advantages of both and even beyond; low-cost operation & high separation efficiency and dismantling depth comparable with those informal sectors from developing countries, yet solving the environmental problems and workers safety & health issues without using Cyanide or Mercury & without the need of burning while semi-automatically retrieve electronic components and keep the high re-usability by using eco-friendly leachant to remove lead/tin at room temperature initially, and the subsequent hydrometallurgical process to leach gold or PMs are also without using Cyanide or Mercury, yet the leaching rate are 4 times faster than Cyanide and gold leaching yield comparable with those integrated smelter-refinery, without the need of expensive Dioxin and Cyanide pollution control equipments.

The revolutionary UWIN e-waste processing technology provide the Best-of-2-Worlds (Bo2W) solution for both developing countries & developed industrial nations (for example, a better way for 2020 Olympic medals in Tokyo from e-waste) towards more eco-friendly way extending the life of electronic products/components, as well as its ability to be recycled and reused, a systematic e-waste optimum treatment solutions in environmental, economic and social performance comply with the new circular economy direction envisioned by UN E-waste Coalition.

Audience Take Away:

- E-waste problems world-wide, opportunities and trends
- E-waste treatment in developing countries, its advantages & disadvantages
- E-waste treatment in developed industrial nations (such as Japan), its advantages & disadvantages
- A new eco-friendly E-waste processing technology UWIN, combines the best of the above two
- Business and research collaboration opportunities expanding UWIN technology world-wide

Biography

Mr. Gordon Yu received BS in Control Engineering 1979 at National Chiao Tung University in Hsinchu, Taiwan, and MS in Electrical Engineering 1985 at University of Texas in Arlington, Texas, USA. After working several years in Semiconductor industries for UMC, Taiwan, SGS Semiconductor, Singapore, ST Microelectronics at Carrollton, Texas, AMD at Austin, Texas and LSI Logic at Milpitas, California, Mr. Yu has founded (or co-founded) a few electronics and environmental companies including C-ONE Technology, then merged by M-systems, and then merged by SanDisk (merged by Western Digital now), the largest solid state storage company in the world; Pretec Corp., then merged by Premier (merged by Foxconn now), the largest digital camera manufacturer in the world. Holder of more than 150 patents in Taiwan, China, USA and EU, Mr. Yu is currently the Chief Strategy Officer at UWin, Managing Director & CSO at EVP, Chairman & CEO at eTouch Innovation Co. Ltd., and Managing Director at Taiwan Hsinchu Green Industry Association.

$Cu_xCe_{1-x}O_2$ nanoflake type catalysts with improved catalytic activity and good thermal stability for diesel soot combustion

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In the present study, nanoflakes (NF) of CeO_2-NF and $Cu_xCe_{1-x}O_2$-NF (x = 0.1, 0.2, 0.3 and 0.4) were prepared with the polyvinylpyrrolidone(PVP)-assisted co-precipitation method. The prepared samples were first characterized with FE-SEM, HR-TEM, XRD, N_2 adsorption, O_2-TPD, H_2-TPR, Raman and XPS. Then, their catalytic performance and thermal stability were examined for the applications in soot combustion. It was found that $Cu_xCe_{1-x}O_2$-NF exhibited much better activity in tight contact mode than CeO_2-NF that has no Cu doping. Furthermore, the highest activity was observed for the sample of $Cu_{0.2}Ce_{0.8}O_2$-NF, which was most likely due to its moderate doping that induced both a large amount of surface adsorbed oxygen species and a special flake morphology, thus providing effective contact area. However, in NO_x-assisted loose contact mode, the catalysts exhibited relatively lower activity with a T_{50} higher than that of tight contact mode due to the reduced solid-solid contact points. Finally, both the cyclic and accelerated aging tests demonstrated that $Cu_{0.2}Ce_{0.8}O_2$-NF was able to keep a good thermal stability.

Audience Take Away:

- Nanoflakes of CeO_2-NF and $Cu_{0.2}Ce_{0.8}O_2$-NF were synthesized with the PVP-assisted co-precipitation method
- Doping of Cu in CeO_2-NF significantly promoted the formation of oxygen species that replenished the vacancies
- $Cu_{0.2}Ce_{0.8}O_2$-NF exhibited superior catalytic performance in soot oxidation with a T_{50} as low as 312 °C for tight contact mode and 360 °C for loose contact mode
- $Cu_{0.2}Ce_{0.8}O_2$-NF kept good catalytic activity and thermal stability after five cycles or the accelerated aging tests

Biography

Dr. Liu studied Chemical Engineering at Dalian University of Technology, China, graduated with BS and MS degree in 1985 and 1988 respectively. He then joined the College of Chemical Engineering at East China University of Science of Technology as an Assistant Professor and worked for six years before going to US for pursuing advanced study. He received his PhD degree in 1998 from Oklahoma State University, and then worked in industries (in US companies like Chevron) for more than 12 years before returned to China and became a Professor at Xiamen University in 2010. Dr. Liu's research areas include Biomass & Bioenergy, Hydrogen Production & Fuel Cells, and Environmental Catalysis. He has published more than 60 research papers, and holds 10 US patents and more than 20 Chinese Patents.

Study of performance for various catalysts for the oxidation of carbon monoxide reaction

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The single pellet studies for two different catalytic converters were simulated using MATLAB and the effects of perturbation of various parameters was carried out to increase the performance of the converter. The effect of various parameters of the converter system such as flow rate of incoming gas, the composition of inlet gas stream, density of pellet and dispersion on the performance of the system was done considering the oxidation of carbon monoxide by solving the coupled partial differential equations resulting from mass and energy balances by reducing the system of equations to a set of ordinary differential equations using the Galerkin method. The results indicate that platinum is far better catalyst compared to Copper Oxide. Based on these studies some heuristics are suggested to increase the efficient of the converter

Audience Take Away:

- Helps in use of a technique for predicting the performance of a converter
- Helps in identifying the heuristics for increase the efficiency of a converter
- Helps in Solving PDEs by reducing them to ODEs

Biography

Dr. P. S. T. Sai is a Professor in Department of Chemical Engineering at the Indian Institute of Technology Madras. He has been actively involved in teaching and research for the past 30 years. His research interests include fluidization, reaction engineering and air pollution control. He has published over 90 research papers. His paper entitled 'Esterification of ethanol with sulfuric acid: A kinetic study' was awarded as the best paper published in the 12-month period in The Canadian Journal of Chemical Engineering in 2001. He is also recipient of Chemical Weekly Award, IIChE NRC award and Kuloor Memorial Award in 2012.

Fabrication of new types, environmentally-safe fire-protective covers based on fire-extinguishing powders of raw materials

Lali Gurchumelia[1*], **Murman Tsarakhov**[1], **Salome Tkemaladze**[2], **Feliks Bejanov**[3], **Lasha Tkemaladze**[3]
[1]TSU Rafael Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
[2]Ivane Javakhishvili Tbilisi State University, Georgia
[3]G. Tsulukidze Mining Institute, Georgia

The aim of the presented investigation is the fabrication of new types, environmentally-safe fire-protective covers on the basis of halogen-free, highly efficient composite fire-extinguishing powders of local mineral raw materials. The technology for production of these materials differs from the conventional production. It is imply and is not associated with significant economic costs, which is reflected in the low cost price of materials. Fire-protective covers we made only by mechanical mixing of binders - Polyurethane resins and fillers - High-dispersed fire-extinguishing powders of our preparation, does not need addition of expensive, phosphorous and halogen-containing flame retardants. Such fire-extinguishing powders are manufactured by mechanical treatment and blending of local mineral raw materials, which does not require modification with expensive, halogen containing, organic hydrofobizing additives, what makes the extinguishing powders far cheaper than imported analogues. Here it should be noted, that obtained fire-extinguishing powders similarly of efficient flame retardants, are characterized by high inhibition properties and fire-extinguishing ability. Therefore, such powders we used as fillers, which in composite fire-protective materials are functioning, in itself, as efficient inert flame retardants. Mentioned fillers, similarly to serial inert flame retardants, don't participate in the process of polymer preparation and in contrast to them are characterized by high performance properties.

Experimental data confirm that the developed fire-protective covers by fire-resistance are qualified as hardly combustible materials and their performance properties are not worse than performance properties of the standard protective materials of common production.

Thus, such fire-protective materials are environmentally-safe, very effective and far cheaper than imported analogues. Therefore they are fulfilling completely requirements posed by normative documentation to the materials used in building processes.

Biography

Lali Gurchumelia, Chemist, Doctor of Technical Sciences. I work TSU Rafael Agladze Institute of Inorganic Chemistry and Electrochemistry (Georgia). Scope of scientific interests: chemical science, chemical engineering, ecological engineering, ecological biotechnology. I have 55 publications, including in the Infactactatorial Journal -12. The last 10 years I have participated in 5 scientific grant. Currently I am a manager of the grant # 216770 - " New type fire-extinguishing powders and foam-suspensions based on local mineral raw materials" funded of the National Science Foundation. I participated in many international conferences and congresses: Nürnberg, Germany; Toledo, Spain; New Forest, UK; Montreal, Canada; Istanbul, Turkey; Elenite Holiday Village, Bulgaria; Rome, Italy; Paris, France; Yerevan-Vanadzor; Tbilisi, Georgia and Ureki, Georgia. I have many years of experience in the study and evaluation of fire–extinguisghing and fire- protective materials.

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DAY 1

VIDEO PRESENTATION

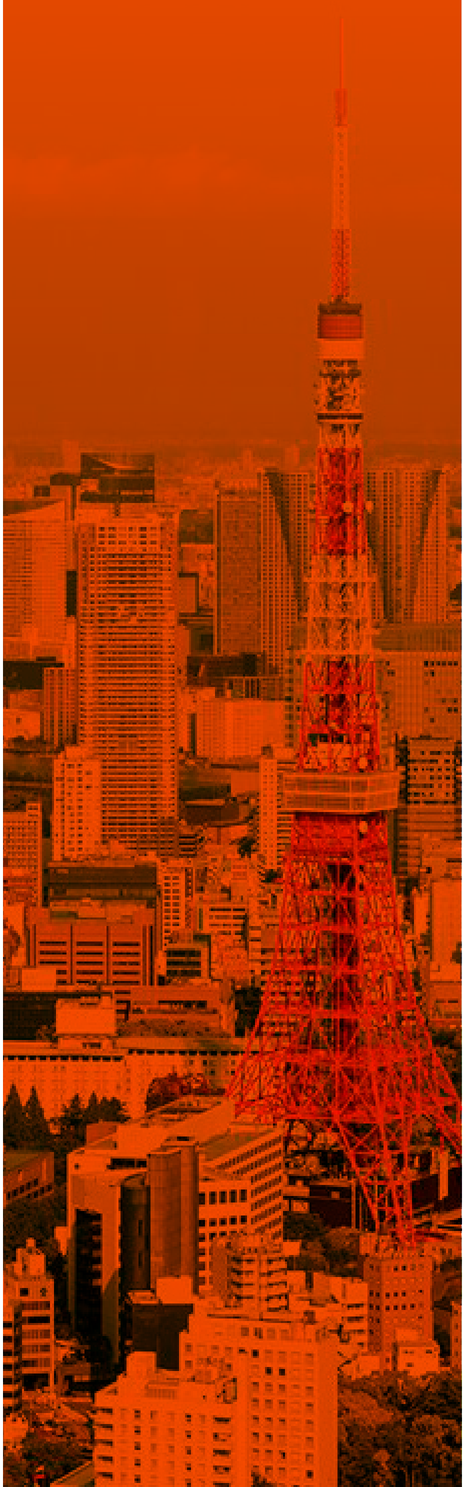
4th Edition of

INTERNATIONAL CONFERENCE ON

CATALYSIS AND GREEN CHEMISTRY

MAY
13-14, 2019

TOKYO, JAPAN



ICG 2019

Biography

Dr. Nicolas Abatzoglou is Professor and ex-Head of the Department of Chemical & Biotechnological Engineering of the Université de Sherbrooke. He is specialist in Process Engineering involving particles and Director of GRTP-C&P (Group of Research on Technologies and Processes in the Chemical & Pharmaceutical Industry). He is a Fellow of the Canadian Academy of Engineering. He is holder of the Pfizer Chair. He is co-founder of the company Enerkem Technologies, precursor of Enerkem, a spin-off in the field of energy from renewable resources. His scientific production includes 100+ publications, reviews, conferences, keynotes, plenaries, invited lectures, patents and three book chapters.

A new catalyst for the conversion of aromatics to HC and CO-rich gas

Professor Nicolas Abatzoglou

Department of Chemical & Biotechnological Engineering, Université de Sherbrooke, Sherbrooke, QC, Canada

A novel autothermic pyrolysis process followed by a hybrid mobile-fluidized bed catalytic reactor is used to produce carbon nanofilaments (CNF) from waste plastic streams.

The autothermic pyrolysis unit produces a gaseous stream rich in aromatic compounds which are precursors of polymeric carbon rather than the targeted CNF. The catalytic production of CNF is favoured by the presence of CO and unsaturated light hydrocarbons (HC), such as ethylene.

The main target of this work is the formulation and testing of a new catalyst able to reform toluene, an aromatic compounds surrogate molecule, in a way to maximize its conversion into CO and light unsaturated HC.

The new catalyst is made of olivine functionalized with alumina and nickel. The catalyst was prepared by the incipient wetness method through mixing olivine with nickel and aluminium nitrates, then drying and calcining the mixture for 8 hours at 900°C.

The reforming experiments are conducted in a fixed bed reactor. Toluene and water were emulsified with H2O/C ratio equal to one then injected into the reactor.

Preliminary tests, performed at 750° C with two catalytic formulations show that the Ni content is an important parameter. Thus, the toluene conversion was 93% for the 5% Ni catalyst while a 36% conversion was reached with the 1% Ni formulation.

Outlet gases from the reactor were analysed by GC. It was found that the main products were H2 and CO, with 55% and 30% yields, respectively. The formulation containing lower Ni gave a gas product containing more unsaturated HC. The reaction optimization is underway and detailed results along with full mass balances will be presented during the conference.

The catalyst is analysed before and after the experiment through X-ray diffraction, BET, and FEG/SEM microscopy. These analyses provide useful information concerning the crystalline phases present in the catalyst, the specific area changes as well as the changes of the catalyst morphology.

Audience Take Away:

- This presentation will provide the audience with the following information:
  - A novel autothermic pyrolysis reactor configuration.
  - A way to convert residual (non-recyclable) plastics into a homogeneous gas stream having a high potential as (a) feedstock for the production of high value CNF and (b) a renewable fuel.

  - A new catalyst able to convert aromatic-rich streams coming from pyrolysis or gasification into a HC+CO-rich product with high potential for the production of CNF.
  - A general overview of the technology used for the production of CNF using all of the above.
- The presentation will be done under the form of an educational seminar useful for chemical engineers in this area.
- This work can give to research-oriented faculty the opportunity to learn about the ongoing activities and enrich their literature review and eventual funding endeavors.
- This work is funded by both Quebec and Canada government as well as by two private companies. Their motivation rises from the possibility to invent a new technology capable to convert a negative value stream to a high plus-value commercial product.
- A new catalytic formulation and its testing will be presented. Moreover, the design component of the overall endeavor is an important component of the work.

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DAY 2

KEYNOTE FORUM

4th Edition of

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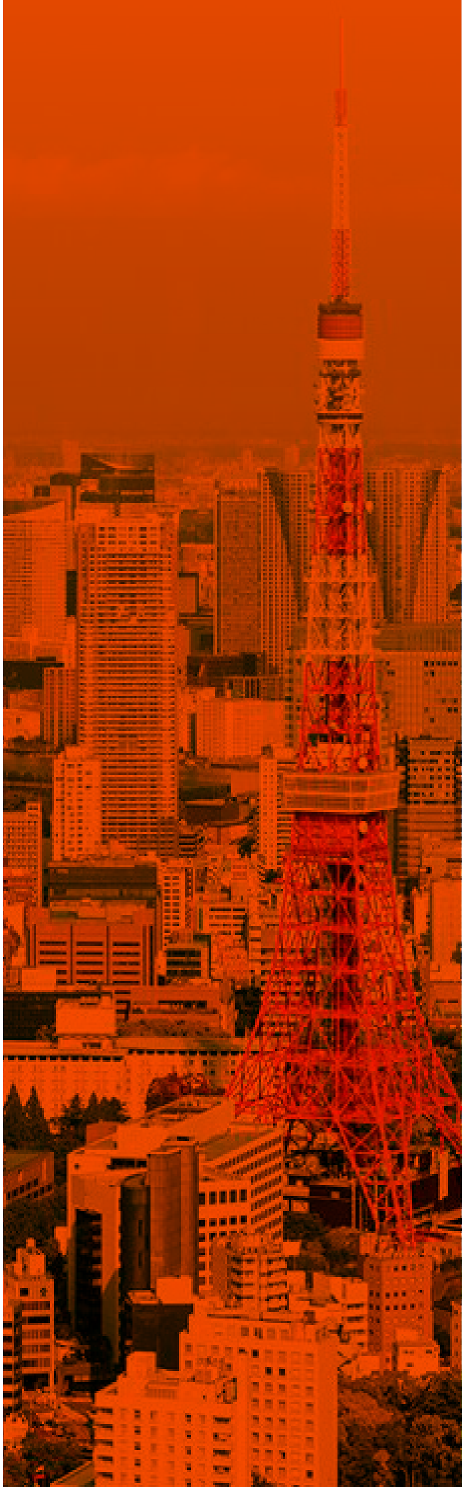

Biography

Prof. Dr. Leszek Moscicki studied Agricultural Engineering at Lublin Agricultural University, Poland and graduated as MS in 1973, than started his scientific carrier there. He received his PhD degree in 1977 and habilitation in 1983 at the same institution. After postdoctoral fellowship and number of practical works in laboratories of Food Process Eng. Dept. at the Wageningen University and Groningen University of Life Sciences, the Netherlands, since 1994 he obtained the position of an Professor – Head of Food Process Engineering. Dept. at Lublin University of Life Science, Poland. He has published more than 150 research articles in SCI journals.

Green chemistry in processing of degradable and recycled polymers

Prof. Dr. Leszek Moscicki

Department of Thermal Technique and Food Process Engineering,
Lublin University of Life Sciences, Lublin, Poland

The global polymer and plastic material production increased substantially in the last decade reaching in 2016 the staggering amount of about 500 million metric tons. China is the largest producers with around 25% of the global production and 20% by NASFTA countries (USA, Canada, and Mexico). In Europe, there are 60,000 plastics factories, with direct employment of 1.45 million people. Today, an average person in developed countries consumes over 100 kg of plastic each year (packaging materials and household items).

The Green chemistry of polymers with degradable products and bio-based plastics are considered in the right direction for sustainability in the polymer field. PolyLactic Acid (PLA - globally marketed in 2003) has been implemented into a commodity plastic and nowadays is produced in a large amount. Its applications included packaging, durable plastics, and fibers. There are promising market segments for biodegradable polymers: plastic bags for household bio waste, barriers for sanitary products and diapers, planting cups, disposable cups and plates as well as foamed fillers. Commercial markets for biodegradable polymers are expected to increase substantially in the coming years. Its low toxicity along with its environmentally benign characteristics has made an interesting material for food packaging and for other consumer products. Let me show a most spectacle samples of the development in this field. In 2015, the world's largest beverage company Coca-Cola Co showed off its new recyclable 100% bio-based bottles at the Expo Milano. The new recyclable PlantBottleTM was the first plastic to be made 100% from sugar cane in Brazil. The consortium of BASF, Cargill, and Novozymes has selected a method to make biobased acrylic acid for superabsorbent polymers. In 2014 Invista introduced a new version of its Lycra brand spandex that it touts as being 70% from dextrose derived from corn. BASF developed a compostable polyester film that called Ecoflex® and Ecovio® - fully biodegradable product based on cassava starch and calcium carbonate. In the paper, many practical aspects as well as prospects for the further development of biopolymers application in the production of biodegradable packaging are discussed.

One of the particular example can be production of foamed packaging materials, commonly used during transportation of various types of products. Plastics origin they are a source of difficult to handle waste. Many inventors are convinced that the substitution of polymeric porous materials with starch-based products encounters difficulties due to limited moisture resistance and poor mechanical properties. Basically they are right but using of PLA or the blands with LDPE polymers together with natural substances as plant fibbers can improve the properties of the final product. The lack of industrial solutions in this area encouraged us to undertake the experimental program aimed at obtaining fully biodegradable foamed fillers, useful in the packaging. Presented in the paper results, along with some conclusive remarks have to be taken as a concrete example of Green Chemistry practical applications in processing of degradable and recycled polymers.

Audience Take Away:

- Short review of state of art in biopolimers application in production of packaging materials.
- Future trends in that field
- Practical research results of the processing of starchy foamed fillers and provide new information to assist in a design problem.

Biography

Professor Victor M. Kogan graduated from Oil and Gas University in 1975 as a chemical engineer, specialty – radiation chemistry. Since 1979 he has been a researcher at the Institute of Organic Chemistry of the Russian Academy of sciences. From 2009 he heads the Institute Laboratory of Catalysis by Transition Metals and their Compounds. Some fundamentals in the field of catalysis by transition metal sulfides has been obtained and commercially used. His research interests include mechanisms of catalytic reactions, such as olefin and ring olefin metathesis; thiophene hydrodesulfurization, Fischer-Tropsch and alcohol over transition metal compounds.

Interlayer dynamics of the active sites of transition metal sulfide-based catalysts and the mechanisms of hydrodesulfurization of oil fractions and synthesis gas conversion into higher alcohols and other oxygenates

Professor Victor Kogan

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Recently suggested concept on the dynamic nature of active sites (AS) of the catalysts (Dynamic Model - DM) based on transition metal sulphides bases a hypothesis, that AS formed and functioning under the reaction conditions can oscillate between layers of promoted molybdenum sulphide. The DM assumes the existence of the AC of different types and the possibility of their mutual transformation due to the reversible migration of sulphur and promoter between the crystallite layers in a hydrogen atmosphere. The DM explains a series of “structure – property” correlations. The results suggest that the catalytic activity in hydrodesulphurization (HDS) and hydrogenation (HYD) reactions depends on the shape of crystallites of the active phase. Alkali-modified CoMoS is a promising catalytic system both for hydrotreating of FCC gasoline and synthesis of higher alcohols from synthesis gas. According to quantum chemical calculations potassium donates electronic density onto the Co atoms of CoMoS phase AS. Reduction of metal atoms of the AS leads to a decrease in Lewis acidity and in the CO and H2 adsorption energy as well as promoting the oxidative addition of H2. The influence of ethanol addition to synthesis gas on its conversion and the product composition results in sharp increase of CO conversion in the presence of ethanol. A reaction network of CO conversion on the KCoMoS catalyst active sites depending on the catalyst composition and reaction conditions was suggested. The proposed model makes it possible to develop criteria for the evaluation of the efficiency of catalytic performance for HDS of oil crudes of various types, for syngas conversion with formation of higher alcohols and their followed conversion into wide range of oxygenates.

DAY 2

SPEAKERS

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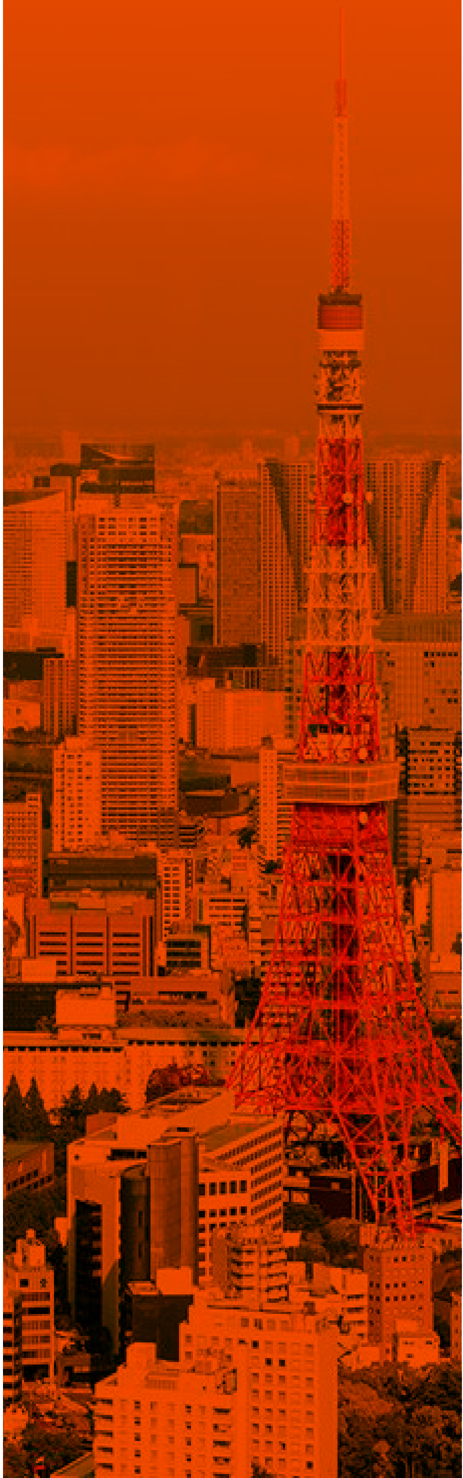

Adding value to biomass through catalytic transformation

Tuulamari Helaja*, Matti Reinikainen

VTT Technical Research Centre of Finland Ltd, Espoo, Finland

Chemistry has been the driving force behind progress for centuries - resulting in our lives becoming easier, more comfortable and healthier. These improvements however came at an environmental cost, which is associated with the way we have been using our resources and sourcing our energy. A global shift towards sustainable ways of doing chemistry is necessary to make sure that we continue to meet the needs of our society for chemicals and products, without jeopardizing those needs for future generations.

This transformation requires constant innovation and new technologies, but also support of all stakeholders - from academy, industry, policy-makers and society.

VTT Technical Centre of Finland actively participates in all areas of sustainable development - with special emphasis on climate action and sustainability. We recognize the value that sustainable chemical technologies provide and we actively pursue the development of new bio-based monomers, bio-oils and biofuels, biochemicals, evaluating waste streams as new raw materials sources, carbon capture and reuse, wood-based high value products, bio-based packaging or innovations such as thermoplastic cellulose. In many of our processes and research, catalysis is the key enabler for technologies - making the process commercially viable - reducing costs, increasing energy efficiency and product selectivity. The presentation will highlight VTT's expertise and catalytic technologies related to biomass, waste and CO_2 conversion to added-value chemicals - including liquid hydrocarbons, waxes and aromatics.

Audience Take Away:

- Overview of VTT and research activities related to sustainable chemical technologies
- Biomass gasification strategies and Fischer-Tropsch synthesis
- VTT's development of Bio-BTX and other added-value chemicals
- VTT's multipurpose Mobile Synthesis Unit

Biography

Tuulamari Helaja graduated with a Ph.D. in Chemistry from the University of Helsinki in 2000. Following a post-doctoral fellowship at the University of Münster in 2000-2001, she joined Borealis Polymers to work with olefin polymerization catalyst technologies. In 2006, she obtained an eMBA from Aalto University and joined VTT, where she has held various positions. Since 2016 she has been the Vice President for the Sustainable Energy and Chemical Technologies research area covering thermochemical conversions and chemical process technologies incl. scale-up, industrial synthesis and catalysis, polymer and plastic processing, metals and materials recovery, and computational chemistry incl. process concepts and models.

Development of Pt catalysts using graphene supports for polymer electrolyte fuel cells

Jian Xie
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Two of the major challenges for development of polymer electrolyte membrane fuel cell (PEMFC) systems, especially for automotive applications, are cost and durability of the precious metal group (PGM) based cathode electrocatalysts. We have been addressed these issues by improving the catalyst performance and durability using graphene as the supports. The dispersion of Pt nanoparticles on surface of the graphene sheets were improved, the performance and the corrosion resistance of graphene supports were enhanced. In addition, the interaction of Pt nanoparticle with the graphene support is investigated using the XPS to determine the strength of the Pt-C interaction, which will provide the mean to improve the Pt catalyst stability and durability by mitigating the Pt nanoparticle surface migration. Development of high performance and durability membrane electrode assembly (MEA) using the Pt/Graphene catalyst will also be discussed focusing our bottom up approach—from catalyst ink to the structure of the solid catalyst layer in MEA. We have developed a methodology to study the catalyst powder and Nafion ionomer dispersion in the catalyst ink using small angle x-ray scattering (USAXS) combined with cryogenic TEM. The effect of Nafion ionomeer binder on the structure of the catalyst layer in an MEA was studied using Hg porosimetry, TEM, SEM and its fuel cell performance was characterized. The property-structure-performance relationship was established.

Audience Take Away:

- The audience can learn the basics of graphenes and their applications in electrocatlysis process. In addition, they can learn how to use the graphenes and graphene based materials in the electrocatalysis for oxygen reduction reaction in the proton exchange membrane fuel cells as well as in other catalysis processes in which a highly stable and electric conductive catalyst support is needed. The audience will also learn how to use the graphenes in the catalysis and energy conversion applications.
- Graphenes are newly developed materials, which have many unique properties such as extremely high conductivity, chemical stability and mechanical strength. Appearance of the graphenes opens a new avenue for many fields, which could lead for breakthroughs in many applications such as display, flexible electronics, batteries, fuel cells, semiconductors, composite materials, etc. Grephenes can help to solve many practical problems by providing high electric conductivity and chemical stability. For examples, graphenes can be used in batteries, fuel cells, conducting materials, super-conducting, composites to improve or alter their properties.

Biography

Dr. Xie is a professor of Mechanical and Energy Engineering at the Purdue School of Engineering and Technology, IUPUI. He has published more than 55 journal papers and 2 book chapters, has 11 patent applications (6 issued), and has been awarded more than $5.86 million in research grants over 10 years. He has served as a reviewer for more than 12 journals including Nature and Science. He serves as a panelist reviewer for the US National Science Foundation, the Advanced Research Project Agency-Energy, Fuel Cell Technology Office, the Office of Technology Transfer of the US Department of Energy,, and the Canadian National Science Foundation. He received his PhD in chemistry from Miami University, and a BS in chemical engineering (emphasis on electrochemical engineering) from Tianjin University, China.

Modelling thermokinetics using the sestak-berggren equation: A calcium carbonate case study

Rebecca Gibson[1,2*], Prof Mark Simmons[2], Prof Athanasios Tsolakis[3], Prof Hugh Stitt[2], Dr John West[1], Robert Gallen[1]
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During the production of catalysts there are many energy-intensive thermal processing steps, and these can be critical to both the performance of the final product and the economics of the manufacturing process. To design efficient, specialised calcination and drying processes for new catalyst products, kinetic information must be extracted from thermal analysis data.

This presentation will discuss the methodology developed to extract kinetic parameters from thermal analysis data using the Sestak-Berggren equation, specifically the decomposition of calcium carbonate studied through thermogravimetric analysis. The thermal decomposition of calcium carbonate has been selected as a case study, as calcium carbonate is an industrially relevant mineral and the product calcium oxide can be used as a carbon dioxide capture material.

The Sestak-Berggren equation is a mathematical model which describes the behaviour of solid-state reaction mechanisms, many of which occur during the thermal processing of a material. The parameters estimated from the Sestak-Berggren equation are used to inform which of these solid-state mechanisms are occurring. Models for these mechanisms, such as three-dimensional diffusion, can also be found in the literature.

Initially conventional kinetic experiments were completed, varying the temperature ramp rate. Parameter estimation was carried out using Athena Visual Studio, along with the statistical analysis of the quality of fit. Following the results of the Sestak-Berggren modelling, discrimination between candidate mechanistic models was completed. It was found that the decomposition of calcium carbonate is dominated by a two-dimensional interphase-controlled mechanism.

This case study further utilises design of experiments to explore the impact of temperature ramp rate, space velocity and particle Reynolds number. It was found that the particle Reynolds number had minimal impact on the results, however the ramp rate and space velocity do have an impact on the regime encountered. The problems associated with including the space velocity will be discussed and possible improvements highlighted.

Audience Take Away:

- This presentation will outline a method for extracting kinetic information from thermogravimetric analysis data, specifically using the Sestak-Berggren equation to inform the mechanism occurring during a decomposition reaction.
- The presentation will highlight the use of statistical model discrimination in thermal analysis.
- The value that the use of design of experiments can bring to a kinetic study.
- The problems which arise when space velocity is considered in thermogravimetric analysis experiments.

Biography

Rebecca Gibson studied Chemical Engineering with Energy Engineering at Heriot Watt University, graduating in 2017. Since then she has started a Formulations Engineering Doctorate, studying at the University of Birmingham with Johnson Matthey as industrial partners. Rebecca's research is specifically focused on the kinetic modelling of thermal processes, with the aim of informing the scale up of materials manufacture to improve product quality and the efficiency of the processes used.

Thermal utilization of biochar in the process of steam gasification oriented on hydrogen rich gas generation

Adam Smolinski

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Increasing energy demand, limited resources of fossil fuels and environmental aspects are the main rationales behind the research efforts aiming at wider utilization of biowaste (e.g. sewage sludge) in energy generation systems. Gasification as an alternative to combustion offers increased efficiency, lower negative environmental impact and wider application range of the main product – synthesis gas – in power generation and chemical synthesis. It is also considered as one of the most viable options for hydrogen production, as an environment friendly energy carrier. An increased interest in renewable energy resources has resulted in numerous studies on biomass and biowaste gasification. Municipal solid wastes, sewage sludge and industrial residues are also considered as potential gasification feedstock. In the paper the experimental results on steam gasification of biochar in a fixed bed reactor under atmospheric pressure and at the temperature of 700, 800 and 900oC are presented. The effectiveness of the biochar gasification process was tested in terms of the total gas and hydrogen yield, gas composition, carbon conversion rate and biochars reactivity.

Biography

Prof. Adam Smolinski, Scientific Secretary, Central Mining Institute (Katowice, Poland). Specializes in clean coal technologies including solid fuels gasification, carbon dioxide sequestration, sorbents and catalysts application in hydrogen production. His expertise covers also exploratory environmental data analysis, multiway data analysis, clustering, data mining, missing elements and outlier detection methods, calibration and autoassociative neural networks. Author of over 200 scientific, peer-reviewed papers.

In his professional career, he has held numerous research and teaching positions. In 2000-2004, he worked as a lecturer in the Institute of Chemistry at the University of Silesia. From 2005 to 2006, he occupied several research positions at the Department of Mechanical Engineering and Energy Processes of Southern Illinois University in Carbondale, USA, Coal Research Park of Southern Illinois University in Carterville, USA, and the Department of Material Engineering at the Central Mining Institute.

Professor Smolinski serves on various international committees including the Energy Strategic Working Group of the European Strategy Forum on Research Infrastructures (ESFRI), World Energy Council, Polish Committee for Standardization (PKN), and the Scientific Association of Chemists at Polish Academy of Sciences. He is also the Head of the Silesian Environmental PhD Program in the field of Sustainable Energy and Environmental Technologies and a member of the Scientific Council of the Central Mining Institute. He sits on the editorial boards of several international peer review journals.

Clean biogas as a renewable economic source of syngas and hydrogen

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[2]Department of Science and High Technology, University of Insubria, Via Valleggio 9, 22100 COMO (Italy)

The steam reforming (SR) of natural gas plays a key role in the production of syngas (CO + H_2) and hydrogen, widely used to produce chemicals, fuels or energy. However, the depletion of fossil fuels together with the environmental drawbacks associated to their utilization, have in the last decades prompted the attention towards new and renewable fuels. The main candidate to replace the natural gas is the biogas obtained by anaerobic fermentation of organic wastes or not edible biomass that, after purification from pollutant compounds, is a mixture of CH_4 and CO_2 (clean biogas or CB). Although the removal of CO_2 to obtain bio-CH_4, that can be directly introduced in energy grid, is a feasible way, a full valorization of CB is more desirable from both economic and environmental point of view. In this context, the utilization of CB in the SR process is an attractive option, although the CO_2 fraction is barely converted in presence of a high steam content in the feed, decreasing the overall productivity. From this point of view, the Dry Reforming (DR) represents an attractive way to produce syngas from CB, although its many drawbacks (high reaction temperature and coke formation) limit its commercialization. An interesting option is represented by the combined Steam/Dry Reforming (S/DR) reaction, in which the additions of a limited amount of steam to the DR process can mild the reaction conditions and limit the phenomena leading to the catalyst deactivation. In this process, the S/CH_4 (Steam/CH_4) molar ratio in the feed drives the composition of the outlet stream, allowing to obtain syngas directly exploitable in hydrocarbons (Fischer-Tropsch) or CH_3OH synthesis. The syngas can be further upgrade through the Water Gas Shift process, that allows to tune the H_2/CO ratio or to improve the production of H_2 for the chemical or energetic markets (for example to feed Solid Oxide Fuel Cells) as a function of catalyst formulation and reaction conditions. In this study, Ni-Rh and Cu-based catalysts prepared from hydrotalcite-type (HT) precursors, investigated in the S/DR of CB and WGS of the obtained syngas, were deeply characterized before and after reaction to collect useful information to improve the performances by tuning catalyst composition and properties. A study of the deactivation mechanism allowed to suppress the carbon formation in the harsh reaction conditions of the reforming processes. The feasibility of the integrated process to obtain syngas directly exploitable in various downstream applications was successfully demonstrated by using new catalysts able to fully valorize the CB, without significant deactivation phenomena with time-on-stream.

Audience Take Away:

- Clean biogas as valuable alternative to fossil CH_4 to produce syngas or H_2
- Advantages of the combine reforming process
- Way to tune the H_2/CO ratio as a function of the downstream applications
- Role of catalyst composition on the activity and stability with time-on-stream
- Advantages of the catalyst preparation from hydrotalcite-type precursors.

Biography

In 1972, Prof Vaccari graduated in Industrial Chemistry with honors at ALMA MATER STUDIORUM – University of Bologna, were 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 Universitad 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, 265 Congress Communications and 20 Patents (16 EU or WO), with H-index = 43 and 10934 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.

Photocatalytic production of hydrogen from biomass or wastewaters using solar energy

Alberto V. Puga
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Hydrogen, a key chemical for manufacturing processes, and a clean source of energy for fuel cells, is mainly produced from fossil gas and oil, a fact which calls for alternative routes. Biomass-derived feedstocks offer a distinct possibility for this technological challenge. However, typical thermocatalytic biomass-to-hydrogen processes are energy intensive and their selectivities are often moderate. Sunlight-driven photocatalysis represents a promising alternative, given their mild operation conditions and the small extent of substrate degradation involved.

The processes considered in our research team imply the use of processed lignocellulose, resulting in aqueous streams containing a range of biomass-derived substances. In particular, the substrates we study may derive from either of the following: (1) hydrolysis, (2) pyrolysis, or (3) industrial or domestic activities which generate wastewaters. Light-promoted photocatalytic reforming (photoreforming) of such aqueous streams on titania-supported metal photocatalysts (M/TiO_2) is then carried out to produce hydrogen.

In general, where the processes start from raw lignocellulose (1 and 2), treatment leads to deconstructed chemical entities of lower structural complexity, ideally mono- and oligomers, which are then subjected to photoreforming for H_2 generation, whereas direct use of wastewaters combines remediation with energetic valorization of residual organic substances.

The synthesis of the photocatalytic materials is performed by impregnation or deposition-precipitation of the desired metal (Au, Pd, Pt, Cu or Ni) on titania, aiming at obtaining materials of small metal nanoparticle sizes (< 5 nm) and high dispersion. The photocatalysts are characterised by standard techniques (powder XRD, TEM, ICP-MS elemental analysis or DURV-Vis spectroscopy). A considerable research endeavour is focused on mechanistic aspects of the photoreforming of model biomass-derived oxygenates (e.g. mono- and oligosaccharides, carboxylic acids or aldehydes).

The ultimate goal of these processes is the extensive yet decentralized valorisation of residual biomass or wastewaters, powered by the harnessing of solar energy for the ultimate goal of producing hydrogen as a valuable energy product.

Audience Take Away:

- Solar production of hydrogen from biomass-derived aqueous streams is a surprisingly versatile and selective strategy.
- Conditions are mild, and solar irradiation is the only energy input.
- Photocatalysts based on Earth-abundant metal co-catalysts, such as copper, can be optimized to boost H_2 selectivity and productivity.

Biography

Dr. Alberto V. Puga studied Chemistry at the University of Barcelona, and received a PhD in Chemistry at the Autonomous University of Barcelona in 2007. He has been a post-doctoral research fellow at the Queen's University of Belfast (UK) and a Marie Curie researcher at Rovira i Virgili University (Tarragona, Spain). Dr. Puga is a research associate at Instituto de Tecnología Química (Valencia, Spain), and will be shortly taking on a tenure-track position at Universitat Rovira i Virgili. Topics of interest to his research include heterogeneous catalysis, photocatalysis, solar energy, hydrogen production, carbon dioxide capture and reduction, or biomass valorisation.

Key factors for the design of active iron-based oxygen evolution catalysts

Toshihiro Takashima
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The oxygen evolution reaction (OER, $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$) has received considerable attention in recent years as a promising method for utilizing water as a sustainable electron source. By coupling the OER with a reduction half-reaction such as hydrogen evolution ($2H^+ + 2e^- \rightarrow H_2$) or carbon dioxide reduction (ex. $CO_2 + 8H^+ + 8e^- \rightarrow CH_4 + 2H_2O$), the intermittent energy from renewable sources, including solar energy or wind power, can be captured in the form of chemical fuels.

However, driving the four-electron process to oxidize water to oxygen has proven difficult due to the large overpotential. Among the various OER catalysts examined to date, RuO_2 and IrO_2 have been reported to show good catalytic performance. However, the scarcity and high costs associated with precious metals limit the large-scale applicability of these materials, and therefore it is highly desirable to substitute them with catalysts derived from earth-abundant 3d metals such as Mn, Co, and Fe.

This article reports the investigation of the OER mechanism of hematite (-Fe_2O_3) to gain insight into the critical factors determining its electrocatalytic activity. Using spectroelectrochemimcal measurements, an intermediate species assignable to Fe4+ was identified as the precursor of OER across the entire pH range investigated (pH 4–13). The pH dependences of the onset potentials for OER and Fe4+ formation revealed that -Fe_2O_3 showed higher catalytic activity under alkaline conditions and that there were two reaction mechanisms which switched at approximately pH 10. From the results of kinetic isotope effect experiments, it was found that the manner of proton and electron transfer during Fe4+ formation ($Fe^{3+}–OH \rightarrow Fe^{4+}=O + H^+ + e^-$) was different between the two mechanisms. Whereas proton transfer and electron transfer proceed as discrete reaction steps at neutral pH, they proceed simultaneously at alkaline pH. Because the simultaneous transfer of proton and electron enables to avoid formation of high-energy protonated or deprotonated intermediates, the simultaneous transfer is energetically more favorable than the stepwise one, resulting in the higher activity under alkaline pH conditions. Notably, by adding appropriate pyridine derivatives as proton accepting reagents, the switching of the rate-determining step from the stepwise process to the simultaneous process was demonstrated. As a result, a decrease in overpotential of 250 mV was achieved at pH 7 and the OER activity of -Fe_2O_3 under neutral pH conditions became comparable to that under alkaline pH conditions. Furthermore, when the pyridine derivatives were replaced with a solid proton accepting material that is robust against anodic decomposition, the enhanced activity was maintained in the long-term operation. These findings will be helpful to design active Fe-based OER catalysts and offer the opportunities to achieve high OER activity under neutral pH using 3d-metal catalysts which often show remarkable activities under alkaline pH conditions.

Audience Take Away:

- Reaction mechanism of oxygen evolution reaction on iron oxide
- Strategy for design of active oxygen evolution catalyst
- Spectroelectrochemical method for identification of intermediate species

Biography

Toshihiro Takashima received his Dr. Degree in Engineering in 2012 from The University of Tokyo under the supervision of Prof. Kazuhito Hashimoto. After working as a Japan Society for the Promotion of Science (JSPS) postdoctoral fellow at National Institute for Materials Science (NIMS, Japan) for half a year, he joined University of Yamanashi as an assistant professor and was promoted to an associate professor in 2017. His major research field is electrochemistry, photochemistry, and material science. He is particularly interested in the development of multi-electron transfer catalysts for sustainable energy conversion.

Competitive reactions in hydrogenation of aqueous acetic acid by flow-type reactor with Ni-Sn/TiO_2 catalyst for bioethanol production

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A novel bioethanol production process from lignocellulosics via acetic acid fermentation has been proposed in our laboratory as a “third-generation” technology for minimizing the by-production of CO_2. This paper focuses on the last step of this process, which includes three consecutive steps, that is, hot-compressed water treatment to hydrolyze lignocellulosics, acetic acid fermentation, and hydrogenation of acetic acid into ethanol. As the effective catalysts, we exploited TiO_2 (Lewis acid)-supported Ru-Sn and Ni-Sn for direct hydrogenation of aqueous acetic acid into ethanol. A high yield (88mol%) production of ethanol from aqueous acetic acid was also successfully demonstrated with 8wt%Ni-8wt%Sn/TiO2 catalyst by using a flow-type reactor [liquid hourly space velocity (LHSV): 1.31 h^{-1}]. However, the hydrogenation reaction into ethanol was slowed down when the reaction temperature reached 280-300°C under the reaction pressure of 10 MPa, and acetaldehyde that is the intermediate to ethanol started to be detected. In the present paper, the slowdown mechanism is studied by investigating the reactivity of acetaldehyde as the intermediate.

Aqueous acetaldehyde solution was treated with the flow-type reactor in the temperature range of 200 to 380°C at 10 MPa under the catalytic (4wt%Ni-4wt%Sn/TiO_2) or non-catalytic conditions. Cannizzaro-type reaction giving acetic acid and ethanol, oxidation into acetic acid, and gasification were found to occur as the competitive reactions to hydrogenation into ethanol. These three side-reactions occurred without the addition of any hydrogen but required the presence of the catalyst. Because acetaldehyde did not react at all on TiO_2, all these reactions were suggested to be catalyzed by 4wt%Ni-4wt%Sn/TiO_2. The selectivities of these side reactions and hydrogenation into ethanol were determined in the temperature range of 200-380°C, which suggests that the slow-down mechanism is related to the oxidation of acetaldehyde to acetic acid that becomes important at temperatures > 300°C.

The slow-down temperature in acetic acid hydrogenation shifted to the lower temperature region when the reaction pressure decreased from 10MPa. In addition, the slow-down temperature was very close to the boiling point of water at each reaction pressure. Based on these results, the slow-down mechanism is discussed focusing on the influence of boiling of solvent water on hydrogenation and three side reactions.

Audience Take Away:

- Highly efficient ethanol production from aqueous acetic acid through hydrogenation over Ni-Sn/TiO_2 catalyst with a flow-type reactor.
- Cannizzaro-type reaction, oxidation into acetic acid, and gasification occur for acetaldehyde that is the intermediate in hydrogenation of acetic acid into ethanol.
- Particularly, oxidation to acetic acid becomes competitive at high temperatures >300°C (at 10 MPa), where the reactivity of hydrogenation into ethanol is slowed down.
- The boiling of the solvent water, which is affected by the reaction pressure, is suggested to cause the slowdown of the hydrogenation of acetic acid into ethanol.

Biography

Ms. Yuanyuan Zhao studied Chemical engineering at the Kagoshima University, Japan and graduated as BC in 2016. She then joined the research group of Prof. Kawamoto at the Graduate School of Energy science, Kyoto University, Japan, and graduated as MS in 2018. The same year she started her PhD study at the same institution.

Percolation and additional active centers as key factors for performance of highly productive Fischer-Tropsch synthesis catalysts

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The Fischer–Tropsch synthesis (FTS), which is important for energy and alternative fuels, is a strongly exothermic and temperature sensitive process. Therefore, the use of a catalyst with low thermal conductivity may lead to rapid deactivation. It means that efficient heat removal by thermally conductive additives is of crucial importance. Efficient mass transfer is also important for the viscous product removal. This work shows that a percolating heat-conductive network (characterized by newly introduced interconnectivity function) in combination with extended pore system provides an unmatched performance of composite catalysts in FTS. The electron microscopy and X-ray tomography support the conclusions. Both methods showed that the catalyst pellet represents an interconnecting network of transport pores and percolating metallic heat-conductive flakes. The improved interconnectivity effect is manifested if a condition of fast enough diffusion of liquid hydrocarbon products is met. This can be accomplished by introduction of additional active centers into the catalyst. For example, the introduction of some zeolites can help as shown by experimental practice.

Audience Take Away:

- Catalytic processes with high thermal effect and high temperature sensitivity can still be controlled by introduction of a thermally conductive network into the catalyst pellets.
- A newly introduced function of interconductivity may help in understanding and engineering such reactions.
- Additional active centers, which help changing product viscosity, can help in further intensification of a process.

Biography

Vladimir Mordkovich earned his degrees from the Moscow State University (MS in 1981; Ph.D. 1984). The upper degree of Dr.Sci. awarded in 1995. Vladimir Mordkovich has dedicated his career to R&D in chemistry and technology of fuels and materials. He had spent 11 years in Japan working for R&D companies before returning to Russia. Since 2009 he leads the New Chemical Technologies and Nanomaterials Research Department at the Technological Institute for Superhard and Novel Carbon Materials in Moscow. He serves as a full professor in Moscow Physico-Technical Institute (since 2010). 52 inventions in the field, 160 publications in peer-reviewed journals.

Scale-up of an integrated formic acid-to-power system

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Transitioning from fossil fuels to sustainable and green energy sources in mobile applications is a difficult challenge and demands sustained and highly multidisciplinary efforts in R&D. Liquid organic hydrogen carriers (LOHC) offer several advantages over more conventional energy storage solutions, but have not been yet demonstrated at scale. Herein we describe the development of an integrated and compact 25 kW formic acid-to-power system. Formic acid is introduced as a viable liquid energy carrier for future mobile and static applications. Formic acid is effectively one CO_2 molecule carrying one H_2 molecule. In an energy storage system this CO_2 is hydrogenated and subsequently dehydrogenated. This second part, a formic acid to power system, was developed and is schematically presented.

In short: the formic acid is dehydrogenated inside a generator, the hydrogen/CO_2 gas flow is used in a tailored fuel cell system to produce power. Several dehydrogenation-catalysts were screened. A Ru-TPPTS water-based catalyst was eventually chosen because of its stability, commercial availability, ease of activation and low CO production. Tests show remarkably fast activity upon formic acid input and give stable gas outputs at moderate temperatures. Challenges remaining are: Purification of the hydrogen gas flow and energy integration to increase system efficiency. Economic viability requires sustainable produced formic acid at a target price below $450 per ton. Few companies are working on formic acid production using renewable sources of energy. More scale up projects are needed to accelerate this development. CO_2 capture and storage at location would ensure a closed carbon cycle.

Audience Take Away:

We highlighted a number of key engineering challenges encountered during scale-up of the technology and discuss several aspects commonly overlooked by academic researchers

- High intrinsic catalytic activity was found to have little impact on the viability of the developed technology, whereas availability and stability of the utilized catalytic solution were found to be of critical importance. A high TOF catalyst is not the first objective for a scale up system. Many catalysts have been reported with TOFs exceeding a million. Often, they are not stable or very sensitive to e.g. water, oxygen or other common impurities in for example the formic acid feed. Research can focus more on the application of the catalyst. System design should be considered when developing catalyst and can compensate for low turnover frequencies.
- Lab scale experiments do not automatically show the same behaviour in scaled up systems. For example, we encountered CO production (poisoning the fuel cell) at larger scale but at lab scale the catalyst was tested to be 100% selective towards CO_2. Also, the scale up system at elevated pressure was less sensitive to foaming and more responsive upon formic acid input or depletion.
- The goal is not to reach a high reaction rate but a high productivity. Catalyst costs are relatively small compared to e.g. fuel cell costs. Catalyst concentrations can be varied and often deviate from research. In scientific publications, concentrations are deliberately kept low to reach high TOF, while higher concentrations increase productivity and give more insight in the applicability of the catalyst.
- The solvent choice has great influence on the required system design. Water is the preferred solvent but requires above-ambient-operating pressures to prevent unacceptable boil-off rates and high cooling duties. Other solvents such as ionic liquids degrade over time and poison the fuel cell with organic residues. Effluent gas flow purification is required to protect the fuel cell.

Biography

Tim Wissink studied Chemical Engineering and Applied Physics at the Eindhoven University of Technology and graduated as MSc in April 2019. His graduation project about photo-electrochemical CO_2 reduction was conducted in the research group 'Inorganic Materials and Catalysis' lead by Prof. dr. Emiel Hensen. In the same research group, during his bachelor, he started a project to develop formic acid as an energy carrier. He then continued leading the research in the student team 'Team FAST', to develop a formic acid to power system. This led to the founding of the start-up 'DENS', bringing the formic acid to power generator to market.

Development of auto-thermal catalytic reforming of tars and hydrocarbon gases derived from pressurized fluidized-bed gasification of wood residues

Ilkka Hiltunen*, Esa Kurkela, Minna Kurkela
VTT Technical Research Centre of Finland Ltd, Espoo, Finland

One of the major global energy challenges is the need for decarbonizing transportation, which will require new sustainable alternatives to replace fossil-based fuels in all transport sectors. While electric vehicles may become the key solution for light-duty transport, there is still a growing demand for renewable fuels in the heavy-duty road transport, maritime and air traffic sectors that cannot be electrified. Highly efficient tri-generation concepts have been developed in Finland for converting biomass residues and wastes into renewable transport fuels or chemicals through gasification and synthesis, while the by-product heat from the process and synthesis off-gases are utilized for generating energy in the combined-heat and power plants.

Fluidized-bed gasification is a feedstock-flexible technology, which is especially suitable for high volatile and highly reactive feedstocks, which can be readily gasified at 800-950 °C. However, in low-temperature gasification an abundance of tars and hydrocarbon gases are produced in addition to targeted carbon monoxide and hydrogen. Consequently, auto-thermal catalytic reforming is a key front-end conversion technology enabling high syngas yields and making it possible to apply conventional final gas cleaning and synthesis technologies developed for coal and oil gasification.

This paper highlights the ten-year R&D programme carried out in Finland on developing catalytic reforming technology as part of a pressurized fluidised-bed gasification process. Different reactor designs applying monolith catalyst elements as well as granular catalyst in fixed beds are described and the results from pilot-scale test facility are presented. In this process, the raw gas is led into a high temperature filter unit, where the ash and char particles are removed. Then the particulate-free gas is reformed in a multi-stage catalytic reformer. One of the key technical challenges, soot formation resulting from thermal cracking reactions, has been avoided by using staged reforming and innovative combination of different catalysts. In addition, the way of oxygen and steam introduction turned out to be a critical design factor. The key results and conclusions from 4000 hours of pilot-scale testing are summarised and best practical designs suggested. Typical raw gas of fluidised-bed biomass gasifier contains 5-10 vol% methane, 1-3 vol% C2-hydrocarbon gases and 10-25 g/m3n benzene and 10-15 g/m3n tars. Under optimal operating conditions, 100 % conversion of C2-hydrocarbon gases, over 99 % conversion of tars and benzene and up to 80 % conversion of methane were achieved at relatively mild conditions with the reformer outlet temperature of 900 °C. Scaling-up of the technology as well as the long-term stability of one of the developed reforming concepts as well as the used catalyst materials was also verified at an industrial demonstration plant producing syngas from forest residues and bark.

Audience Take Away:

- Description of a promising concept for converting various biomass residues into transport fuels by a gasification-based technology
- Highlights and main results from a 10 year R&D program on the pilot-scale development of reforming of tars and hydrocarbon gases from biomass-derived syngas
- Comparison of various reactor alternatives and catalyst materials
- Present a practical solution for solving the key challenge of biomass gasification - converting also tars and hydrocarbon gases into syngas components H2 and CO
- Show the significant effect of reforming technology on the competiveness of gasification based routes to renewable transport fuels and chemicals

Biography

Ilkka Hiltunen, M.Sc. (Tech). Research Team Leader of the Thermochemical Conversions Research Team at VTT. He has over 10 years of experience on biomass and waste gasification technologies, gasification product gas cleaning technologies and their different applications. He has excellent experience on industrial co-operation projects and pilot-scale activities. He has studied Chemistry at the Technical University of Helsinki and graduated as Master of Science in 2007.

Zeolites: Potential soil amendments for improving agriculture productivity

Vijay Sandeep Jakkula*, Sreenath Dixit
ICRISAT Development Centre, International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), Hyderabad, Telangana, India

Some of the most important applications of zeolites are in water treatment (wastewater and drinking water), agriculture, and metal immobilization in soils. Based on cost effectiveness, four main areas where zeolites are finding application as ion-exchangers are: in detergents; in ammonia/ammonium removal from wastewater effluent; in radioactive isotope removal from spent pile effluent and in agriculture. In agriculture, zeolites have numerous applications, as slow release fertilizers, as heavy metal removers, as soil conditioners, increasing the nutrient and water use efficiency along with increasing crop yield. Farmers add zeolites to soil to control soil pH and improve ammonium retention. Zeolites can increase soil CEC, act as a reservoir of K+ and increase the water-holding capacity of loamy sand soils if very large amounts are added. Studies on synthetic Phillipsite and natural Clinoptilolite supplemented soils showed an increase in water holding capacity (18-19%) and CEC (30-40%). Soils supplemented with both synthetic and natural zeolites can be used as effective fertilizers on saturating the zeolites with ammonium. Nitrogen loss from irrigated cropland, significantly contributes to nitrate contamination of both underground and surface waters. Zeolites (both natural and synthetic) when added as a fertilizer amendment to soil can increase crop yield and prevent water pollution from nitrates and heavy metals, thereby saving the cost for future improvement. Zeolites improve nutrient use efficiency by increasing P availability, improving the use of NH4+-N and NO3-N, reducing leaching losses of exchangeable cations, especially K and also acting as slow-release fertilizer. Zeolite can hold nutrients in the root zone for plants to use when required. This leads to more efficient use of N and K fertilizers - either less fertilizer for the same yield or the same amount of fertilizer lasting longer and producing higher yields. Soil fertilized or amended with organo-zeolite mixtures regulate N release and minimize reactive N (NO3) formation. It can be concluded that N loaded zeolites could be used as a controlled release fertilizer, and continued research in enhanced ammonia supply by zeolite as carrier will result in better nitrogen/fertilization management.

Audience Take Away:

- Zeolites have enormous applications, and their use in agriculture dates back to 1960. My talk will focus on the various aspects of zeolites which would benefit agriculture in semi-arid as well as arid regions of the world. Zeolites have a profound effect on soil physical, chemical and biological properties, therefore my talk will involve past results from all of these aspects. The audience would get a clear picture about the role of zeolites in agriculture as how these microporous materials can mitigate climate change particularly nitrate pollutions of underground water due to excessive usage of fertilizers which is a major problem in most of the developed and developing countries. The audience can start using these materials in their gardens and advice farmers to use these materials keeping in view reduction of chemical fertilizers.
- Zeolite research can be used by many faculties as it has many applications. It definitely provides a practical solution in the form of slow release fertilizers which will reduce N usage and play a vital role in improving soil properties. It will help fertilizer industries to tailor their products and also help in reducing the fertilizer usage by farmers. Researchers working in the field of agriculture can make use of zeolites to increase soil moisture, soil water holding capacity and soil aggregation which all play a vital role in increasing crop yield. Some of the benefits of zeolites in agriculture are: increase in crop yield, reduction in chemical usage, drought proofing and finally environmentally friendly product.

Biography

Dr. Vijay Sandeep Jakkula studied Applied Sciences at the University of Wolverhampton, United Kingdom, and graduated as MS in 2001. He then joined the research group of Prof. Craig D. Williams in his microporous and mesoporous division, University of Wolverhampton and received his PhD degree in 2006 at the same institution. After two year postdoctoral fellowship supervised by Dr Williams at Alpha Adhesives and Sealants Ltd, UK he obtained the position of Visiting Scientist at ICRISAT, India. He has published more than 20 research articles, books, book chapters and bulletins in high impact factor journals.

Preparation of DNA Crown Cells(artifical cells) Using Eggs and Sphingosine-DNA

Shoshi Inooka
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DNA crown cells are artificial cells in which the outside of the cells are covered with DNA; this class of cells is self-replicating. Full application of DNA crown cells will require the development of techniques that are simple and scalable. To date, methods to obtain artificial cells that can replicate have been not established. Therefore, this presentation describes a detailed method for the preparation of these cells.

Materials:

The required materials include sphingosine (Sph), DNA, adenosine, and eggs. Sph is formulated at 10 mM in 50% ethanol (10 mM). DNA (1.7 µg /µl) and adenosine (0.1 M) are formulated in distilled water; the use of distilled water for this purpose is key to this protocol. The edible chicken eggs are obtained from a local market.

Generalized method

Step 1: Sph (90 µl) and DNA (40 µl) are mixed. The mixture is boiled for a few minutes and cooled in ice..

Step 2: Adenosine (300 µl) is added to the Sph-DNA mixtures.

Step 3: Sph-DNA/adenosine mixtures are injected within the egg white and the eggs then are incubated at 37°C.

After 7 days, DNA crown cells will have formed within the egg white.

This protocol permits the ready preparation of DNA crown cells (artificial cells) in essentially un-limited numbers. These cells can be generated with any of various sources of nucleic acid. In the original study, an extract of an *Ascidian sea squirt* was used. Subsequently, I discovered that adenosine was effective to form artificial cells and established the generalized method for preparing DNA crown cells described above. To date, I have successfully prepared DNA crown cells using DNA from *Escherichia coli, Lactobacillus*, human placenta, bovine meat and so on with the extract of an *Ascidian sea squtri* or adenosine.

A key aspect of the method described here is that the cells can be prepared with commercial reagents (Sph, DNA, and adenosine). Many kinds of DNA crown cells can be obtained and recovered from egg white. Thus, this protocol is expected to contribute to new research in the life sciences and to find application in the biotechnology industry.

Biography

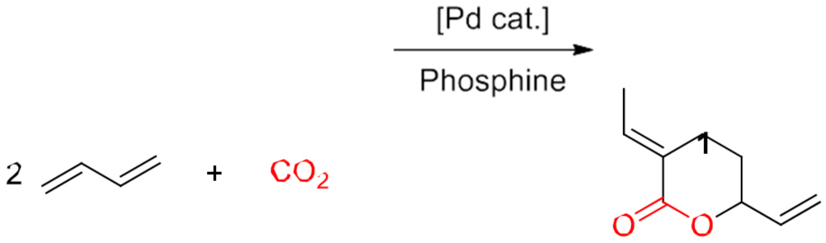
Shoshi Inooka has completed his PhD in Tohoku University in Sendai, Japan. Currently he is working as a President of nonprofit organization: Japan Association of Special Scientists and President of the Japan Academy of Applied Cell Biology.

Selective Palladium-catalyzed synthesis of Diesters: Alkoxycarbonylation of a CO2-butadiene derived δ-lactone

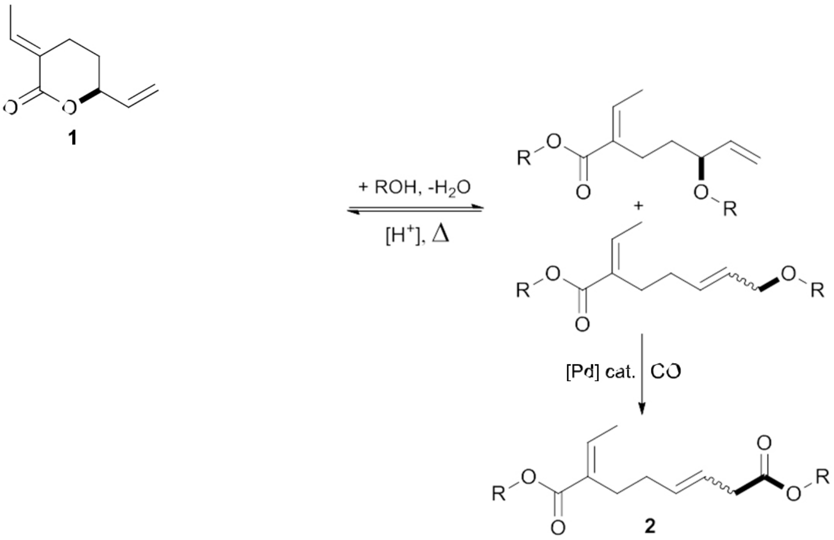
Muhammad Sharif
King Fahd University of Petroleum and Minerals, Kingdom of Saudi Arabia

The development of sustainable processes for chemical synthesis, energy and petrochemical technologies is one of the major challenges and noteworthy task for 21sr century. Notably, catalysis is a key technology for achieving more sustainable processes in the chemical, pharmaceutical and material industries. Currently, more than 80% of all chemical products are made via catalysis. In this regard, the development of more selective, cost-effective and durable catalysts constitutes a key factor for the production of all kinds of chemicals today and in the future.

Novel unsaturated C10 diesters are produced via alkoxycarbonylation of **Δ**-lactone 1 (3- ethylidene-6-vinyltetrahydro-2*H*-pyran-2-one), derived from the telomerization of CO_2 and butadiene. Key for the selective valorization of 1 is the use of a catalytic system based on $PdCl^2$, a chelating phosphine bearing electron-withdrawing groups and an acidic promoter. The unsaturated C10 methyl diester can be easily hydrogenated on Pd/C under mild conditions to afford its corresponding saturated diester. Subsequent hydrogenation using the homogeneous [Ru(acac)3]/Triphos catalysts gives 2- ethyloctane-1,8-diol in high yield. The overall procedure allows synthesizing new building blocks for the manufacturing of renewable polymers and polymers processing materials.



Scheme 1



Scheme 2

Biography

Dr. M. Sharif is currently a Research scientist at Leibniz Institute for Catalysis, Rostock Germany. During his doctoral & postdoctoral research, Dr. Sharif has been heavily involved in synthetic organic chemistry using either classical organic chemistry methodologies or transition metal-catalyzed synthesis of a range of synthetically important organic building blocks for diverse application. Dr. Sharif is also interested in the development of novel efficient synthetic organic methodologies which allow for a "greener" synthesis of fine chemicals for potential use in material, biological and pharmaceutical applications. He has published one patent and 28 research papers in reputed reviewed journals including Chem. Commun., Green Chem., Molecular Therapy and others. He is very well familiar with modern tools of organic chemistry, catalysis and spectroscopy. He held various research positions within academics and has closely worked in industrial driven projects throughout his career with major emphasis on organic synthesis, synthetic methodology development and catalysis for target oriented organic syntheses. His research-experience and expertise cover a wide range of topics in synthetic organic chemistry, green chemistry and homogeneous catalysis. Dr. Sharif is also initiated several collaborations between leibniz Institute for Catalysis, Rostock, Germany and other research institutes/Universities in developing countries. Sharif is also an external committee member for evaluation of PhD dissertations at Jacob University Bremen, Germany. Currently, He is also working as a team leader at leibniz Institute for Catalysis, Rostock, Germany. Sharif is involved in several cooperation projects in Gulf.

The morphology and surface modification effect on the properties of OER

Chuanbao Cao
Research Center of Materials Science, Beijing Institute of Technology, Bejing 100081, China

Water splitting provides an appealing pathway for clean and sustainable energy conversion and storage. Therefore, development of a noble metal-free, efficient and robust electrocatalyst oxygen evolution reaction (OER) is still a great challenge. Herein, we introduced to synthesize nanostructure especially freestanding nanosheets materials such as $Co(OH)_2$, Co_2O_3, CoS, FeNi LDH et.al. We find that the planar sheet area was up to several micrometres and exhibited an ultrathin thickness (< 1 nm) with a mesoporous feature. Hence, the highly exposed surface atoms afforded high electrochemical activity, whereas the ultrathin and mesoporous features facilitated charge and mass transfer along the 2D nanostructure to efficiently perform the surface dependent electrochemical reactions: HER, OER, and the overall water splitting. Furthermore, we demonstrate in situ surface substitution of the hydroxyl functional groups on the surface of $Co(OH)_2$, FeNi LDH et.al, and found that the in situ surface modification maintains the initial structure and morphology while increasing the areal density of active sites and reducing the energy barrier of the OER. These results are embodied by the increase of the electrochemically active surface area (ECSA) and the lowering of the OER onset overpotential, We have found that several substitutes can enhance the properties. The mechanisms are also discussed. The findings provide a new way to improve the OER properties and extend their applications.

Biography

Dr. Chuanbao Cao is currently the Chair Professor of School of Materials Science and Engineering, Director of Research Center of Materials Science of Beijing Institute of Technology. He received B.S (1983) degree in Chemistry from Nanjing University, M.S(1989) and PhD (1992) degrees in Materials Science from University of Science and Technology of China. He was a postdoctoral fellow in Fudan University (1992-1994). In 1994, he joined Beijing Institute of Technology. His current research focuses on the low dimensional materials synthesis and their energy application, . Until now, he was granted more than 40 patents, authored more than 320 peer-reviewed papers, cited by more than 7300 times, H index 46.

Valorization of household waste in hydroponics

Hannachi Abdelhakim
University of Skikda, Faculty of Science. Department of Agronomy (Algeria), HAKHANNACHI@yahoo.fr

The results obtained are related to the fertilizer and the environment, and the cultivation of some cultivated species to give better results. The results of the trials on hydroponic pea, bean and tomato crops at the time of germination and growth for electrical conductivity show that the plants are immersed in the water of potatoes (dilution of bark, coffee waste), the superior electrical conductivity by contribution to the first test because of the presence of the salts. Plants immersed in the infusion of waste allow a greater height of stem compared to the plants plunge into the water because of the presence of a significant amount of mineral salts. The misfortune of hydroponics is to bring together under the same conditions water-saving techniques that produce high nutritional value, and require more nutrients. Products totally devoid of interest, both in terms of nutrition and flavour. Plants always grow well when they need exactly when they need it.

Biography

Hannachi Abdelhakim, PhD in Agronomy, associate professor at the University of Skikda, Department of Agronomy (Algeria). Research area: Plant production, weed science, reuse of wastewater in agriculture, irrigation, fertigation and hydroponics. Baccallaureat: SNV 2000, Engineer: in biology, Mentouri University Constantine 2006, Magister in agronomy, Ferhat Abbas University Sétif 2010, Phd in agronomy, Ferhat Abbas University Sétif 2018.

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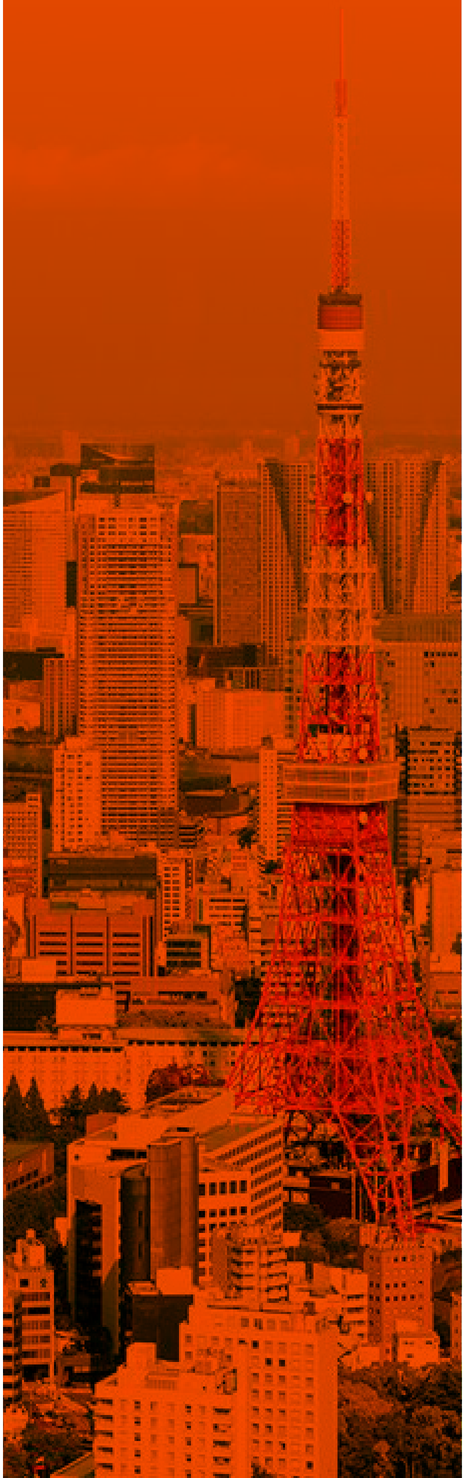


Oscillatory behavior in a cellular automaton based model of metal passivation

Jan Stępień[1], Janusz Stafiej[2 *]
[1]Department of Complex Systems and Chemical Information Processing, Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland
[2]Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, ul. Wóycickiego 1/3, 01-938 Warsaw, Poland

Passivating systems display potential or electric current oscillations in galvanostatic or potentiastic control, respectively. Their occurrence is related to the negative differential resisitivity observed on the potenial vs electric current dependence commonly called polarization curve. Our cellular automata based model reproduced such polarization curves for the stationary regime.Here we show that our simulations reproduce either potential or electric current oscillations in galvanostatic or potentiastic conditions respectively. Compared to other modelling approaches we can see morphology variations during several oscillations periods.

Audience Take Away:

CA automata based approach is a nice method of choice for complicated system modeling. In particular it correctly reproduces the qualitative features of passivating systems now including the oscillatory behavior.

It can be used for a range of problems such as surface mask at nanoscale, inflence of aggressive ions on the passive layer structure, depassivation healing etc. It can have potential applications in surface nanosttructuring for subsequent enzyme or another catalyst deposition.

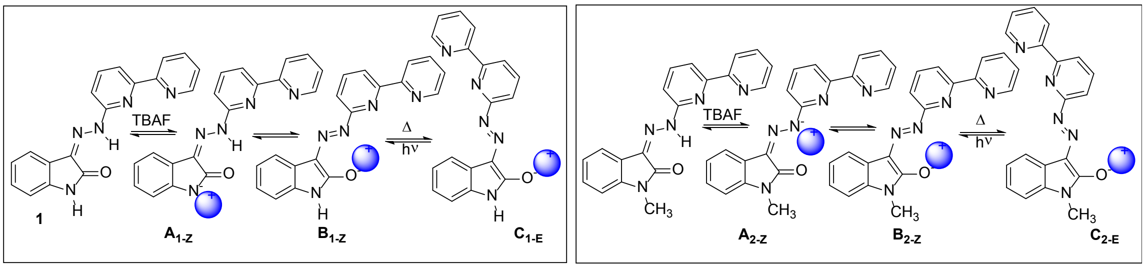
Biography

Dr J. Stafiej graduated from the Department of Physics, Warsaw University, 1980. In 1991 he defended PhD thesis supervised by prof. Zofia Borkowska, Institute of Physical Chemistry, Warsaw, (ICHF). He collaborated with JP. Badiali in Paris for over 20 years on statistical field theory for interfacial electrolytes. His habilitation thesis concerns branching pattern of differential capacitance caused by ionic profile depletion (ICHF 2002). Since 2014, as a professor in the Institute of Chemistry, Cardinal Stefan Wyszynski University, Warsaw, he works on corrosion, passivation, nanopore formation and oscillatory phenomena within cellular automata approch. He authors 59 SCI papers.

Photochemical and thermal reactivity of bipyridyl-functionalized hydrazones and their ON / OFF functionality

Pavol Tisovský*, Klaudia Csicsai, Jana Donovalová, Anton Gáplovský
Faculty of Natural Sciences, Institute of Chemistry, Comenius University, Ilkovičova 6, 84215 Bratislava, Slovakia

Arylizatin hydrazones in the presence of basic ions (F-, CH_3COO^-) provide the corresponding anions by the NH group hydrogen cleavage located on the hydrazone moiety. The charge delocalization in the anion molecule is reflected in the UV-VIS spectra by the formation of a new, intensively batochromically shifted absorbent band. Hydrazone 1 titration with fluoride ions results in formation of new intensive but hypsochromically shifted absorbent band. By NH-hydrogen substitution for the methyl group is achieved the fact that the UV-VIS titration record is the same as in the above cited works – with hypsochromically shifted absorbent band. The different behavior of the studied hydrazones in the presence of F- ions is illustrated on the scheme 1.



Scheme 1: The behavior of the studied hydrazones in the presence of F- ions.

By the NH hydrogen cleavage from the hydrazone, respectively B_{1-Z} or B_{2-Z} anion formation, the intramolecular hydrogen bond is extinguished. The thermodynamic stability of the *Z* isomer is reduced. Suitable conditions for the thermal *Z-E* isomerization of anion A_{2-Z}, respectively B_{2-Z} are formed. In the case of hydrazone 1, the N-anion A_{1-Z} transformation to anion B_{1-Z} must be carried out first. Anions C_{1-E} and C_{2-E} are photochemically transformed to *Z* isomers of this anions and they undergo the thermic *Z-E* isomerization again.

Audience Take Away:

- The audience can get information about behavior of new bipyridyl-functionalized hydrazones.
- This information can help them to use hydrazones as photoswitches in their research.
- This work can help other researchers to explain behavior of hydrazones in the presence of basic anions.

Biography

Pavol Tisovský has completed his PhD in organic chemistry from Comenius University in Bratislava in 2014. He is the researcher in the Institute of Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Slovakia. He has published 9 papers in SCI(E) journals. His research interests are materials for organic electronics and two photochemistry areas: molecular photoswitches and colorimetrical/fluorescent chemo-sensors.

Synthesis of comb type fluorine containing siloxane polymers and solid polymer electrolyte membranes on their basis

Tamar Tatrishvili*[1,2], JimsherAneli[2], Omar Mukbaniani[1,2]
[1]Department of Macromolecular Chemistry, Ivane Javakhishvili Tbilisi State University, Chavchavadze I. Ave 3, Tbilisi 0179, Georgia
[2]Institute of Macromolecular Chemistry and Polymeric Materials, Ivane Javakhishvili Tbilisi State University, Chavchavadze I. Ave., 3, Tbilisi 0179, Georgia

Energy conversion and energy storage are becoming more and more important in today's society due to the increased demand for stationary and mobile power. In particular, electrochemical energy conversion and storage devices using battery technologies have recently attracted attention worldwide in terms of technology development and commercialization.

For example, lithium-ion batteries have been considered one of the most promising energy con¬version and storage devices due to their intrinsic advantages such as high energy density, high efficiency, superior rate capability, and long cycling life compared with other batteries.

It is well known that polysiloxanes are characterized with very low glass temperatures such as T_g= -123oC for polydimethylsiloxane, very high free volume and high segmental mobility and present best matrix for Li-ion transportation. The high solubility of the corresponding salt in the polymer is another one factor for achievement of high ion-conductivity. This condition is created by introduction to the polymer-electrolyte main chain or side group of such „host"donor group, as ester oxygen imide group, halogen, especially fluorine groups. Formation of the grid like structures increases the mechanical properties of polymer-electrolytes. Among organosilicon compounds, the comb-type polymers with donor fragments at silicon atoms are of interest.

The aim of presented work is synthesis of D_4^R type methyltetrafluoroorganocyclo¬tetrasiloxane with 2.2.3.3-tetra¬fluoropropyl propionate side group at silicon atoms, via hydrosilylation reaction of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane (D_4^H) with 2.2.3.3-tetrafluoropropyl acrylate in the presence of platinum catalysts at 80-900C temperature. Determination of structure and composition of obtained addition adduct is carried out by FTIR and ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy. The polymerization reaction of D_4^R type methyltetrafluoroorganocyclotetrasiloxane in the presence of anhydrous powder-like Potassium hydroxide and tetramethylammonium fluoride, at 90-100oC temperature has been studied. The structure, composition and properties of obtained comb-type polymers was de¬termined using DSC, GPC, WAX, SEM, FTIR and NMR spectral methods of analysis.

Via Sol-gel reaction of hydroxyl terminated comb-type polymers and tetraethoxysilane doped with 5-20 mas.% Lithium salts, lithium triflate or Lithium bis(trifluoromethanesulfonyl)imide, transparent solid polymer electrolyte membranes is obtained.

By electrical impedance spectroscopy the ion conductivity of solid polymer electrolyte membranes is determined and the ionic conductivity of solid polymer electrolyte membranes at 25oC changes in the range 1.2×10^{-6} - 6.2×10^{-8} Siem¬ens/cm.

Acknowledgments. The financial support of the Georgian National Science Foundation and Technology Centre in Ukraine, STCU-2016-16 (6301), is gratefully acknowledged.

Audience Take Away:

- By us will be first presented the synthesis of new type fluorine containing organocyclotetrasiloxanes; investigation polymerization reactions of organocyclotetrasiloxanes in the presence of various catalysts; investigation of sol-gel reactions of obtained comb-type polymers with regular arrangement of side groups; obtaining solid polymer electrolyte membranes on the base of Lithium salt: Lithium triflate and Lithium bis(trifluoromethanesulfonyl) imide and investigation of their ion-conductivity
- For obtaining of comb-type polymers with regular arrangement of electro donor side groups they will use suggested by us this method.
- This suggested way of synthesis of comb-type polymers with regular structure for obtaining of solid PE membranes will be used by another researcher in their research and teaching, which will be make their research more efficient, informative and interesting.

Biography

Dr. T.Tatrishvili studied at Tbilisi State University, Faculty of Chemistry and graduated in 1990. She received her PhD degree in 2002.T.Tatrishvili works at the TSU up to day at the Faculty of Exact and Natural Sciences and Head of the department of the Institute of Macromolecular Chemistry and Polymeric Materials. She is a Member of Georgian Chemical Society; T.Tatrishvili is a supervisor of Bachelor, Master and PhD Students thesis. She was participant of local and International Grants and has got Individual fellowships too (DAAD -2013-2016; Max-Planck Institute for Polymer Research; Mainz; Germany). She has published more than 160 research publication.

Ruthenium based multimetallic nanoparticles: Probe the local structure

Capucine Sassoye[1*], Laura Ellezam[1,2] , Caroline Mellot-Draznieks[2], Clément Sanchez[1]
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[2]Collège de France, CNRS, Laboratoire de Chimie des Processus Biologiques, Paris, France

Ruthenia and ruthenium based nanomaterials are versatile and attractive candidates for various technological applications (electrochemical energy storage, catalysis, electrocatalysis…). As catalysts, they are well known for their high activity and selectivity. Oxide based materials are used as oxidation catalyst[1] while metallic ruthenium is mainly used for hydrogenation reaction.[2] In order to decrease the price of nanocatalysts and to increase the stability, we are introducing heteroatoms such as cobalt and are studying the consequences on the atomic structure and catalytic activity. Indeed, a rational understanding of the catalyst evolution[3] is crucial to further elaborate more efficient or new catalysts.

Nanoparticles are prepared using a one-step oxidative aqueous route knowing that the further reduction under H_2 is easy and straightforward and that the deposition process is mastered. These nanoparticles are highly hydrated: water molecules are present on the surface but can also be directly inside the structure. This lead to many defaults, that explain part of ruthenia high capacitance, electrocatalysis or catalysis properties

To characterize the small (2nm) hydrous and doped nanoparticles, traditional laboratory analysis such as X-Ray Diffraction methods are not sufficient. We have therefore developed Pair Function Distribution analysis from a laboratory diffractometer (Mo anode, reflection or transmission depending the sample, Qmax=15Å^{-1}, D8 Advance diffractometer). Indeed, knowledge of distance histograms, from extremely small coherent length crystalline particles provides direct insight on local structure.

In parallel, DFT calculations are performed to propose structural models. For RuO_2, experimental PDF were successfully compared with DFT optimized models including water. Numerous cobalt insertion schemes are foreseen; For this reason, adapted Monte Carlo methods are used to propose several structural models, screened via DFT energy minimization.

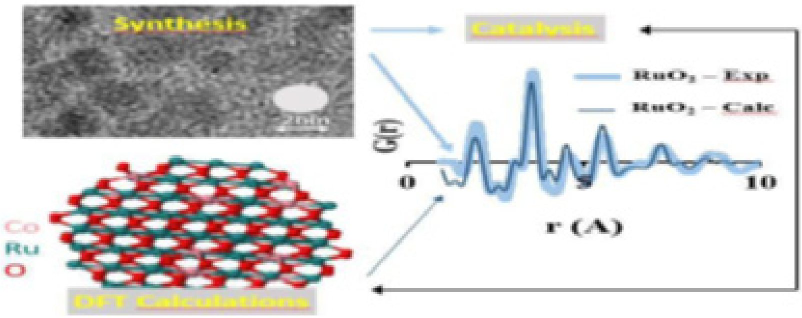

Figure 1: Loop between synthesis, PDF analysis and DFT calculations.

Audience Take Away:

- Comparison of experiments (synthesis, TEM, PDF, catalysis) with calculation (DFT) is an extremely useful tool for understanding particle activity and stability.
- Pair Function Distribution analysis can be performed from a laboratory adapted diffractogram and not only from synchrotron.

Biography

Capucine Sassoye received her PhD degree in 2001 at the University of Versailles Saint Quentin (UVSQ, France) in 2001. After postdoctoral fellowships at Notre Dame University (USA) and the University of California Los Angeles (UCLA, USA), she is currently assistant professor at Sorbonne University (France). Her research deals with inorganic nanomaterials, coupling the sol-gel chemistry with advanced process to tune both macroscopic shape and texture, with sustainability in mind, concerning both material synthesis and its further applications. She is particularly interested in relationship between the atomic structure and properties and has recently developed PDF analysis in her laboratory. She has so far authored/co-authored 32 peer-reviewed journal articles.

Fabrication of new types, environmentally-safe fire-extinguishing powders and foam-suspensions based on raw materials

Lali Gurchumelia, Lasha Tkemaladze*, Olga Chudakova
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G. Tsulukidze Mining Institute, Tbilisi, Georgia.

The aim of the presented investigation is the fabrication of environmentally-safe, high-efficient, fire- extinguishing powders on the basis of local mineral raw materials of silicate origin and production of highly effective foam-suspensions based on such powders. The technology for production of these materials is simple and significantly differs from the serial production technology. Such fire-extinguishing powders are prepared according to the mechanical treatment and mixing of raw materials, which do not require modification with expensive, halogen-containing hydrofobizaing additives. On the one hand it simplifies technological process of production of powder and on the other hand decreases prices of powder. Such powders are characterized by high performance properties as well as fire-extinguishing effect. Also, they have good compatibility with water and foams. The addition of surface active substances into powder suspensions decreases water surface tension, increases permeability and causes powder flotation, which will enable to spray powder together with water and foam. Thus, foam-suspensions are prepared by mechanical blending of waters, obtained fire-extinguishing powders and surface active substances. Thus, foam-suspensions elaborated on the basis of the received powders, have higher cooling effect and permeability compared to powders, while differing from water and foam they make homogeneous, as well as, heterogeneous inhibition of burning process. Therefore, they have higher extinguishing ability than water or powders taken separately.

Fire-extinguishing powders of our preparation may be effectively used for extinguishing of all classes of fires in underground and aboveground objects, within large temperature range, as well as at such low temperatures when CO_2, water and foam cannot be used and in complex with water and foams for extinguishing of large scale fires – forest fires.

Biography

Lasha Tkemaladze physist, undergraduate . I work LEPL G.Tsulukidze Mining Institute (Georgia) at the Department Rock Properties and in-solid Physical Processes Research. Scope of scientific interests: physical science, physical engineering, ecological engineering. I have 10 publications, including in the Infactorial Journal -2. The last 10 years I have participated in 2 scientific grant. Currently I am a partisipant of the grant # 216770 - " New type fire-extinguishing powders and foam-suspensions based on local mineral raw materials" funded of the National Science Foundation. I participated in some international conferences and congresses: Elenite Holiday Village, Bulgaria; Rome, Italy; Paris, France and Tbilisi, Georgia. I have some years of experience in the study and evaluation of fire–extinguisghing and fire- protective materials.

Selective ionic flow cells (SIFC) an alternative to treat wastewater and reduce climate change

Lozada-Castro J.J
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One of the problems that currently occur is the pollution caused by domestic wastewater, as a consequence of the growing world population; this problem affects human health and the environment. For this reason, it is necessary to develop innovative, effective and economic techniques that mitigate this problem. Human excreta (feces and urine) are among the main pollutants present in domestic wastewater, an alternative to solve this problem is to use human excrement to produce energy, since they contain molecules with low oxidation potentials which can be used for the generation of hydrogen in a reduction process, urea is the most abundant organic substance in the urine (product of human excretion), SIFC (national patent registration number NC2017/0012602, international patent application number PCT/IB2018/058596) they are electrochemical systems developed to produce hydrogen from reduction of hydronium ions and oxidation of decomposing organic matter (excrement).

These cells are formed by two semi-cells with stainless steel electrodes: a half anodic cell in which the oxidation reaction of the organic molecules present in the human excrements takes place applying the principle of electrolysis and a cathodic cell in which they reduce the ions hydronium. (H_3O^+) applying the law of chemical equilibrium, these two half cells are separated by a membrane system: a membrane of proton exchange combined with another of exchange of anions and a system of electric bridges, these systems allow selective electric transport and of the masses.

The SIFC technology has demonstrated the production of hydrogen with a purity of up to 96% (w/v). The SIFC technology has the following advantages: the hydrogen produced is a source of clean energy in the combustion process produces only water vapour and high amounts of energy, degrades organic matter through electrolysis at high potentials (12 V) thus providing an alternative treatment to matrices containing large amounts of organic matter such as domestic wastewater, the conditions allow to obtain the electrical energy for the reactions of photovoltaic cells (solar energy), gaseous hydrogen can substitute several conventional energy sources (gasoline, diesel, residential gas and hydroelectricity); therefore SIFC technology aims directly at the reduction of atmospheric emissions and the prevention of the greenhouse effect and acid rain.

The idea of using electrochemical techniques for water treatment is not a new idea, currently two techniques are known; electrolysis and electrocoagulation, electrolysis is an electrochemical technique that is based on the oxidation of organic matter using inert electrodes, such as diamond electrodes doped with boron (DDB) or stainless steel, electrolysis is commonly complemented with techniques of electrocoagulation, in order to improve the elimination of pollutants from domestic wastewater, the cells perform these processes with low energy consumption, also eliminates microorganisms by their operating conditions.

Audience Take Away:

- produce clean energy from the human excrement
- produce hydrogen with low energy requirements
- finance wastewater treatment
- new technology to produce hydrogen gas thermo-dynamically viable
- implement wastewater treatment plants using SIFC technology

Biography

Dr. Juan Jose Lozada Castro studied Chemistry at the Santiago de Cali University, Colombia 1992, graduated as Mg. in 1997 Valle University, Doctor in Analytical Chemistry from the Complutense University of Madrid in 2013. he directs the research group “Study of Contaminant Systems” Nariño University, Pasto Colombia. Associate Professor at the Nariño University. he has published more than 10 research articles, currently processes two patents in national and international phase and prepare two more.

Integrated two stage processing of biomass conversion to HMF esters using ionic liquid as green solvent and catalyst: Synthesis of mono esters

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In this study a two stage process were established for the synthesis of HMF esters using ionic liquid acid catalyst. Ionic liquid catalyst with different strength of the Bronsted acidity was synthesized in laboratory and characterized using ^{1}H NMR, FT-IR and ^{13}C NMR spectroscopy. Solid acid catalyst from the ionic liquid catalyst was prepared using immobilization method. The acidity of the synthesized acid catalyst was measured using Hammett function and titration method. Catalytic performance was evaluated for the biomass conversion to 5-hydroxymethylfurfural (5-HMF) and levulinic acid (LA) in methyl isobutyl ketone (MIBK)-water biphasic system. Good yield of 5-HMF and LA was found at the different composition of MIBK: Water. In case of MIBK: Water ratio 10:1, good yield of 5-HMF and LA was observed at ambient temperature 150 ˚C. Upgrading of 5-HMF into mono esters from the reaction of 5-HMF and reactants using biomass derived mono acid were performed. Ionic liquid catalyst with -SO_3H functional group was found to be best efficient in comparative of solid acid catalyst for the esterification reaction and biomass conversion. A good yield of 5-HMF esters with high 5-HMF conversion was found to be at 105 ˚C using the best active catalyst. In this process, process A was the hydrothermal conversion of biomass and its monomer into 5-HMF and LA using acid catalyst. And the process B was the esterification followed by using similar acid catalyst. All mono esters of 5-HMF synthesized here can be used in chemical, cross linker for adhesive or coatings and pharmaceutical industry. A theoretical density functional theory (DFT) study for the optimization of the ionic liquid structure were performed using Gaussian 09 program to find out the minimum energy configuration of ionic liquid catalyst and their comparative Bronsted acidic strength.

Audience Take Away:

- Ionic liquid synthesis and their acidity characterization using Hammett acidity function.
- Immobilization of the ionic liquid on to the solid support for the synthesis of solid acid catalyst.
- Finding the minimum energy configuration using density functional theory (DFT) probably that structure is responsible for catalytic activity.
- Using DFT calculation we can find out the reaction pathway for the esterification reaction of 5-HMF with different acids.

Biography

Komal Kumar is a research scholar in Indian Institute of Technology Delhi in the department of chemical engineering. Earlier he did his M. Tech. in Molecular Engg. Chemical Synthesis and Analysis from the department of chemistry Indian Institute of Technology Delhi. Currently he is working on his PhD thesis entitled “Catalytic conversion of lignocellulosic biomass into value-added chemicals and their upgrading” at Indian Institute of Technology Delhi, India. His current interest is involved synthesis and characterization of the ionic liquid catalyst and their application in the field of biomass degradation into value-added chemicals.

Synthetic, Biological evaluation of Bis Tetrathiomolybdate compounds of Pt, Pd and Ni Ions

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The Chemistry of compounds containing Transition metals bound to sulfur containing ligands has been actively studied. Interest in these compounds arises from the identification of the biological importance of Iron-sulfur containing proteins as well as the unusual behaviour of several types of synthetic metal-sulfur complexes. Metal Complexes $(C_6H_5)_4P)_2$ Pt $(Mos_4)_2$, $(C_6H_5)_4P)_2$ Pd $(MoS_4)_2$, $(C_6H_5)_4P)_2$ Ni $(MoS_4)_2$ of Bioinorganic relevance were investigated. The complexes $[M(M'S_4)_2]_{2-}$ were prepared with high yield and purity as salts of the variety of organic cations. The diamagnetism and spectroscopic properties of these complexes confirmed that their structures are essentially equivalent with two bidentate $M'S_4^{2-}$ ligands coordinated to the central d^8 metal in a square planer geometry. The interaction of the complexes with CT-DNA was studied. Results showed that metal complexes increased DNA's relative viscosity and quench the fluorescence intensity of EB bound to DNA. In antimicrobial activities all complexes showed good antimicrobial activity higher than ligand against gram positive, gram negative bacteria and Fungi. The antitumor properties have been tested in vitro against two tumor human cell lines, Hela (derived from cervical cancer) and MCF-7 (derived from breast cancer) using a metabolic activity tests. Result showed that the complexes are promising chemotherapeutic alternatives in the search of anticancer agents.

Biography

Dr V.K Srivastava received his M.Phil and Ph.D Degree from Institute of Basic Sciences Dr B.R Ambedkar university Agra After completing his PhD he joined RBS Engineering College Agra as Lecturer in Applied Chemistry and currently as Associate Professor (Inorganic Chemistry) in D.S College ,Aligarh, UP India

His current area of Research expertise is focused on synthetic inorganic, Bioinorganic and Coordination chemistry of metal complexes.He has been recipient of several awards and honors few of them are like young scientist award, Best research paper award on tungsten chemistry, Award for excellence in research, Distinguished faculty award and Professor of the year(Biochemistry) 2018 etc. He has published numerous research papers in Journal of high repute and contributed to academic National and international conferences. He also published Book chapter and Books on Bioinorganic chemistry and Medical Bioinformatics springer publication.

New fluorine containing solid polymer electrolyte membranes

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Chavchavadze Ave., 3, Tbilisi 0179, Georgia
[2]Institute of Macromolecular Chemistry and Polymeric Materials, Ivane Javakhishvili Tbilisi State University, I. Chavchavadze Ave., 3, Tbilisi 0179, Georgia

Polymer electrolytes (PE) play an important role in electrochemical devices such as batteries and fuel cells. To achieve optimal performance, the PE must maintain a high ionic conductivity and mechanical stability at both high and low relative humidity. The polymer electrolyte also needs to have excellent chemical stability for long product life and robustness.

According to the prevailing theory, ionic conduction in polymer electrolytes is facilitated by the large-scale segmental motion of the polymer backbone and primarily occurs in the amorphous regions of the polymer electrolyte. Crystallinity restricts polymer backbone segmental motion and significantly reduces conductivity. Consequently, polymer electrolytes with high conductivity at room temperature have been sought through polymers which have highly flexible backbones and have largely amorphous morphology.

The interest to polymer electrolyte was increased also by potential applications of solid polymer electrolytes in high energy density solid state batteries, gas sensors and electrochromic windows. Conductivity of 10^{-3} S/cm is commonly regarded as a necessary minimum value for practical applications in batteries. It is well established also that lithium ion coordination takes place predomi-nantly in the amorphous domain and that the segmental mobility of the polymer is an important factor in determining the ionic mobility important. So, investigation in the field of creation new solid polymer electrolyte membranes with new host fluorine groups is important.

By hydrosilylation reaction of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane (D_4^H) with 2.2.3.3.4.4.5.5.6.6-octafluoropentyl acrylate and vinyltriethoxysilane at 1:3:1 ratio of initial compounds in the presence of platinum catalysts $D_4^{RR'}$type adduct has been obtained. Via ring opening polymerization reaction of $D_4^{R,R'}$ in solution, in the presence of anhydrous powder-like potassium hydroxide, new comb-type siloxane matrixes with pendant octafluoropentyl propionate side groups and triethoxysilane groups have been obtained. So, ssynthesized comb-type polymers were analyzed by FTIR, ^1H, ^{13}C, and ^{29}Si NMR spectroscopy, DSC and GPC methods. Sol-gel reactions of polymers doped with lithium trifluoromethanesulfonate (triflate) and lithium bis-(trifluoromethanelsulfonyl)imide have been studied and new solid polymer electrolyte membranes have been obtained. The ion conductivity of the membranes was determined via electrical impedance spectroscopy. The ion conductivity of solid polymer electrolyte membranes at 25°C changes in the range 7.8x10^{-5} - 9.1x10^{-7} S/cm.

Acknowledgment: The financial support of the Georgian National Science Foundation and Technology Centre in Ukraine, STCU-2016-16 (6301), is gratefully acknowledged.

Audience take away:

- Synthesis of new D_4’ type organocyclotetrasiloxanes containing 2.2.3.3.4.4.5.5.6.6-octafluoropentyl propionate groups and ethyltriethoxysilane crosslinking moieties at silicon; investigation polymerization reactions of organocyclotetrasiloxanes in the presence of various catalysts; investigation of sol-gel reactions of obtained comb-type polymers with regular arrangement of side groups; obtaining solid polymer electrolyte membranes on the base of Lithium salt: Lithium triflate and Lithium bis(trifluoromethanesulfonyl) imide and investigation of their ion-conductivity
- For obtaining of comb-type polymers with regular arrangement of electro donor side groups they will use suggested by us this method.
- This suggested way of synthesis of comb-type polymers with regular structure for obtaining of solid PE membranes will be used by another researcher in their research and teaching, which will be make their research more efficient, informative and interesting.

Biography

From 2009-now, Iv. Javakhishvili Tbilisi State University (faculty of Chemistry) - Head of laboratory 1993-2006 Iv. Javakhishvili Tbilisi State University (Department of Macromolecular Chemistry)-Senior Researcher.1982-1992 Iv. Javakhishvili Tbilisi State University (Department of Macromolecular Chemistry)-Researcher. Author more than 210 publication, where: 8 books, 2 monographs and 1 inventions.Under guidance 1 doctor dissertation and 6 bachelor works has been prepared.

Electrocatalytic enhancement of oxalic acid oxidation using platinum/carbon black-nickel-reduced graphene oxide on screen-printed carbon electrode

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[1,2,3]Applied Science & Engineering for Social Solution Unit, Faculty of Science, King Mongkut's University of Technology Thonburi, 126 Pracha-utid Road, Bang Mod, Thungkru, Bangkok, 10140, Thailand

The platinum/carbon black-nickel-reduced graphene oxide (Pt/CB-Ni-rGO) nanocomposites were prepared by reduction method. Graphene oxide (GO) support was synthesized from natural graphite powder using a modified Hummer's method. Then, nickel ions were reacted with surface functional groups of GO via an ionic adsorption process at pH 11. The carbon black was decorated into this nanocomposite to obtain the CB-Ni-GO nanocomposite. Reduction of platinum by ethylene glycol produced Pt/CB-Ni-GO catalysts. Their morphology and chemical component were characterized by scanning electron microscopy (SEM) and energy dispersive and X-ray (EDX), respectively. The results clearly demonstrated the achievement in Pt/CB-Ni-rGO nanocomposite formation. The spectrum of EDX confirmed the presence of exclusively carbon (C), oxygen (O), nickel (Ni) and platinum (Pt), which indicated the success of the composite formation with a high purity. Moreover, the deposition and distribution of Pt nanoparticles on CB-Ni-rGO was investigated by transmission electron microscopy (TEM). The nano-sized particles (2.89±0.54 nm) of Pt were excellently loaded on CB-Ni-rGO. The cyclic voltammetry (CV) technique was applied to investigate the electrocatalytic activity of the Pt/CB-Ni-rGO on electrode. It was indicated that appropriate amount of Pt could enhance the catalytic activity of Pt for oxalic acid electro-oxidation. In addition, different metal loaded on CB-Ni-rGO were also investigated. The result showed that the oxidation peak current of oxalic acid on Pt/CB-Ni-rGO modified screen-printed carbon electrode was highest and occurred at lowest potential among Ag/CB-Ni-rGO, Au/CB-Ni-rGO and Pd/CB-Ni-rGO. The linearity and limit of detection were found in the range of 20-60,000 µM and at 2.35 µM, respectively.

Audience Take Away:

- Synthesis of the platinum/carbon black-nickel-reduced graphene oxide nanocomposites
- Characterization of the platinum/carbon black-nickel-reduced graphene oxide nanocomposites
- Application for oxalic acid electrochemical analysis using the platinum/carbon black-nickel-reduced graphene oxide nanocomposites

Biography

Kamolwich Income is a Ph.D. candidate in the Department of Chemistry at King Mongkut's University of Technology Thonburi. He received his B.S. in Chemistry in 2006 and his M.S. in Chemistry in 2015, both from the Chiang Mai University. He joined the research group of Asst. Prof. Wijitar Dungchai at the Organic Synthesis, Electrochemistry & Natural Product Research Unit, King Mongkut's University of Technology Thonburi. His research interests include graphene-based catalytic materials and electrochemical sensors research.

Synthesis and characterization of Tetranuclear Palladium complexes of abnormal N-heterocyclic Carbene ligands and their catalytic application in C—C Coupling reaction

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Based on the ligand scaffold of an imidazolyl/benziimidazolyl moiety and an N-$CH_2C(=O)NHPh$ amide substituent, we prepared two novel series of ligand precursors with an ortho hydroxy group incorporated on the N-phenyl ring. We demonstrated that the structural fine tuning of the ligand scaffold allowed the facile synthesis of tetranuclear palladium complexes including the first example of such multinuclear complexes with abnormal NHC (aNHC) ligands. For those precursors with C2-phenyl group, tetranuclear complexes featuring a tridentate ligand of aNHC, amidate, and bridging phenoxide donors was produced. For those with C2-methyl group, an extra addition of pyridine was essential leading to the production of mononuclear tridentate palladium aNHC complexes or tetranuclear complexes with tridentate ligands of methylene, amidate, and bridging phenoxide donors. Representative mononuclear and tetranuclear palladium aNHC complexes were structurally characterized by X-ray diffraction studies, revealing extremely short Pd—C bond distances. The tetranuclear palladium aNHC complexes were used Mizoroki-Heck reaction in ionic salt, delivering higher activities than the mononuclear complexes. The structures of three of the new complexes were further established by single-crystal X-ray diffraction studies.

Audience Take Away:

We demonstrated that the structural fine tuning of the ligand scaffold allowed the facile synthesis of tetranuclear palladium complexes.

Enantioselective [4 + 2]-annulation of oxadienes and allenones catalyzed by an amino acid derived phosphine: Synthesis of functionalized dihydropyrans

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An enantioselective [4 + 2]-annulation process between cyano-activated oxadienes and allenones is developed. An L-valine-derived phosphine was efficient in catalyzing the reaction, and a wide range of highly functionalized dihydropyrans were prepared in high yields and with excellent enantioselectivities.

Audience Take Away:

- Oxadienes is used as a C4 synthon, in combination with allene ketones to produce structurally unique ring motifs.
- A wide range of highly functionalized dihydropyrans can be synthesized by adopting to our synthesis method
- The audience would realize a new methodology of constructing synthetically useful molecular architectures

Biography

Prof. Nisar obtained his PhD from the University of Graz, in 2001. He then assumed postdoctoral positions in McMaster University and University of Guelph, Canada, for one year each. He joined KFUPM as an Assistant Professor in 2007 where he is now a Professor of Organic Chemistry. His research is mainly centered on the organic synthesis, designed based drug development and environmental chemistry. He has authored more than 85 papers in reputed journals and is the recipient of Diligence, Dedication and Performance Award by Pfizer Ann Arbor, USA in 2005 and Excellence in Research Award, KFUPM, in the year 2019.

Carbon nanodots for mercury ions detection

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In this research work, carbon nanodots were developed for determination of mercury ions. CDs were performed according to a simple one-step by microwave method. In the synthesis of CDs, citric acid was added in ultrapure water followed by ethylenediamine for produced nitrogen doped on CDs surface. The mixed solution was then put in microwave within 5 min. It was appeared the red-brown foamy solid and purified by using centrifugal filter unit. Characterization of carbon nanodots was studied by XRD, UV-vis, Fluorescence spectroscopy, TEM and FTIR. For the optical properties, the absorption spectra were shown at 350 nm which was the n-π^* electron spectra of C=O and the sp3 hybridization. The emission wavelength was presented in a high intensity at 450 nm. The structure and functional group of carbon nanodots were studied by spectroscopic method using FTIR. The appearing peaks at the 1400 and 1320-1100 cm-1 wave positions were shown the bending vibration of C-N and C=N in the structure and the surface of the carbon nanodots. From the TEM image, it has good dispersion with a narrow size distribution in the range of 2 to 5 nm. The average diameter of the CDs was shown in 3 nm. The Hg2+-CDs complex was provided bigger size of CDs at 90 nm. In the presence of mercury ions, the fluorescence emission of CDs was gradually quenched by photo-induced electron transfer. The fluorescence turn-off of carbon nanodots obtained by Hg2+-CDs complex which didn't interfere from other metal ions. The occurring interaction of mercury ions and CDs was applied on paper-based device by control with the black-light. The application on paper-based device provided several advantages that are simple, inexpensive material and the fabrication is cost effective. Moreover, it will be suitable for on-site environmental monitoring.

Audience Take Away:

- Synthesis of carbon nanodots
- Characterization of carbon nanodots
- Application for mercury detection and alternative method using paper-based device

Biography

Benjawan Ninwong studied Chemistry at the Chulalongkorn University, Thailand and graduated as MS in 2012. Now, she studying in PhD at King Mongkut's University of Technology Thonburi. She received a scholarship from Royal Thai Government Scholarship for PhD. She joined the research group of Asst. Prof. Wijitra Dungchai at the Organic Synthesis, Electrochemistry & Natural Product Research Unit.

Synthesis, characterization and catalytic applications of Au@Pd heteroparticles

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The catalytic and optical properties of nobel-metal nanoparticles can be tuned by controlling the shape and dimensions. Multicomponent nanomaterials consisting of two or more than two noble metals can enhance these properties not only due to the presence of more than one domain but also because of the interfacial electronic communication. We present the synthesis of different shape multicomponent Au@Pd nanoparticles by controlling the nucleation and growth steps in non-aqueous medium. Moreover, we have explored the role of different morphologies on the catalytic activity for the reduction of 4-nitrophenol to 4-aminophenol with sodium borohydride. The composition and crystal structure of all bimetallic NPs were analysed using high resolution transmission electron microscopy (HR-TEM) equipped with energy dispersive X-ray spectroscopy (EDX), X-ray diffraction and electron diffraction (ED).

Audience Take Away:

- Synthesis of bimetallic multicomponent nanoparticles
- Control on nucleation and growth processes on nanoscale
- Efficient use of advanced nanoscale characterization techniques

Biography

Dr. Muhammad Nawaz Tahir received his PhD in 2006 from Johannes Gutenberg University (JGU) of Mainz, Germany with distinction "Summa Cum Laude" under the supervision of Prof. Wolfgang Tremel. Later, as post-doctoral fellow, he underwent many research projects funded by DFG, MWFZ and Max Plank Society. In 2010, he joined the Institute of Inorganic and Analytical Chemistry JGU Mainz, as senior scientist. Since September, 2017 he joined the Chemistry Department, King Fahd University of Petroleum and Minerals as assistant Professor. His research interests involve synthesis of innovative nanomaterials, characterization, surface functionalization, for biomedical and energy storage applications.

DAY 2

E - POSTERS

4th Edition of

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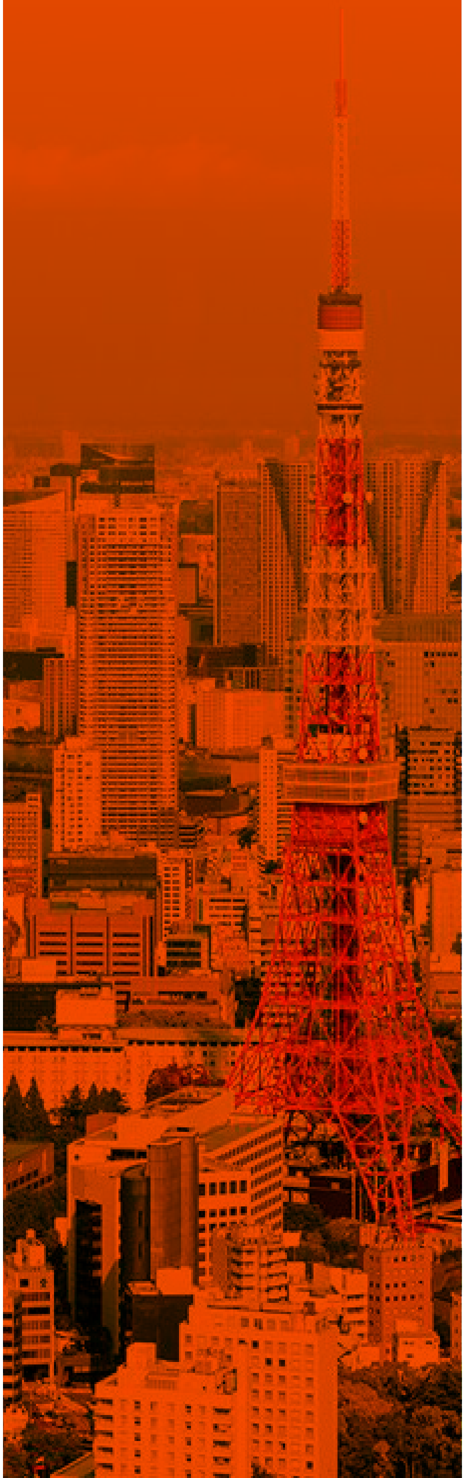

The use of aerosol nanocatalysis technology is one of the new directions of industrial development

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Currently, the success of the chemical industry is associated with the use of heterogeneous catalysis on carriers. It is also called traditional catalysis. The majority of modern scientific works in the field of catalysis include:

- The search for catalytically active substances and mixtures,
- The improvement of their structure and the choice of carrier material,
- The technology of preparation and methods of fixing the active substances on the surface of the carrier.

The most important problems considered the problems of activity, poisoning and regeneration of catalysts. Despite the technology with a catalyst on a carrier has a development in chemistry and covers a wide range of raw materials and processes. The difficulties of this catalysis are associated with both a reduction in the possibility of full use of the technology, and a rapid deactivation of the catalyst. The technology of aerosol nanocatalysis (AnC), developed by us, reduced the effect of these difficulties.

This technology is based on the use of a catalyst without a carrier in the aerosol. It is crushed to nanoscale in a reactor in situ. The constant mechanical and chemical activation of the surface of the catalyst nanoparticles in the reactor allows:

- Maintains high catalyst activity;
- Increases the reaction rate (10^4–10^6 times based on the weight of the catalyst when compared with traditional catalysis);
- Reduces the catalyst concentration (up to 0.3–5 g/m^3 of the reaction volume);
- Reduces the reactor volume (2–10 times);
- Allows you to even reach the catalyst surface with reagents;
- Uses reagents in any aggregate state.

The first publication on AnC technology appeared in the journal The Theoretical Foundations of Chemical Technology in Russia in 1996. The technology AnC began with the technology with a fluidized bed reactor. During the development of technology, about 50 individual substances and about 30 real industrial wastes were investigated. The obtained results of laboratory studies were confirmed in four pilot plants in Russia, Ukraine and Sweden. Unfortunately, the technology of aerosol nanocatalysis has not received further industrial development.

The technology AnC under laboratory conditions develops in a vibro-fluidized bed reactor. It is convenient for studying the kinetics of chemical reactions in the laboratory. Also, there is a new development in the reactor with a rotating bed. It is effective in chemical interaction and easy to use in industry. The technology of aerosol nanocatalysis has proven itself well in both ecological processes and some syntheses of chemical compounds.

The table presents some of the processes studied in the reactor aerosol nanocatalysis.

Table. Some processes investigated by aerosol nanocatalysis technology

process	temperature, K	catalyst		reaction rate	
		g/m^3	composition	kg/m^3*hour	kg/g$_{cat}$*hour
cracking process:					
n-pentane	873	5,0	V_2O_5	849,6	169200
vacuum gas-oil	873	1,0	CaA	1265,2	421745
	723	3,0	Si/Zr	1177,6	392526
	873	2,0	Nexus-345	434,1	217000
oxidation processes:					
1,2-dichloroethane	853	3619	CuO	135,97	117,36
	903	2,4	CuO	3033,6	1264,2
natural gas	973	4,8	Fe_2O_3	92,16	70056
tarsil water	873	0,5	Fe_2O_3	168,4	168426
waste lubricant drain	873	0,1	Fe_2O_3	14,3	143200

Audience Take Away:

- The technology of aerosol nanocatalysis is one of the new promising areas for the development of the chemical and petroleum refining industry.
- The technology of aerosol nanocatalysis will be interesting for enterprises and companies related to environmental issues.
- The technology of aerosol nanocatalysis will allow scientific organizations to take a fresh look at the kinetics of chemical and physical processes simultaneously.
- The technology of aerosol nanocatalysis is universal and mobile for various chemical transformations.

Biography

Dr. Glikina I. graduated as MS in 1998 in Severodonetsk Technology Institute (now Volodymyr Dahl East-Ukrainian National University). While studying at the institute Iryna was engaged in research activities. Her work is related to scientific research in the field of catalytic processes, research and development of promising global chemical industry technologies. She received her PhD degree in 2005 at the at the National University Lviv Polytechnic and degree of Doctor of techninal science in 2015 at the same university. She is the author of over 150 research publications on chemical technology of organic substances and fuel.

Whole-cell bioconversion of naringenin using *Yarrowia lipolytica* 2.2ab in surface and liquid cultures

Christian Hernández-Guzmán[1], Angélica Román-Guerrero[1], Arely Prado-Barragán[1], Miquel Gimeno[2], Sergio Huerta-Ochoa[1*]

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Naringenin is a polyphenolic molecule considered within the subgroup of flavanones that in addition to the important antioxidant activity, several beneficial effects on health have been attributed to this molecule. Flavonoids are natural phenolic compounds that exert several biological acivities suchlike antioxidant, anti-inflammatory, antibacterial, antiviral, estrogenic, vasodilator, hepatoprotective, antihemorrhagic, and many others. Naringenin is a polyphenolic molecule considered within the subgroup of flavanones, which in addition to the important antioxidant activity, several beneficial effects on health have been attributed to this molecule. For this reason, the study of this molecule has attracted the attention of various research groups. The flavanones also called bioactive compounds, are plant origin and their industrial production is limited due to their complex extraction from vegetal substrates and the low extraction obtained. To overcome these limitations, the microbial biosynthesis may represent a suitable alternative to increase its production. The antioxidant activity exerted by the flavonoids is related to the hydroxyl groups in the polyphenol B ring, reason why the increase of the antioxidant activity in the flavonoids is directly related to the hydroxylation degree. The increase in the hydroxylation degree of the flavonoid molecules can be directed from specific molecules by means of its bioconversion by enzymes or whole microbial cells. This study aims to identify the resulted products from naringenin bioconversion by whole cells of *Yarrowia lipolytica* 2.2ab (Yl2.2ab) either superficial and liquid culture media. Identification of the hydroxylated products was performed by HPLC and HPLC-MS-MS. Antioxidant activity was measured by ABTS and DPPH methods. Increase on hydroxylated and dehydrogenated groups from naringenin bioconversion by Yl2.2ab was observed in both culture media; apigenin, luteolin, aromadrine, ampelopsin and myricetin compounds were identified. These molecules are highly desired by the pharmaceutical and food industries; then are considered as compounds with high value added. Additionally, the compounds obtained have greater antioxidant activity with respect to naringenin, the molecule used as precursors during bioconversion by complete cells of Yl2.2ab shown in this work

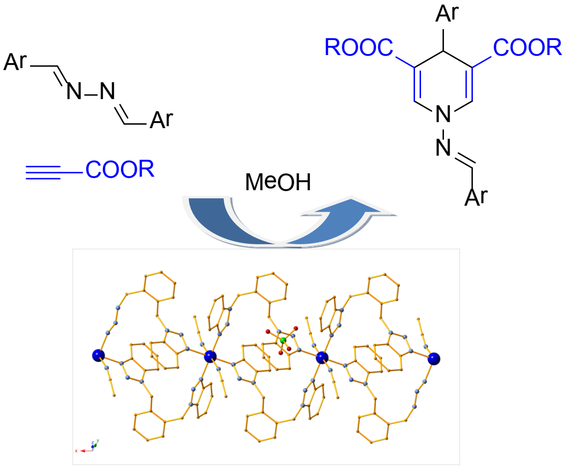
Audience Take Away:

- The audience will learn that the biological properties of flavonoids with important beneficial effects on human health might be enhanced by increasing the adding more hydroxylated and / or methoxylated groups of an original precursor. They will also learn that bioconversion processes consist of enzymatic modifications to a given substrate by biological systems (microbial whole cells) as biocatalysts.
- The industrial production of flavonoids is restricted due to low concentrations in plant tissues, low presence in species, and difficulties find during its extraction from plants. To overcome these restrictions a promising strategy is the bioconversion mechanism. In this study, the biological properties of the flavonoids are analyzed focusing on the relationship between their antioxidant activity and the degree of hydroxylation which occur through alternative processes such as microbial bioconversion, obtaining compounds with greater added value.
- This simple process of microbial bioconversion for the efficient production of polyhydroxylated compounds from naringenin by yeast *Y. lipolytica* 2.2ab gives rise to future research projects where this type of process is carried out with whole cells and bioactive compounds serving as a direct antecedent and as a basis for an optimization of the process.
- Because this process of bioconversion is simple it represents a practical and efficient solution in the obtaining of compounds of interest.
- The bioconversion process can be optimized to provide new information, selection of the appropriate bioreactor and obtain better production.

Copper-benzotriazole based coordination polymer as catalyst towards the one-pot synthesis of N'-substituted-hydrazo-1,4-dihydropyridines

Michael G. Kallitsakis,[1*] Edward Loukopoulos,[2] George E. Kostakis[2], Ioannis N. Lykakis,[1]
[1]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece
[2]Department of Chemistry, School of Life Sciences, University of Sussex, Brighton BN19QJ, UK

1,4-dihydropyridines (1,4-DHPs) represent one of the most important class of *N*-containing heterocyclic compounds, used as L-type calcium channel blockers in the treatment of cardiovascular diseases.[1] Therefore, useful synthetic strategies for 1,4-dihydropyridines have been developed.[2] Recently, much attention has been directed toward the synthesis of *N*-substituted-1,4-dihydropyridines with interesting biological properties.[3] In this respect, we elaborate the efficient one-pot synthesis of novel symmetrical (*N*'-substituted)-hydrazo-4-aryl-1,4-dihydropyridines in moderate to good yields from electron-rich azines and propiolate esters catalyzed by a one-dimensional copper-benzotriazole based coordination polymer.[4] The reaction proceeds with low catalyst loading, under mild catalytic conditions and without the need of inert atmosphere and base additives. Fine-tuning the catalyst allowed us to gain more insights regarding the plausible reaction mechanism.[5]



Audience Take Away:

- Metal-catalyzed organic synthetic methodology
- Homogeneous catalysis in the area of Green Chemistry
- Cu(II)-benzotriazole based one-dimensional coordination polymers chemistry
- Synthesis of (*N*'-substituted)-hydrazo-4-aryl-1,4-dihydropyridines as molecules with biological activity

Biography

Dr. Kallitsakis, received his Bachelor (2007) at the Chemistry Department of the Aristotle University of Thessaloniki, and he earned his Master's Degree (2009) and his PhD at the same institution (2014) under the supervision of Prof. Litinas. Since 2015, he is working as a post-doctoral researcher under the supervision of Prof. Armatas and Prof. Lykakis, with an ERC grand and IKY fellowship. During his post-doctoral period (2016) he worked as a visiting Researcher at the School of Life Sciences of University of Sussex in collaboration with Assoc. Prof. G. Kostakis. So far, he has 12 publications in peer reviewed journals.

Synthesis and features of formation of hydrated oxides at the nanoscale level

Olga V. Artamonova*, Mariya A. Shvedova
Department of chemistry and chemical technology of materials, Voronezh state technical university, Voronezh, Russia

Formation of nanoscale particles (NSP) with controlled properties complicated insufficient study of the processes of nucleation and growth of particles of different chemical nature, their structuring at separate stages of formation. Disclosure of the process of formation of a solid at the phase formation stage (nucleation at the nanoscale level) is most significantly, since the processes occurring at this stage predetermine the structure and properties of the solid. At the nanoscale level, the formation of materials is subject to the same fundamental laws of structure formation, which is important both for understanding effective, purposeful management of changes in the composition, size and morphology of the NSP and for obtaining multifunctional composite materials with the required characteristics.

Present study aims to establish correlations between the conditions of preparation, composition, structure, dispersion, morphology and properties of oxide nanosystems at all stages of their phase formation, starting with the formation of hydrosols and suspensions of hydrated oxides from salt solutions.

In this work theoretical issues and experimental results of the investigation of the formation of the solid phase of hydrated oxides at the nanoscale level in different oxides systems are considered. The research systems have been received by sol-gel method (systems $SiO_2 \cdot H_2O$, AlOOH, FeOOH, NaX), as well as by hydrothermal synthesis (nanotube of chrysotile [$Mg_3Si_2O_5(OH)_4$], synthetic montmorillonite $(Na, Ca)_{0.3}(Al, Mg)_2Si_4O_{10}(OH)_2 \cdot nH_2O$). Based on experimental research the evolutionary models of formation of particles of hydrated oxides at the nanoscale level are proposed. She includes the following stages: hydrolysis of aquaions, their polycondensation with the formation of polymer hydroxocomplex, the formation of the fetus, their further increase, aggregation and crystallisation. The most effective nanoscale additives for hydration-synthesis (cement) and hydrothermal-synthesis (silicate) hardening systems can be the $SiO_2 \cdot H_2O$ system and chrysotile nanotubes, since they have a related crystal-chemical structure with new growths of the solid phase of building composites.

Audience Take Away:

- Theoretical issues and experimental results of the investigation of the formation of the solid phase of hydrated oxides at the nanoscale level in different oxides systems are considered.
- The evolutionary models of formation of particles of hydrated oxides at the nanoscale level are proposed.
- The results of this research can be useful research fellow and specialists working in the field of material science, construction of the composites and products, as well as in their research and scientific activity.

Biography

Olga V. Artamonova studied Chemistry at the Voronezh state university, Voronezh, and graduated as MS in 2001. In 2004 she defended her thesis for the Degree of Chemistry Candidate of on the theme «Synthesis of nanoceramic materials based on zirconium dioxide stabilized with indium oxide» and received her PhD degree. From 2004 she works in Voronezh state technical university (VSTU). From 2006 up to she is Associate Professor of department of chemistry and chemical technology of materials of VSTU. Between 2010 and 2013 she trained in full-time Doctoral studies of VSTU. She has published more 120 scientific publications, including 3 monographs, and 25 teaching materials, including 10 training manual. Scientific activities are synthesis nanostructures and nanotechnology of inorganic hardening systems and composites, as well as elaboration of nanoadditives for modification of structures of construction composites.

On thermodynamics & experimental evidences of the Kurdjumov and spillover effects in carbon nanostructures, under self-intercalation of high density hydrogen

Yury S. Nechaev
Kurdjumov Institute of Metals Science & Physics, Bardin Central Research Institute for Ferrous Metallurgy, Moscow, Russia

Experimental evidences and thermodynamics of the self-intercalation of high-density gaseous molecular hydrogen ($\rho_{H2} \approx 0.045$ g/cm^3, at 300 K) into surface nanoclusters in highly oriented pyrolytic graphite and epitaxial graphene, as well as the self-intercalation of high density solid molecular hydrogen ($\rho_{H2} \approx 0.5$ g/cm3, at 300 K) into graphite nanofibers are considered, with regard to the problem of compact and efficient hydrogen on-board storage. The manifestation and physics of the Kurdjumov and spillover effects in carbon nanostructures, under self-intercalation of high density hydrogen, are discussed. Perspectives of a further development of these results are considered, as well. This work was financially supported by the RFBR (Project # 18-29-19149 mk).

Audience Take Away:

- They will be able to use the thermodynamic approach and these fundamental results in their studies.
- This research could be used to expand their research or teaching, with respect to perspectives of solving the urgent problem of compact and efficient hydrogen on-board storage, and other clean energy applications.

Biography

Yury S. Nechaev is Professor of Materials Science & Metals Physics (Dpt.), Doctor of physical-mathematical sciences (Dr.Sc.)). He is a chief researcher-analyst of G.V. Kurdjumov Institute of Metals Science and Metals Physics, within Federal State Unitary Enterprise “I.P. Bardin Central Research Institute for Ferrous Metallurgy” (I.P. Bardin TsNIIChermet), RF, 105005, Moscow, Radio Str., 23/9, Build. 2. Phone: +8(495)777-93-01. He has published more than 150 research articles in SCI(E) journals.

Effect of doping on Physicochemical characteristics of lead titanate and of barium titanate

Mrharrab Lamiae*, S. Sayouri [1], Y. Ababou[2]
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[2]LPTA, Physics Department, Faculty of Science DM, Fes, Morocco

Since their discovery in 1920 until the mid-1940s, the ferroelectrics constituted a class of materials fragile and difficult to exploit. This has radically changed with the discovery of ferroelectric simple oxides; the synthesis of these new materials, mainly in the form of ceramics, marked the beginning of the exploitation of the ferroelectricity, in the first rank of which is the barium titanate ($BaTiO_3$)(BT) and lead titanate ($PbTiO_3$)(PT). Today, the electro-ceramics industry produces several billion $BaTiO_3$-based capacitors each year. Also, Due to their interesting piezoelectric properties, non-linear optics, electro-optics and holographic, the lead titanate derived materials have become popular in various fields of application.

Thus the doping of BT and PT is still the subject of numerous studies for the realization of agile functions at microwave frequencies (BST), or in the manufacture of transducers (PZT ceramics near the morphotropic phase boundary.

The present work deals with the effect of substitution of Ba by Gd in $BaTiO_3$ (BGT) and of Ti by Zr in $PbTiO_3$ (PZT) on crystalline structure and dielectric properties of these perovskite structured compounds. The $BaTi_{1-x}Gd_xO_3$ (BGT) powders , x= 0, 1, 2, 3 and 4%, were synthesized by the sol gel method and calcined in air at different temperatures and their structure characterized by X-ray diffraction (XRD). Besides, the analysis of the electric impedance of these BGT ceramics in a wide frequency range (0.1Hz-1MHz), at room temperature, have also been performed, and parameters such as capacitance, relative permittivity and dielectric losses have been determined.

$Pb(Zr_x ,Ti_{1-x})O_3$ (PZTx) powders, x=0, 26, 39, 52, 65, 78 and 91%, have been prepared by the conventional solid state reaction, and characterized by X-ray diffraction (XRD), Raman and Fourier transform infrared techniques, and their microstructure was investigated using Scanning Electron Microscopy (SEM). XRD spectra of the PZTx samples revealed a behavior in conformity with the phase diagram established by Jaffe et al. Dielectric analysis showed the presence of an anomaly in the ferroelectric phase of PZT, located at about 275 °C. Few studies have reported the existence of such anomalies, which we have interpreted based on structural results.

Biography

Dr. Mrharrab Lamiae is born in Fes, Morocco, 1983. She received her Ph.D. degree in 2014 at Sidi Mohamed Ben Abdellah University, Morocco, whose subject is the study of physicochemical properties of $PbZr_xTi_{1-x}O_3$ ($0\leq x\leq 0.91$) and pure and doped $PbTiO_3$ by Cu; Bi; V; Mn; Mg; La; Ca produced by the conventional solid state reaction. His work concerns the ceramic materials with perovskite structure and its dielectric properties. She is a Professor of physics at Ibn Zohr University, Ouarzazate, Morocco.

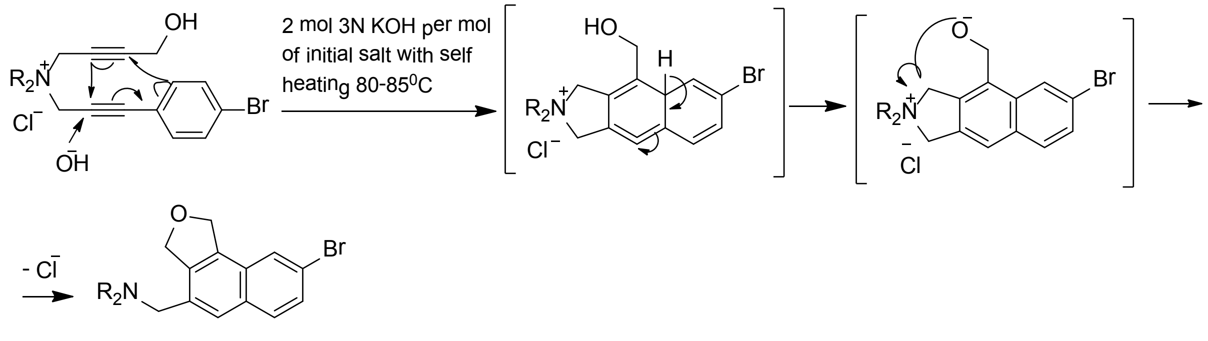
Synthesis of derivatives of 4-hydroxymethylisoindolinium chlorides and their intramolecular recyclization

Chukhajian E.O. *[1], **Ph.D., Shahkhatuni K.G.** [1], **Ph.D., Gevorgyan H.R.** [1], **Ph.D., Khachatryan A. A.** [2], **Ph.D.**
[1]The Scientific Technological Centre of Organic and Pharmaceutical Chemistry of National Academy of Sciences of the Republic of Armenia, Yerevan, Republic of Armenia
[2]Gyumri State Pedagogical Institute after M. Nalbandyan, Gyumri, Republic of Armenia

Base catalyzed intramolecular cyclization, discovered by acad. A.T. Babayan, prof. E. O. Chukhajian with co-authors, is a absolutly new direction in organic and fine organic chemistry and includes excellent possibilities for the synthesis of di-, tri- and tetracyclic condensed isoindolinium and also linearly annulated benzo[f] isoindolinium salts. In continuation of the research, it was found that in the base catalysed conditions -(4-hydroxybut-2-ynyl)(3-alkenyl- or 3-aryl-prop-2-ynyl)ammonium chlorides undergo intramolecular cyclization. For cyclization of above mentioned salts in contrast of the propargylic analogs the reaction mixture is heated at 40–45 °C during 10–15 min, then takes place cyclization with self-heating. The cyclic products - chlorides of -4-hydroxymethylisoindolinium- and –benzo[f]isoindolinium were obtained with high yields. In 2003 it was established that the above mentioned salts in water-base cleavage reaction conditions undergo intramolecular recyclization. As a result are formed derivatives of 1,3-dihydroisobenzo[c]furan, the formation of which include nucleophilic attack of the alkoxy ion on the partially positively charged carbon atom of the isoindolinium cycle. This leads to breaking of N-C bond of the isoindolinium as well as to formation of new C-O bond.

Recently it was established that the cyclization of dialkyl(4-hydroxybut-2-ynyl)(3--bromphenylprop-2-ynyl)ammonium chlorides in water-base condition is accompanied by the subsequent recyclization of cyclic products.W

Scheme



In the case of piperidinium and morpholinium analogs it was possibile to isolate the corresponding salts: chlorides of 2,2-pentamethylen-4-hydroxy-6-brombenzo[f]isoindolinium and spiro[4-hydroxymethyl-6-brombenzo[f]isoindolin]-2,4'-morpholinium. The recyclization of these salts under the conditions of water-alkali cleavage is realized at the room temperature. The observed phenomenon is unique in the field of intramolecular recyclization.

The study revealed the influence of substituents at nitrogen atom, in aromatic ring and the number of aromatic rings on the base-catalyzed cyclization as well as the intramolecular recyclization of cyclic products. For the first time revealed by us intramolecular recyclization is a domino process and, in contrast to intermolecular recyclization, is not accompanied by a narrowing or an increase of the cycle, and instead of a five-membered isoindolinium cycle, a dihydrofuran cycle is formed.

Audience Take Away:

- The audience will learn how to expand the area of base catalized intramolecular Cyclization and Recyclization for synthesis of new bioactive nitrogen-containing heterocycles, 1,3-dihydrobenzo[c]furans and their condensed analogs.
- These compounds have proved to be very attractive and useful for the synthesis and design of molecules of potential drugs.
- The involvement of new dienes and dienophiles in base catalized intramolecular Cyclization and Recyclization will

help to synthesize compounds, the synthesis of which by another methods is difficult.

Biography

Prof. Emma Chukhajian is Leading Scientist and Head of the laboratory of aminocompounds of STCOPHCH NAS RA. She obtained her Ph.D. in 1970, postdoctorial in – 1985. In 1969 she discovered base-catalized intramolecular Cyclization of unsaturated ammonium salts, in 2003 - intramolecular Recyclization of 4-hydroxymethylbenzo[f]isoindolinium salts, in 2008 – isomerisation of 3a,4-dihydroisoindolinium salts, in 2011 – Stevens rearrangement of the salts, containing allylic type group along with 4-hydroxybuth-2-ynyl, in 2016 – deamination of 3-(dialkylamino)-1,4-diarylhex-5-en-1-yns during vacuum distillation, leading to terphenyles, established the mechanisms of mentioned reactions. She has published more than 160 Scientific works.

Loading metal phthalocyanine on modified graphene oxide for photocatalytic effect

Melika Ghaeini*, Mohammad Ali Zanjanchi
Department of Chemistry, Faculty of science / Guilan University, Rasht, Guilan, Iran

Nowadays emission of harmful and dangerous substances which is released from various chemical industries is a major concern. Dichlorophenol (DCP), which is commonly used as herbicide, biocide and wood preservative are extremely dangerous pollutants due to its high toxicity towards all organisms. Over the past decades, different techniques for the treatment of organic-contaminated wastewaters have been applied including photocatalysis and recently, cobalt phthalocyanine (CoPc), a two-dimensional 18-π electron aromatic macrocycle with a Co atom located at the central cavity, has been intensively studied as an effective catalyst. CoPc is thermally and chemically stable, and cost-effective. 2, 4-dichlorophenol (DCP) is one of the pollutants which are regarded as a very high risk compound. The present work has attempted for degradation of this compound. For this purpose, cobalt phthalocyanine (CoPc) is immobilized on graphene oxide (GO) and on the modified graphene oxide prepared as a nitrogen-doped graphene (NG) or the reduced graphene oxide (RGO). The efficiency of these prepared photocatalyst is studied. A conventional Hummers' method is used for the preparation of GO. NG sheets are prepared by either the thermal annealing graphene oxide using melamine (as a source of nitrogen) or a hydrothermal method using graphene oxide and ammonium carbonate (source of nitrogen). Also, RGO is synthesized using hydrazine hydrate for reduced GO. The synthesized samples are characterized by X-Ray diffraction (XRD), Fourier- Transform spectroscopy (FT-IR), Field emission scanning electron spectroscopy (FESEM), Energy dispersive X-ray (EDX), UV-Vis spectra, Raman spectroscopy, transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). The degradation of DCP was tested under visible light using prepared photocatalysts. The prepared photocatalyst based on NG (synthesized by thermal annealing and using a 1:10 ratio of graphene oxide/melamine) and containing CoPc showed the highest activity. In this regard complete degradation of some DCP with a 40 ppm concentration using only 6.5 mg of CoPc/NG (1:10) has taken place within 135 min.

Biography

Melika Ghaeini studied Applied Chemistry at the Azad University ShahreQods Branch, Iran and graduated as BC in 2016. She then joined the research group of prof. Zanjanchi at the University of Guilan, Iran. She received her M.S degree in 2019. She is cooperating with food and drug administration of Iran and also cooperated in 3 of chemistry conferences named: National Conference on Treatment of Water, Air and soil (TWAS ,2018), The 5th Iran International Zeolite Conference (IIZC) and research and technology week of Guilan university chosen as the best poster.

Deep sleep simulation

Vdovenkova T.A.
T.V.A., Saint-Leonard, Quebec, Canada

Observed at the beginning of sleep, deep sleep nonREM stages are different in frequency and amplitude of brain waves. This difference is caused by thalamus, which passes to cortex perception states action potentials (a. p.), but generates its own σ a. p. of encoding states at its reticular nucleus depolarization. Its highest depolarization at deep sleep is caused by Ado accumulation, but ILN are inhibited not only due to GABA release from reticular nucleus but also due to less Ach release from MPN/MRF. Consistently, influencing solely GABA receptors sleep promoting medication reduces deep sleep.

ILN inhibition at less Ach release from MPN/MRF creates conditions for retransmission to PFC 5th and 3rd layers of mainly matrix area of relay nuclei σ a. p., grouped with frequency of delta and slow oscillation (SO). Thus, posterior fast spindles located on peaks of SO and travelling along perception pathways are accompanied by anterior slow spindles travelling along attentional pathways. Cortical T-type Ca^{2+} channels reactivation determines the beginning of nonREM IVth stage, when half-period of SO exceeds the reactivation time. Thereby, simulation of low frequency and high amplitude SO is the deep sleep simulation.

In the present work, SO are simulated by linear oscillation of electric charge along neurites of PFC 3rd layer neurons: emitted by oscillating charge electric field E_y creates force, accumulating positive charge q^j_m of Na^+ ions at axon terminal neuronal membrane. This charge creates membrane potential increase up to thresholds of opening of VGCC, which leads to neurotransmitter release and subsequent SO travelling.

Calculated E_y amplitude and q^j_m maximums at the end of each linear oscillation increase with time. q^j_m accumulation during oscillation of 4^x10^{-7} C with amplitude 0.15 m, frequency 0.75 Hz and at distance 1 m for cytosol relative permittivity 3.84^x10^5 demonstrates that neurons with higher resting membrane potential initiate SO first: its increase from -90 to -60 mV reduces duration of charge oscillations necessary for activation of R- / N-type Ca^{2+} channels from 22 / 27 to 3 / 5 min. Resting membrane potential heterogeneity reduction by Cl^- inflow through activated $GABA_A$ channels reduces contribution of H_2O orientational polarization into cytosol relative permittivity and number of necessary oscillations up to 6 / 7. Increase in value of oscillating charge up to 35^x10^{-7} C accelerates q^j_m accumulation, leading to decrease in required for vesicle fusion and neurotransmitter release time interval in 9 times. Number of necessary oscillations is also less for shorter distance and for longer projection of axon along the direction of emitted electric field. On the contrary, negative charge of RNAs / RNA polymerase, in neurons experienced E-LTP with IEG activation, prevents Cl^- inflow, increasing cytosol relative permittivity and number of necessary oscillations.

Initiated in vPFC, SO travel over the entire cortex. They are accompanied by spindles and ripple a. p., incorporating AMPA and NMDA receptors into neuronal membrane. Consistently, their support by oscillations of static electricity charge from 4^x10^{-7} C to 35^x10^{-7} C during age-dependent circadian cycle's minima of spindle frequency, should enhance memory.

Audience Take Away:

- Audience will be able to switch from sleep promotion by chemical compounds to sleep promotion by contactless simulation of deep sleep waves, which could be interesting from the point of view of Green Chemistry.
- This research provides a practical solution to a problem: simple oscillation in front one person, of static electricity charge, accumulated on hands of another person, with certain frequency, amplitude, at certain distance and time intervals would enhance first person deep sleep and memory.
- This research could be used by other faculty to expand their research in the field of nanothechnology of memory formation.
- Simplicity of implementation would provide new information to assist in understanding of nanotechnology of memory formation.

Biography

Dr. Vdovenkova studied Radiophysics at TSN University of Kyiv, Ukraine and graduated as Radiophysicist Engineer-Researcher in 1984. She obtained positions of Engineer, Junior Researcher, received her PhD degree in Physical and Mathematical Sciences in 1989, obtained positions of Assistant Professor, Researcher, Senior Researcher at the same university, obtained positions of Researcher at Ghent University, Belgium, Research Associate at Trent University, Canada, Research Assistant at Douglas Hospital Research Centre, Canada and now fulfills contracts for TB (Federal Government of Canada). She has more than 60 scientific publications.

Novel study on the effect of TiO_2 nanosol addition on properties of Iraqi engine oil

Quraish Abbas Kadhim[1], Riyadh Mohammed Noaman[2], Alwan Nsaif Jassim[*3]
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[2]Chemical and Petrochemical Research Center, Corporation of Research and Industrial Development, Iraqi Ministry of Industry and Minerals/ Baghdad, Iraq
[3] Corporation of Research and Industrial Development, Iraqi Ministry of Industry and Minerals/ Baghdad, Iraq

Nano fluid of lubricating oil for internal combustion engines was prepared by adding TiO_2 sol as a source for Nano TiO_2 particles. TiO_2 sol was prepared via sol-gel route. The Nano sol was found to improve thermal conductivity, heat transfer and other physical properties of lubricants. The prepared TiO_2 sol, with bright golden color, was added to the local lubricant oil (Al-Rasheed brand) with 2 vol.% of the oil.

The addition of TiO_2 Nano sol to Iraqi oil increased significantly heat transfer and thermal conductivity of pure lubricant oil. The heat transfer increased by 38.4% with time lag of 25 min.

Also, other physical properties of Nano fluid oil were improved to fulfill the requirements of Iraqi specification (1197/2000) and as follows:

1-	Viscosity	form	274	to	368	Cp	at 25°c
2-	Pour point	from	-7	to	-18.5	°c	
3-	Density	from	0.90	to	0.95	g/cm^3	
4-	Flash point	from	164	to	232	°c	

The originality in this work resides in the new combination of TiO_2 – Nanosol with lubricating oil to produce Nano fluid which used successfully in this experiment.

Audience Take Away:

It is a simple and facile liquid-liquid stable mixture with negligible phase or precipitation of particles for more than one year without chemical change of the nano fluid.

1. The nano fluid was homogeneously mixed using magnetic stirring for 2 hours and was further mixed using high energy sonicator at 40 °C for another few hours to improvise the stability of the nano fluid without adding any additives.
2. We observed 38.4% enhancement of the effective thermal conductivity in this method comparing with 33% enhancement reported by other researchers when TiO_2 nano powder was used.
3. The thermo-physical tests concluded that the prepared nano fluid was excellent comparing with plane engine oil.
4. However, addition investigations are necessary to verify the impact of temperature and other variables, on the effective thermal conductivity of nano fluid.

Biography

Alwan Nsaif Jasim was born in Baghdad, Iraq, 1945. He received his professional degree from College of Education University Baghdad, Baghdad in the year 1966. He had completed his Ph.D in Physical Chemistry on the topic entitled :Studies of Quenching of Excited States of Aromatic Molecules in Polymer Matrices under the supervision of Dr J. R. Mac. Callum in the year 1980. He has published about 20 research article, besides three Iraqi pantents.

Professional	Experience
1975-1984	Head of Construction Department, Central Organization for Standardization and Quality Control, Government of Iraq.
1984-1997	Chemist, Iraqi Atomic Energy Commission.
1999-2004	Assistant Professor of Physical Chemistry and Head of Department of Chemistry , Faculty of Education,Zabid , Hodeidah University , Hodeidah. Yemen
2004 – 2008	Chemist , Ministry of Science and Technology, Iraq.
2008 – 2017	Consultant , Corporation for Industrial Research and Development

Problems of the pollution in transboundary rivers basin of the aral sea and the ways of their solution

Chembarisov E.I
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The article describes the hydrochemical condition of the transboundary rives in Central Asia. Cause of water pollution is increasing human pressure on surface water re-sources from population growth, increased economic activity and increasing intake of users, low level operation of irrigation systems, the exiting discharge of untreated industrial of sewages and drainage water to irrigation areas. The recommendations for reducing pollution of transboundary rivers streams Aral.

1. In the last years hydrochemical state of many rivers and reservoirs of Aral Sea has deteriorated significantly. This applies particularly to the basins of transboundary rivers Syrdarya , Amudarya, Zarafshan. If the upper reaches of these rivers salinity of river water does not exceed 0.4 -0.5 g/l, in the lower reaches of the rivers in increases up to 1.2 – 1.4 g/l. In this case, the water content increased sulphate and chloride ions, and the ions of magnesium and sodium. As part of water downstream is also observed excess of the maximum permissible concentration (MPC) of other pollutants, phenol, petroleum copper, chromium and other;

2. The cause of the existing water pollution of transboundary rivers is increasing human pres-sure on surface water resources from population growth increased economic activity and in-creasing intake of users, low level operation of irrigation systems, the existing discharge of un-treated industrial sewage and drainage water irrigation areas.

3. To minimize cross-border pollution of surface water must have the following:

-expansion of hydrochemical monitoring along the river, which includes quantitative and qualitative assessment of the degree of contamination and salinity in agreement with the international norms and standards on water quality.

It should be — subject to monitoring water samples for chemical analysis in cross-sections are located at the boundaries of different states on the output and the input to the different countries, located a major river basin. For example, in the Syrdarya river basin to hold water sampling at the exit of Kyrgyzstan, at the entrance of the river in Uzbekistan, at its exit from Uzbekistan, at the entrance to the Republic of Kazakhstan— in the mouth.

-Reduction of discharge of drainage water into the river system through better use in place of formation, improve the technical condition of existing drainage systems (GMS) lead mineralized drainage water into desert denkessions, local application of advanced methods of highly mineralized water desalination individual collectors.

-The creation of closed water systems in industrial plants, which not only exclude discharge of sewage , but also to minimize their consumption will drive the outside.

4. Remember that the management of water quality in the transboundary rivers, is part of the overall management, of water resources. It is therefore necessary to improve the practical implementation of the existing mechanism, international agreement on water management. In particular, you need to get signed and the implementation of paragraphs Helsinki Convention (1992) on international rivers and lakes.

5. In the future it is necessary for state government level to implement the ideas and meth-ods to integrated water resources management (IWRM), which is a continuous current process ensuring sustainable development in each country, as well as the monitoring and allocation of water resources in the context of the existing social, economic and environmental problems.

Biography

Chembarisov Elmir Ismailovich was born in 1948, Doctor of Geography, Professor, Chief Researcher of the Laboratory of Hydrometry and Metrology of the Research Institute for Irrigation and Water Problems (RIIWP). He devoted 49 years of his life to scientific and social activities. E.I. Chembarisov is a leading scientist of the Republic of Uzbekistan in the field of hydrology, hydrochemistry and hydroecology, water resources and the protection and rational use of natural resources. Under his leadership and with direct participation extensive hydrochemical studies were conducted on the rivers and reservoirs of the Aral Sea basin.

In 1970, he graduated with honors from the geographical department of Tashkent State University. In 1975 at the Faculty of Geography of Moscow State University, he defended his thesis on “The change in river water salinity in Central Asia due to irrigation”. Subsequently, it became the basis of the monograph “The Influence of Irrigation on the Mineralization of River Waters” and in 1990 at the Institute of Geography of the Academy of Sciences in Moscow - his doctoral thesis on “Collector Drainage Waters of Central Asia”.

In 2005 E.I. Chembarisov was awarded the title of professor in the field of hydrology of land, water resources and hydrochemistry. He is the author of a basin landscape halochemical method for analyzing changes and forecasts of the mineralization and chemical composition of river and collector-drainage waters, which is widely used in practice.

E.I. Chembarisov - author of 182 scientific and popular science works, among which are the "Hydrochemistry of the river and drainage waters of Central Asia" (1989), "Hydrochemistry of irrigated territories (using the example of the Aral Sea basin)" (1988), "Collecting - drainage waters of the Republic of Karakalpakstan "(2008)," Practical hydroecology (on the example of the Republic of Karakalpakstan) "(2012)," Genesis, formation and regime of surface waters of Uzbekistan and their impact on salinization and pollution of agricultural landscapes (on the example of the Amudarya river basin) " (2016), "Hydrological and geological features ical surface water monitoring Kashkadaria region "(2018) and others.

E.I. Chembarisov is a member of the Scientific Councils for the award of the degrees of PhD and PhD (DSc) in the specialties of Land Hydrology, Water Resources, Hydrochemistry and Environmental Protection and Rational Use of Natural Resources. He is elected professor at the American Hydrological Institute. He participated in many international conferences, including at the University of Bloomington in Indiana in the United States on the Aral problem, which was organized by Professor Yury Bregel in 1991.

Under the leadership of E.I. Chembarisov eight candidate dissertations were defended, three of them are representatives of Karakalpakstan. The research results of E.I. Chembarisov and his practical recommendations are used in projects on the integrated use and protection of water resources in the Central Asian river basins.

Potential use of Algae from Red Sea in Bioremedation

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Industrial pollution is an area of growing concern to legislators and the scientific community alike. In particular, organic pollutants present a real threat to human and wild-life, especially if they enter the food-chain. In the last two decades, there has been increasing interest on the use of bioremediation for removal of environmental pollutants. This study was undertaken to investigate the efficiency of four types of marine plants (micro-algae) in removing organic pollutants under different conditions. The study showed a significant reduction (up to 88%) in pollutants. In a related investigation, these species were also efficient in removing nitrogen oxides and ammonia from polluted water. Studies are continuing to fully characterize the structure of pollutants removed by these species and to find other applications of their usage in pollution reduction.

Audience Take Away:

- The audience will appreciate the general benefits of using algae in pollution reduction
- The audience will be introduced to organisms from the Red Sea which are being used for phytoremediation for the first time.
- This study will open the door for researchers in the field to collaborate. There maybe even a business opportunity in the application of these species in pollution control and green environment sustainability.

Biography

Dr. Suleiman Bifari holds an MSc in Environmental Engineering &Biological Technology (2005) from the King Abdulaziz University, Saudi Arabia. After working with the Saudi Ministry of Health for several years, Dr. Bifari was awarded a scholarship to pursue his doctoral studies. He joined the group of ProfessorMunetaka Ishikawa at Osaka University, Japan, in 2009 and graduated in 2013 with a PhD inEnvironmental Engineering. Dr. Bifari then joined the department of Environmental Engineering at the Royal Commission as a researcher and consultant. Currently, Dr. Bifari holds the position of Research Associate at the Jubail Research & Innovation ClusterHUB, Jubail Industrial College, Saudi Arabia, where he is active in bioremediation research.

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