

CATALYSIS  
2019



3<sup>rd</sup> Edition of International Congress on

# Catalysis AND CHEMICAL SCIENCE

*Theme: Accentuate innovations and emerging novel research in Catalysis and Chemical Science*

March  
11-13, 2019  
Singapore



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*3<sup>rd</sup> Edition of International Congress on*  
CATALYSIS AND  
CHEMICAL SCIENCE

*Theme:*

*Accentuate innovations and emerging novel research in  
Catalysis and Chemical Science*

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SINGAPORE

# CATALYSIS 2019



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# CATALYSIS 2019



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**Pusparatu**

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Thank You  
All...

# Welcome Message



Dear colleagues,

I am pleased to welcome you to the 3rd edition of International Congress on Catalysis and Chemical Science. A glance through the list of scientific sessions planned by organizers reveals the amazing diversity of the works focused on Catalysis and Chemical Science. They range from advanced synthesis, to industrial catalysis, treating many applications. Photocatalysis covers a wide range of applications, such as pollutant removal, water splitting hydrogen production, dye-sensitized solar cell, disinfection, etc. Most of them are related to Environment and Energy fields, which are main priority areas of many government programs. Water treatment by photocatalysis has received special attention as a suitable technique for the removal of different pollutants (organic and inorganic ones) using solar



light as energy source. Appearing as a low-cost, environmental friendly and sustainable technology for water treatment. Recent progresses explore different strategies to achieve high efficiencies and reduce the toxicity of wastewaters. They cover many options that include the study of the chemical nature of the catalyst, improve the use of solar energy or improve the technological properties of the catalysts, among others.

*Carolina Belver*

**Carolina Belver**  
Autonoma University of Madrid  
Spain

# Welcome Message



Dear all our attendees for Catalysis 2019, it is great honor and pleasure to write a few welcome notes. Asymmetric catalysis today makes unprecedented progress, since the Nobel Prize in Chemistry 2001 was divided to Drs. William S. Knowles and Ryoji Noyori for their work on catalytic enantioselective hydrogenation reactions and to Dr. K. Barry Sharpless for his work on catalytic enantioselective oxidation reactions. In contrast, the development of asymmetric catalysis for carbon-carbon bond formation reactions is much more divergent. The development of green and sustainable catalysis is also one of the most important subjects in current organic synthesis. As you know, the Nobel Prize in Chemistry 2005 was awarded jointly to Drs. Yves Chauvin, Robert H. Grubbs and Richard R. Schrock for the development of the catalytic metathesis, and the Nobel Prize in Chemistry 2010 was awarded

jointly to Drs. Richard F. Heck, Ei-ichi Negishi and Akira Suzuki for palladium-catalyzed cross couplings. The further development of highly efficient catalysts has been still demanded directed towards the green and efficient organic synthesis.



**Prof. Kazuaki Ishihara**  
Nagoya University  
Japan

# keynote speakers



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*About*

## MAGNUS GROUP

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

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

## *About* CATALYSIS 2019

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Magnus Group is pleased to invite you to participate in the '3rd Edition of International Congress on Catalysis and Chemical Science (Catalysis 2019)' during March 11-13, 2019 in Singapore.

This Catalysis 2019 is the International platform which brings together the collection of investigators who are at the forefront in the field of chemistry, catalysis and chemical science. The scientific program will include oral presentations of sub-disciplines, keynote sessions led by eminent scientists and poster sessions presented interactively by junior scientists and graduate students. It is the ultimate meeting place for all the experts worldwide for new interdisciplinary scientific collaborations and networking.

With its scientific sessions, you are provided assurance to explore the latest technologies and breakthroughs that are specific to your area of work. No doubt the event has a broad scope of topics and continued in parallel sessions relative to the specific area of research.



# About Exhibitor



**Anton Paar**

Anton Paar develops, produces and distributes analytical instruments used in the research, development and quality control worldwide.

We are the market leader in the field of density, dissolved CO<sub>2</sub> measurement and rheology.

Our product portfolio include viscometers, polarimeter, refractometer, microwave digester and extraction system and a full range of powder and structural characterization instruments for various industry ranging from pharmaceuticals, food, chemical, petroleum, water and environmental. Today, Anton Paar also offers complete customized robotics and automation solutions to our customers to optimize process reliability and efficiency.

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KEYNOTE FORUM

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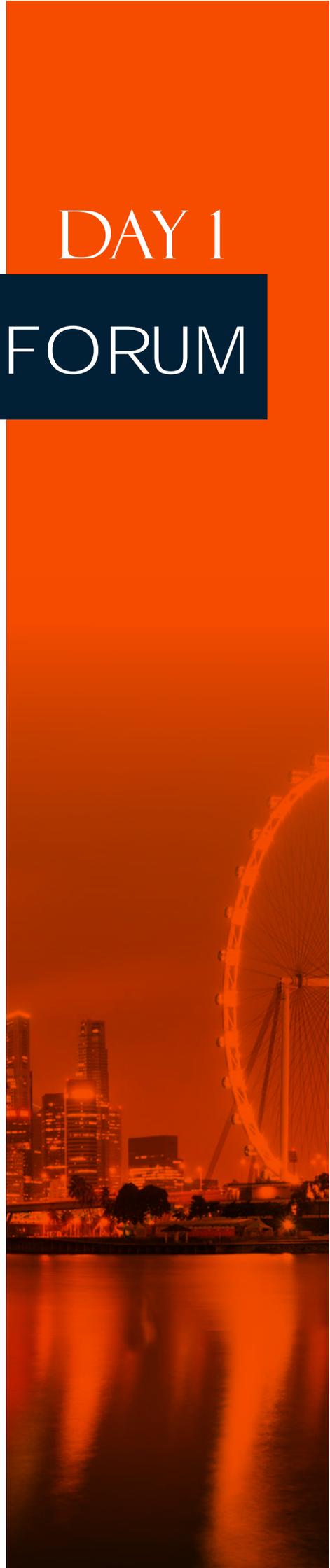
CATALYSIS AND  
CHEMICAL  
SCIENCE

MARCH

11-13, 2019

SINGAPORE

CATALYSIS 2019





#### Biography:

Professor Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris) he obtained in 1990 a position of contract researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements he received the title of professor. His published work includes more than 150 papers published in reputable international journals.

## Design of Ta- and Nb-single site zeolite catalysts for production of 1,3-butadiene from renewable sources

### Stanislaw Dzwigaj, Ph. D.

Sorbonne Université-CNRS, UMR 7197, Laboratoire de Réactivité de Surface, France

The metal ions well dispersed at zeolite framework are considered to be active sites of catalytic processes. Therefore, the incorporation of these metals into these materials as isolated tetrahedral sites appears to be the important challenge. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions involve a reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite.

During my keynote talk the design of new Ta- and Nb-single-site zeolite catalysts will be described and characterized by different physical techniques both at the macroscopic and molecular levels.

The application of Ta- and Nb-single-site zeolite catalysts in production of 1,3-butadiene from renewable sources, including ethanol obtained from biomass will be discussed.

This two-step postsynthesis method applied in this work allowed obtaining single sites Ta- and Nb-containing zeolite catalysts with mononuclear metal species active in above mentioned cascade reactions. Their catalytic activity strongly depends on the speciation and content of metal incorporated into zeolite structure as well as their acidity.

#### Audience Take Away:

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



### Biography:

Dr. Ishihara studied chemistry at Nagoya University, Japan and graduated as BEng in 1986, MEng in 1988, and DEng 1991, under supervision of Prof. H. Yamamoto. He then joined the research group of Prof. E. J. Corey at Harvard University, USA, as a postdoctoral fellow. He obtained the position of an assistant professor of Nagoya University in 1992, and then promoted an associate professor in 1997 and a full professor of Nagoya University in 2002. His research interests are synthetic organic chemistry, design of acid–base combined catalysts, halogen chemistry, asymmetric catalysis, Green & sustainable chemistry, design of supramolecular catalysts, etc.

## Rational design of High-Performance Catalysts based on Acid–Base combination chemistry

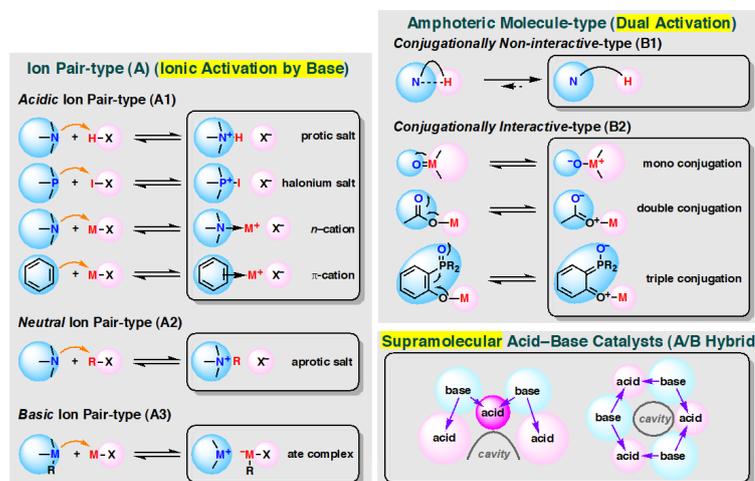
### Kazuaki Ishihara, Ph. D.

Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa, Nagoya 464-8603, Japan

Catalysts are the most important substances for efficiently controlling the reactivity and selectivity of organic reactions. Although enzymes control a huge number of reactions in living systems with extremely high substrate-, chemo-, regio-, site- and stereoselectivity, their substrate scopes and applicable conditions are quite limited. We established a rational methodology for designing high-performance unimolecular or supramolecular catalysts based on the chemistry of acid–base combined catalysis for numerous types of organic reactions.

The rational design of catalysts using non-covalent bonding interactions is useful for controlling their catalytic activities and selectivities.

We classified acid–base combined catalysts into two types: ion pair-type (A) and amphoteric molecule-type (B). Furthermore, type A can be subclassified into acidic ion pair-type (A1), neutral ion pair-type (A2), and basic ion pair-type (A3). On the other hand, type B can be subclassified into conjugationally non-interactive-type (B1) and interactive-type (B2). We developed various high-performance catalysts based on acid–base combination chemistry. I will talk about some recent topics on high-performance acid–base catalysts.



### Audience Take Away:

- How to design high-performance catalysts.
  1. Reaction mechanism.
  2. Acid-base combination chemistry.
- My presentation gives audiences significant information to develop high-performance catalysts.
  1. My presentation gives not only academia but also industrial researchers valuable information to develop efficient synthetic methods of target molecules.



#### Biography:

Assoc. Prof. Dr. Ng Eng Poh received his BSc (first class honors) degree (2004) in industrial chemistry and MSc in chemistry (2006) from the Universiti Teknologi Malaysia, Malaysia. He obtained his PhD degree in 2009 from University of Upper Alsace, France under the supervision of Prof. Dr. Svetlana Mintova. After postdoctoral work in the University of Caen, France, he was appointed as a senior lecturer (2010) at the Universiti Sains Malaysia. His main research is devoted to the synthesis, characterization and application of microporous and mesoporous silica-based materials for catalysis and new applications. He has published more than 70 peer-reviewed papers and his H-index is 20.

## Fast hydrothermal synthesis of nanocrystalline Cs-Aluminosilicate zeolites catalysts free of organic template

Eng-Poh Ng, Ph. D.

Universiti Sains Malaysia, Malaysia

**Z**eolites are crystalline aluminosilicates which have well defined channels and cavities. Zeolites are commonly used in ion exchange, catalysis and separation processes due to their unique crystalline structure and tunable surface properties. Subdivision of zeolites into fine particles (<100 nm) leads to immense external surface areas, and affects the magnetic, optical, electric and catalytic properties.

As a result, such nanocrystals brings unique properties to the structures prepared and expand the area of zeolite applications toward atomic energy production, food, paper, drug delivery, ceramics, paints, electronics, recording materials, lubricants, detergents and so on. While more than 200 zeolites are known today, only 14 types of aluminosilicate zeolites can be synthesized in nanometer scale.

Synthesis of zeolite nanocrystals involves hydrothermal treatment using harmful organic additives as the templates and to control the size of zeolite crystals. Cesium counter-balanced aluminosilicate zeolites (Cs-zeolite), are highly demanded due to their strong basicity for catalytic applications and good host-guest property for immobilization of radioactive cesium. The synthesis of Cs-zeolites, however, is rarely reported considering their tedious and dangerous syntheses that require high temperature (700-1200 °C), high pressure (>1000 bar) and long crystallization time and also, their nanocrystalline form has not been reported so far.

Thus, mild and safer synthesis condition with lower heating temperature and pressure remains challenging in Cs-zeolites synthesis. In this presentation, we intend to report the successful synthesis of two types of organotemplate-free nanosized Cs-zeolites using traditional and microwave-assisted hydrothermal techniques.

Besides discussing the crystallization for synthesizing the molecular sieves, the properties of zeolites are studied before they are investigated in several catalytic reactions.

#### Audience Take Away:

- gain knowledge on the new approach of synthesis of nanocrystalline zeolites
- know the properties of these nanocrystalline zeolites
- have basic knowledge on zeolites
- have other alternative solid base catalyst for their catalytic reactions
- have potential research collaboration



#### Biography:

Tarik CHAFIK is currently full Professor, Research Director and Master courses coordinator at the Faculty of Sciences and Technique of Tangier (Morocco), where he is teaching Thermodynamic, Chemical engineering, catalysis and atmospheric pollution control. Before his appointment at University Abdelmalek Essadi, he was Post doc researcher at University of Patras (Greece) than he worked at National Institute for Resources and Environment (AIST, Tsukuba Japan). He was awarded as Fulbright visiting researcher at University California Berkeley (USA) in 1999 (with Prof. A. T. Bell). He was visiting Professor positions at Alma Mater University of Bologna for research and teaching assignments within European Master Advanced Spectroscopy in Chemistry as well as at the University of Lille, France. He was, also, several times invited lecturer at the universities in France, Spain, Portugal, Germany. Prof. T. Chafik's research is focused on sustainable development technologies such as those involving adsorbents and catalysts for VOC removal and methane reforming as well as nanomaterials for winds turbine lubricant additive and nanoporous carbon for energy

## Determination of the Heat of Adsorption and Desorption of a Volatile Organic Compound Under Dynamic Conditions Using Fourier-Transform Infrared Spectroscopy

**Tarik CHAFIK, Ph. D.**

University Abdelmalek ESSAADI, Faculty of Science & Techniques

Tanger, Morocco

Quantitative Fourier-transform infrared spectroscopic analysis was used for the determination of adsorption capacity of a model volatile organic compound (VOC) under dynamic conditions. The analytical method used also offers the possibility of distinguishing between reversible and irreversible adsorption as well as further detection of adsorbed VOC transformation. The obtained adsorbed amounts have been used for the determination of the heat of adsorption and the activation energy of desorption using, respectively, isosteric and temperature programmed desorption methods. The approach has been applied to explore the potential use of local clay and activated carbon as adsorbent material for VOC pollutants.

#### Audience Take Away:

- It will be shown that different values of the heat effect might be obtained following the procedure used. Values ranging from 85 to 40 KJ/mol were obtained for the isosteric heat of adsorption at different adsorbate loadings using adsorption isotherm data measured under static conditions. However, the application of temperature programmed desorption (TPD) experiments carried out under dynamic conditions yields apparent energy of desorption values that cannot be systematically correlated with the heat of adsorption which is a thermodynamic parameter relevant to the adsorption equilibrium. This issue is of interest because the use of accurate values of the heat of adsorption is important for the correct designing and operating of adsorption facilities.

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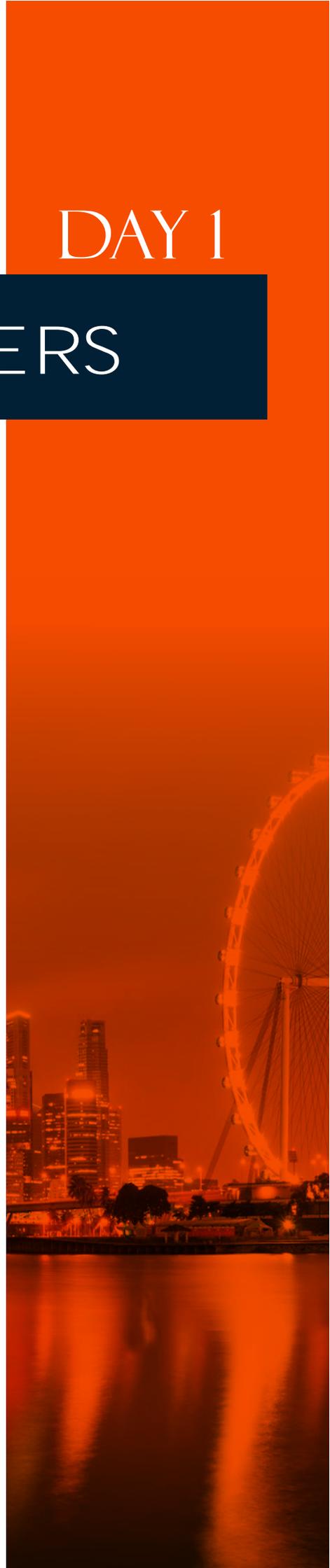
CATALYSIS AND  
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## Synthesis of chiral isoindolinones from chiral (*E*)-*N*-(hex-3-en-5-yn-2-yl) propiolamides via a novel Gold-Catalyzed cycloisomerization reaction pathway

Farzad Zamani, Christopher J. T. Hyland and Stephen G. Pyne\*

School of Chemistry, University of Wollongong, Wollongong, NSW, 2522, Australia

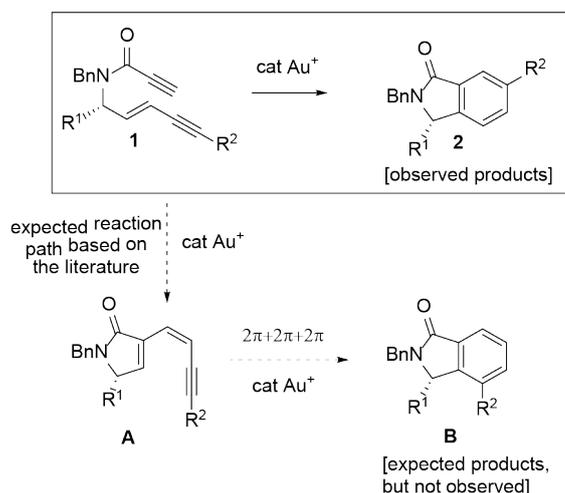
A method for preparing novel chiral (*E*)-*N*-(hex-3-en-5-yn-2-yl)propiolamides **1** and their gold-catalyzed cycloisomerization reactions to give chiral isoindolinones will be presented. Of the gold catalysts screened,  $\mu$ 3-oxotris(triphenylphosphine)trigold(I) tetrafluoroborate,  $[(\text{Ph}_3\text{PAu})_3\text{O}]\text{BF}_4$ , proved to be optimal.

These cycloisomerization reactions gave cyclized products **2** of unexpected regiochemical outcomes (Scheme).

Based on the known reactivity of simple 1,5-enynes the cycloisomerization reactions of (*E*)-*N*-(hex-3-en-5-yn-2-yl)propiolamides **1** was expected to first give the lactam intermediate **A** (Scheme) having a 1,3(*Z*)-dienyl-5-yne moiety which in principle is set up for a gold-catalyzed (formal  $[2p+2p+2p]$ ) cyclization reaction to give the 4-substituted isoindolinones **B** (Scheme).

Surprisingly, the products obtained were 6-substituted isoindolinones **2**. Deuterium labelling and computational studies revealed a novel cycloisomerization reaction mechanism was operating.

The findings from this study and our mechanistic understandings of these cycloisomerization reactions will be presented in this lecture.



### Audience Take Away:

- A new method for preparing usefully functionalized chiral (*E*)-*N*-(hex-3-en-5-yn-2-yl) propiolamides and chiral isoindolinones.
- The discovery of a new mechanism for gold-catalyzed cycloisomerization reactions.
- Compounds **1** could be employed as useful substrates to develop other novel chemistries or libraries of compounds for future drug discovery programs.

### Biography:

Prof. Pyne completed his PhD in synthetic organic chemistry in 1979 with Prof. Lew Mander at the Australian National University. After Post-Doc positions with P. Fuchs (Purdue) and E. J. Corey (Harvard University) he was appointed as a Lecturer at the University of Wollongong in 1985. In 1998 he was promoted to full Professor. His recent awards include, the Birch Medal in 2012 from the Royal Australian Chemical Institute (RACI), and the Archibald Ollé Prize for chemical literature from the RACI in 2015. Research fields include organic synthesis (transition metal-catalyzed reactions), natural product synthesis, medicinal chemistry (antibiotics) and phytochemistry.

## Magnetic field assisted electrochemical synthesis of Co-Ru nanorods for water splitting reaction

I. Dobosz, K. Kolczyk, D. Kutyla, R. Kowalik, Piotr Zabinski\*

AGH University of Science and Technology, Faculty of Non-Ferrous Metals, al. Mickiewicza 30, 30-059 Krakow, Poland

The article presents results of tests on potentiostatic electrodeposition of ruthenium and Co-Ru alloys. The tests applying cyclic voltammetry method with the use of gold disk electrode (RDE) allowed to define a potentials range in which it is possible to obtain ruthenium and its alloys with cobalt from acid chloride electrolytes. The influence of electrodeposition parameters and the electrolyte composition on the composition, morphology and structure of the obtained deposits was determined. Co-Ru alloys underwent XRD tests, an analysis with the XRF method and observations using scanning electron microscopy (SEM). Hydrogen evolution tests have been also performed. Then, cobalt-ruthenium nanorods have been successfully synthesized by electrochemical deposition using an aluminum oxide membrane template with superimposed external magnetic field. The length and average diameter of cobalt alloy nanorods arrays are 4,5 - 9  $\mu\text{m}$  and 100 nm, respectively. For nanorods deposited in applied external magnetic field of 0,6T we observe higher saturation magnetization and slightly higher coercivity field. This method offers a convenient and efficient path to synthesize metal array nanostructures with designed composition.

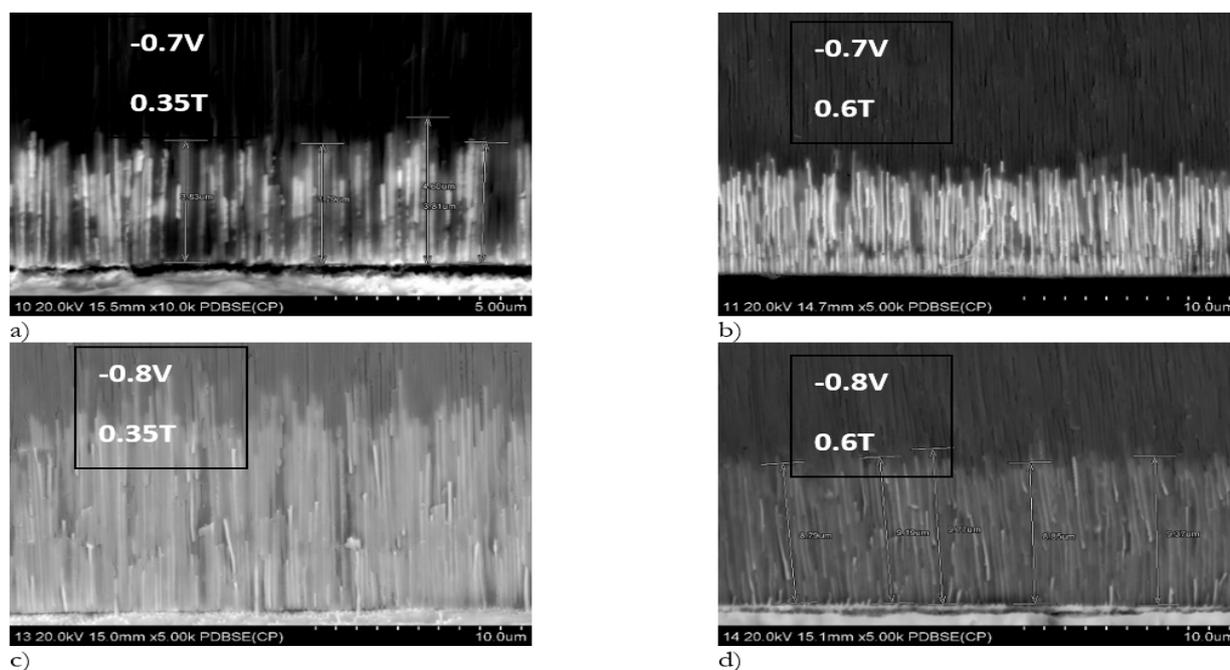


Fig 1. SEM photographs of aluminum membrane cross-section with pore diameter of 100 nm and deposited Co-Ru nanorods at potential of -0,7V and magnetic field 0,35T (a) and 0,6T (b) and -0,8V with applied magnetic field 0,35T (c) and 0,6T (d). Deposition time 60 minutes.

### Biography:

Dr. Piotr Zabinski studied Chemistry at the Jagiellonian University, Krakow, Poland and graduated as MS in 1995. He then joined the research group at the Faculty of Non Ferrous Metals, AGH University of Science and Technology, Krakow, Poland (AGH-UST). He received his PhD degree in 2000 at the same institution. After two years postdoctoral fellowship supervised by Prof. Koji Hashimoto at Tohoku University, Sendai, Japan he obtained the position of an Associate Professor at the AGH-UST. He has published more than 60 research articles in SCI(E) journals.

## H Species reactivity in Hydrogen spillover effect

**Mohammed Bettahar**

Lorraine University, Faculty of Sciences and Technologies, Laboratory of Chemistry and Physical Chemistry, Vandoeuvre-lès-Nancy, France

The hydrogen spillover effect (HSPE) may be involved in both hydrogen storage, an important subject for energy applications, and hydroconversion reactions over metal supported catalysts, key processes in (bio) refineries for the fabrication of high-added value chemical products. Moreover, interactions of hydrogen with solid surfaces, in the presence or not of an organic molecule, is an important topic in fundamental Heterogeneous Catalysis. Also the present talk on the HSPE may be of great interest for people involved in hydrogen energy uses or transformations of carbon feedstocks. It would also be helpful for the teaching of practical surface chemistry.

Briefly, diluting the catalyst by the support leads to both increased hydrogen storage and catalytic activity. This is attributed to the so-called HSPE consisting in the dissociation of H<sub>2</sub> on the metal particles then spreading on the support where they become either a hydrogen reservoir or active species in hydroconversion reactions. This led to debates about the conditions of observation of the effect, observation of the effect, notably the nature of the support observation of the effect, notably the nature of the support. We think that controversies about the HSPE mainly come from a misunderstanding of earlier studies (1960-1970) where the various H-adspecies on the support were not finely discriminated

In this talk we critically review previous works on hydrogen spillover, focussing on characterization and reactivity of surface H atoms incorporated in metal supported catalysts in H<sub>2</sub> or hydrocarbon + H<sub>2</sub> atmospheres. We demonstrate that, contrary to a general belief, H stored species are not the active species in hydroconversion reactions.

### Biography:

Mohammed M. Bettahar held his PhD degree in Physical Chemistry (Paris, 1975). He worked for the CNRS as Attaché de Recherche (Thiais) and Research Director (Caen). He pursued his career as Full Professor in Algiers (1980) then in Nancy (1995). He is Professor Emeritus in Lorraine University since 2015. Main research topics are related to Nanomaterials and Catalysis (Selective Hydrogenation or Oxidation, CO<sub>2</sub> or CH<sub>4</sub> transformations, Hydrogen Storage). Currently his research focuses on Nanomaterials for Biofuels fabrication.

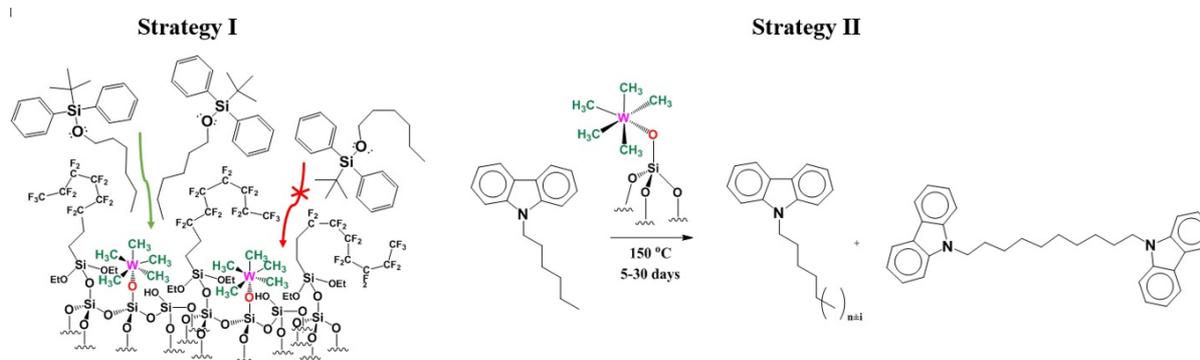
## Metathesis of functionalized alkanes towards the solution to the unsolved problem

Mykyta Tretiakov\*, Yury Lebedev, Manoja Samantaray, Aya Saidi, Magnus Rueping, Jean-Marie Basset

Physical sciences and engineering, KAUST/KAUST Catalysis Center, Thuwal, Makkah Province, Saudi Arabia

Metathesis method is widely used in fundamental research and industrial processes. It allows for the efficient and environmentally-friendly production of a variety of products, such as fuels, pharmaceuticals and organic building blocks. After the breakthrough discovery of the olefin metathesis, which showed the conversion of propene to a mixture of ethylene with 2-butenes and ring-opening metathesis polymerization (ROMP) of norbornene, organometallic chemists became very interested in this new method due to its high potential in synthetic organic and polymer chemistry. In the following years, the metathesis of non-functionalized as well as functionalized alkynes and olefins was reported in the literature. In 1997 for the first time metathesis of linear alkanes was reported and subsequently, this field emerges as an alternative route for the preparation of diesel range alkanes for transportation. To date, a plethora of catalysts has been synthesized and used for alkane metathesis reaction. However, metathesis of functionalized alkanes remains elusive in the scientific community.

In this presentation, we will show the strategies that we have been using to develop a new reaction – metathesis of functionalized alkanes and our work towards the design of catalyst/substrate compatibility. The first strategy to overcome the challenge was based on protection of the catalyst active sites by modification of the support. We have thus grafted octyltriethoxysilane as well as 1H,1H,2H,2H-perfluorooctyltriethoxysilane (protective chains) on dehydroxylated conventional silica and KCC-1 supports followed by grafting the alkane metathesis catalyst precursor –  $W(CH_3)_6$ . The obtained materials with different morphology and ratios between tungsten and protective chains (varying from 15 to 90%) have been thoroughly characterized and subjected to catalysis. Along with that strategy, we designed substrates bearing sterically hindered functional groups to avoid interaction with the catalyst. However, even though the catalysts were active in olefin and alkane metathesis, no metathesis of functionalized alkanes was achieved. The second strategy was aimed to design a compatible substrate for the metathesis of functionalized alkanes. We investigated the pyrrole-based family of substrates bearing in mind that the lone pair of electrons on the nitrogen atom is involved in the formation of an aromatic system and thus is poorly available for coordination. However, metathesis of 1-hexyl-2,5-dimethyl-1H-pyrrole gave only traces of metathesis and isomerization products. These results pushed us to synthesize 9-hexyl-9H-carbazole – a rigid aromatic molecule. While utilizing it on silica-supported  $W(CH_3)_6$ , we reached 5% conversion to lower and higher homologs. This result proved to be the first ever known example of metathesis of a functionalized alkane.



### Audience Take Away:

- In this presentation, we will describe the strategies that have been using to overcome the challenge of metathesis of functionalized alkanes and show, how we succeed with the challenge that was initially considered impossible. The audience will learn the importance of strategy design, persistence, and teamwork when tackling the problem of any difficulty.
- The presentation will be beneficial for scientists and faculties, whose focus of research is not only heterogeneous catalysis and metathesis but for a wide range of backgrounds. We will present a variety of analytical techniques that have been used in our research for characterization and underline the tremendous importance of understanding the failed experiments, why they failed, what knowledge we can get and how we can gain from that knowledge.

- We will explain the significance of the new reaction that we have developed from a fundamental and commercial point of views. That knowledge will be vital for students, postdocs and faculties who may move to study the metathesis of functionalized alkanes in their research.

**Biography:**

Mykyta Tretiakov received his B.Sc. in 2010 and M.Sc. in 2011 from Ukrainian State University of Chemical Technology (USUCT). Between 2011-2013 he worked as a Guest Researcher at Georg-August University of Goettingen (Germany), where his research was focused on the chemistry of N-Heterocyclic and abnormal carbenes. From 2014 he is doing his Ph.D. in Chemical Science at King Abdullah University of Science and Technology (KAUST, Saudi Arabia). He has published 5 research articles and 1 book chapter. He was awarded President of Ukraine grant for outstanding students in 2009 and Dow Chemical Sustainability and Innovation Student Challenge Award in 2014.

## Taking inspiration from molecular chemistry in nanochemistry to tune the properties of metal nanoparticles in catalysis

**Karine Philippot, Ph. D.**

CNRS, France

With the huge development of nanocatalysis, the demand for metal-based nanomaterials has been fast increasing and chemists are looking for effective synthesis methods to achieve well-defined nanocatalysts and to guarantee controllable and reproducible properties. Regarding nanochemistry in solution, the concepts of molecular chemistry allow developing efficient synthetic tools to have metal nanoparticles in a size less than 10 nm. Metal-organic complexes are particularly well-suited precursors to provide well-controlled and functionalized metal or metal-oxide nanoparticles in terms of size and composition. The choice of the stabilizing agent is of prime importance to control the characteristics of the nanoparticles and beyond, their surface properties. This method can be applied for the preparation of mono- or bimetallic nanocatalysts under the form of colloidal suspensions or supported systems. Selected examples of metal nanoparticles prepared through the organometallic approach will be presented with their performance in catalysis, respectively.

### Audience Take Away:

- This presentation is related to nanotechnology, nanochemistry, molecular chemistry and catalysis. Through selected examples, this lecture will provide to the audience a clear view of the benefit when using molecular chemistry concepts to prepare metal nanoparticles of very small size (<10 nm and most often 1-2 nm) and derived materials.
- This synthetic method, also called organometallic approach, can be applied for various systems and is reproducible. More importantly this method is a powerful way to attend nanomaterials that are finely controlled in terms of structure and composition and consequently, to have in hands appropriate systems for investigating the relationships between their characteristics and their properties. Moreover, by playing with the synthesis conditions, it is possible to tune the characteristics of the materials to improve their performance. Applications in catalysis will illustrate the interest to apply this methodology.

### Biography:

After a PhD degree in Chemistry at the University of Toulouse-France and a postdoctoral position at the catalysis department of Rhodia-Lyon, Dr. Karine Philippot integrated CNRS. She is presently Senior Researcher at the Laboratory of Coordination Chemistry (LCC) in Toulouse and head of the team "Engineering of Metal Nanoparticles". Her research interests deal with the synthesis of metal nanoparticles and composite nanomaterials by using molecular chemistry concepts for their application in colloidal or supported catalysis and in the domain of energy. She is co-author of >160 peer reviewed papers (with 5 reviews, 13 proceedings, 9 book chapters, 6 patents) and co-editor of the book "Nanomaterials in Catalysis" (Wiley).

## Chloroform conversion into hydrocarbons by hydrodechlorination with Pd supported on activated carbons obtained by chemical activation of lignin

Jorge Bedia\*, C. Fernandez-Ruiz, J.J. Rodriguez, L.M. Gómez-Sainero

Departamento de Ingeniería Química, Facultad de Ciencias, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain

Conversion of chloroform (TCM) by gas-phase catalytic hydrodechlorination (HDC) has been addressed to maximize the selectivity to ethane and propane hydrocarbons. Several own-made Pd (1 wt.%) catalysts have been tested. The catalysts were prepared by incipient wetness impregnation of five different activated carbons. These carbons were obtained by chemical activation of lignin with different activating agents, namely,  $\text{H}_3\text{PO}_4$ ,  $\text{ZnCl}_2$ ,  $\text{FeCl}_3$ ,  $\text{NaOH}$  and  $\text{KOH}$ . The catalysts were fully characterized by  $\text{N}_2$  adsorption-desorption at  $-196\text{ }^\circ\text{C}$  and  $\text{CO}_2$  adsorption at  $0\text{ }^\circ\text{C}$ , TPR,  $\text{NH}_3$ -TPD, XRD, XPS and TEM. The activating agent conferred important differences on the characteristics of activated carbon supports, and hence to the resulting catalysts, in terms of porous texture, surface acidity, Pd oxidation state and Pd particle size distribution.  $\text{NaOH}$  and  $\text{KOH}$  activation led to carbons with the highest surface areas ( $2158$  and  $2991\text{ m}^2\cdot\text{g}^{-1}$ , respectively) and low  $\text{Pd}^0/\text{Pd}^+$  ratio, while  $\text{ZnCl}_2$ - and  $\text{H}_3\text{PO}_4$ -activated carbons yielded the highest surface acidity and mean Pd particle sizes. The analysis of the TOF values revealed that HDC of TCM on these catalysts is a structure-sensitive reaction, increasing TOF values with Pd particle size. The best results, in terms of selectivity to ethane and propane, were obtained with the catalysts supported on  $\text{KOH}$  and  $\text{NaOH}$  activated carbons. The former allowed 80% selectivity to those target compounds at almost complete dechlorination ( $> 99\%$ ) at  $300\text{ }^\circ\text{C}$ . The  $\text{KOH}$ -based catalysts showed fairly good stability at  $200\text{ }^\circ\text{C}$  reaction temperature.

### Audience Take Away:

- Revalorization of polluted gas streams is possible.
- Chemical activation of residual lignin with different activation agents yields activated carbon supports with very different properties.
- These properties affect considerably the activity and selectivity of the final catalysts in the hydrodechlorination reaction.

### Biography:

Dr. Jorge Bedia received his PhD degree in 2008 at the University of Málaga (Spain). After that, he achieved a postdoctoral position at Autonomia University of Madrid (Spain) where he is now assistant Professor of the Chemical Engineering Department. He is co-author of more than 50 publications in SCI journals (more than 1500 cites; H-index = 22), mostly within 25% of the highest impact in their area of knowledge. He is also co-author of more than 120 communications in national and international scientific conferences and two patents.

## Synchrotron X-ray spectroscopies for catalysis

**Renfei Feng, Ph. D.**

Canadian Light Source, Canada

Synchrotron radiation source is an accelerator-based light source with extremely high brightness and some very unique properties. It enables the researches and applications which are not possible in the regular laboratories. The X-ray spectroscopy techniques available at the synchrotron facilities provide a set of powerful tools for catalysis analysis. This presentation will give an overview of these techniques. As an example of research facilities, Canadian Light Source will be introduced briefly. A few detailed research examples will be presented to show the application in catalysis analysis.

### **Audience Take Away:**

- X-ray spectroscopies available at the synchrotron facilities for catalysis.
- The advantages of synchrotron spectroscopies.
- A few examples of applications as showcases.

### **Biography:**

Dr. Feng is currently a senior scientist and beamline responsible at the Canadian Light Source (CLS) since 2005. He received his PhD degree in atomic and molecular physics in 1993. Before joining CLS, he worked as an assistant (1993) and associate professor (1995) in University of Science and Technology of China; research associate (1997) in University of British Columbia; and staff scientist (2002) in Alberta Synchrotron Institute. He has extensive experience in electron and X-ray spectroscopy and microscopy, and has published ~100 research articles in SCI (EI) journals.

## Alkali-Free NiAl hydrothermally reconstructed layer double hydroxide

Nazrizawati Ahmad Tajuddin<sup>1,2\*</sup>, Adam F. Lee<sup>2</sup> and Karen Wilson<sup>2</sup>

<sup>1</sup>Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, Tapah Road, 35400 Perak, Malaysia

<sup>2</sup>European Bioenergy Research Institute (EBRI), Aston University, Birmingham, B4 7ET, United Kingdom

Recent developments in heterogeneous hydrotalcite (HT) synthesis have led to a proliferation of studies on various preparation steps and its application in many ways. Nowadays, transition metals such as Ni are receiving great interest from researchers due to the promising advantages they possess such as good conductivity, eco-friendliness and inexpensive catalysts, and having the ability to produce various types of host structure with high proton mobility. In terms of catalytic performance, Ni catalysts are preferable due to their active phase especially in hydrogenation reactions, steam reforming, depolymerisation of lignin and their ability to be applied as electrochemical capacitors and high-performance supercapacitors. Nevertheless, the catalytic activity and lifetime of Ni catalysts could vary depending on their physical and chemical properties. Nano-sized NiAl Layered Double Hydroxides (LDH) has gained great attention and been applied in a variety of applications due to its speciality to reconstruct the lamellar structure after calcination-rehydration process. NiAl LDH has been predicted to be hard and challenging to reconstruct due to the rigid formation of mixed oxide after the calcination process. Due to that, a dearth of studies into the reconstruction of NiAl LDH has been reported compared to its mixed oxide which has better stability exhibited from the Lewis basic site. Nevertheless, calcined mixed oxide LDH has a drawback which attributes that include lower catalytic activity. Rehydration alternatively exhibits Bronsted base OH<sup>-1</sup> species which are highly favourable for base catalysed reactions. Generally, reconstruction of NiAl LDH is possible yet needs a special condition such as controlling the calcination temperature or the reconstruction time. In addition to the above reasons, it is important to find an alternative to synthesise and rehydrate NiAl LDH to obtain good morphologies, structural properties and at the same time to improve the catalytic performance. In this study, NiAl LDH has been prepared and reconstructed under hydrothermal conditions. A family of NiAl HT catalysts were synthesised with different Ni:Al atomic ratios ranging from 1.5:1 to 4:1 (pH 9.5) via the green free-alkali hydrothermal reconstructed method. NiAl LDH underwent calcination at 350 °C followed by reconstruction under a hydrothermal process. The successful synthesis has been confirmed via a range of characterisation techniques. Catalyst later has been tested in the transesterification reaction involving lower to bulkier TAG (C<sub>4</sub>-C<sub>18</sub>). The catalytic activity of reconstructed NiAl LDH has been studied and thoroughly investigated.

### Audience Take Away:

- Audience will significantly get new insights of novel NiAl LDH by using alkali-free hydrothermal methods
- Audience will be exposed to LDH physicochemical properties, as well as to explore their effects in biodiesel production via trans esterification especially in the transesterification of bulky triglycerides.
- Catalysis, bioenergy or biodiesel companies could suggestively adopt this catalyst in their production.

### Biography:

Dr. Nazriza received her PhD in Chemistry at the Aston University, UK in 2017. She joined the Surface and Catalysis Research Group of Prof. Karen Wilson and Adam Lee at the European Bioenergy Research Institute (EBRI), Aston University from 2013-2017. Prior to that, she is served as a Chemistry Lecturer at Universiti Teknologi MARA, Malaysia until now-a 10th years of teaching. She has been promoted to Senior Lecturer upon completion of her PhD.

## Electrochemical synthesis of cobalt-selenium coatings as a catalysts for hydrogen evolution

Anna Kwiecińska, Karolina Kołczyk, Dawid Kutyla, Piotr Żabiński, Remigiusz Kowalik\*

Faculty of Non-Ferrous Metals, AGH University of Science and Technology, Krakow, Poland

The electrochemical deposition of transition metal chalcogenides thin films has received recently much attention due to their potential applications in electrocatalysis. Among them the special attention is focused on cobalt-selenium system. Usually, thin films of these materials are prepared by hydrothermal synthesis or high temperature and vacuum techniques. However electrodeposition has been found to be a very good and low-cost method to fabricate thin polycrystalline films of these compounds.

The electrodeposition of thin films of polycrystalline Co-Se system from aqueous baths was studied. The experiments were carried out following the thermodynamic analysis. A conventional three-electrode cell: Cu as working electrode, Pt-sheet as counter electrode and Saturated Calomel Electrode (SCE) as reference electrode was used. The electrodeposition mechanism of pure elements Se, Co and Co-Se phases on copper substrate was studied by chronoamperometry, cyclic voltammetry and hydrodynamic techniques.

Additionally, chronoamperometry and cyclic voltammetry were combined with electrochemical quartz crystal microbalance to analyse this process in details.

This work was supported by the Polish National Center of Science under grant 2016/21/B/ST8/00431.

### Audience Take Away:

- The audience will be familiarize with the electroanalytical techniques used for analysis of electrodeposition processes
- They will be able to synthesis coatings based on transition metal chalcogenides

### Biography:

Remigiusz Kowalik graduated at the University of Science and Technology in Krakowin 2000 (M.Sc.) and 2006 (Ph.D.) under the guidance of Professor Krzysztof Fitzner. He studied electrochemical atomic layer deposition methods with Professor Maria Luisa Foresti (Florence, Italy), electrodeposition of gold nanoclusters with Professor Derek Pletcher (Southampton, UK), electrochemistry of palladium and sonoelectrochemistry with Professor Peter Birkin (Southampton, UK), and electrochemical scanning tunneling microscopy with Dieter Kolb (Ulm, Germany). Now, he is a member of the Laboratory of Physical Chemistry and Electrochemistry, Faculty of Non-Ferrous Metals, AGH University of Science and Technology. His research interests are related mainly to electrochemistry and electrodeposition of metals and semiconductors and electrochemical atomic layer epitaxy.

## Non-hydrolytic sol-gel synthesis of oxide and mixed oxide catalytic materials

**P. Hubert Mutin**

Institut Charles Gerhardt, CNRS-Université de Montpellier, Montpellier, France

Oxides and mixed oxides are used as catalytic supports or as catalysts in all the fields of heterogeneous catalysis. Sol-gel processing is widely used for the synthesis of these catalytic materials. Conventional sol-gel typically involves the hydrolysis and polycondensation of precursors (e.g. silicon or metal alkoxides), but several alternative non-hydrolytic sol-gel (NHSG) routes have been developed over the last decades.

NHSG routes involve the reaction in non-aqueous media of precursors (e.g. chlorides, alkoxides) with an organic oxygen donor (e.g. ether, alcohol).

In this presentation I wish to show the potential of NHSG in the synthesis of catalytic materials. In particular, the reaction of chloride precursors with an ether provides a simple and cost effective route to non-ordered mesoporous mixed oxide xerogels, avoiding the use of multi-step procedures, expensive precursors, reactivity modifiers, templating agents or supercritical drying. This non-hydrolytic route has been applied to the design of mesoporous mixed oxide catalysts:  $\text{SiO}_2\text{-TiO}_2\text{-}(\text{-Me}_3\text{SiO}_{0.5})$ ,  $\text{TiO}_2\text{-V}_2\text{O}_5$ ,  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-MoO}_3$ ,  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-Re}_2\text{O}_7$ ,  $\text{Al}_2\text{O}_3\text{-Nb}_2\text{O}_5\text{-AgO}$ ,  $\text{SiO}_2\text{-ZrO}_2$ , etc. In terms of texture, structure and catalytic performances, the catalysts obtained by non-hydrolytic sol-gel compare well with catalysts prepared by impregnation of supports or by state of the art methods.

### Audience Take Away:

- NHSG offers a powerful toolbox for the design of innovative catalytic supports and catalysts
- NHSG is now a recognized method for the synthesis of non-ordered mesoporous oxides and nanoparticles
- Contrary to conventional sol-gel, NHSG involves organic reaction pathways, and the most popular NHSG routes should be included in a comprehensive course on sol-gel processing

### Biography:

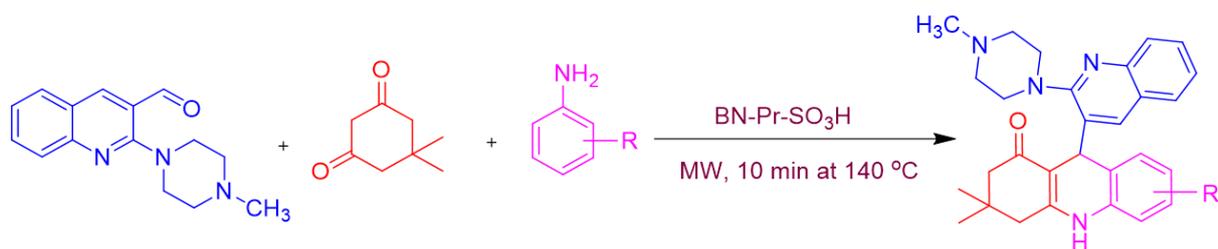
P. Hubert Mutin is a CNRS Research Director at the Institute Charles Gerhardt of Montpellier, where he develops low temperature routes for the synthesis of oxide and hybrid materials. He authored about 160 articles in peer-reviewed journals (>6100 citations, h-index 48), 15 patents, 7 book chapters, and has given more than 100 presentations in international conferences, universities, and companies. He was Invited Scientist at the Australian Nuclear Science and Technology Organisation in Lucas Heights, and at Masaryk University in Brno, and has been a member of the Board of Directors of the International Sol-Gel Society since 2016.

## Boron nitride nano materials based heterogeneous catalyst as an efficient and highly biological active synthesis of methyl piperazinyl-quinolinyl fused Benzo[c]acridinone derivatives

Arul Murugesan\*, R M Gengan, Ph. D.

Department of Chemistry, Faculty of Applied Sciences, Durban University of Technology, Durban, South Africa

**B**oron nitride nano material based solid acid catalyst was found to be an efficient and reusable sulfonic acid catalyst for the synthesis of one-pot Knoevenagel and Michael type reactions in 3, 3-dimethyl-9-(2-(4-methylpiperazin-1-yl) quinolin-3-yl)-3, 4, 9, 10-tetrahydroacridin-1(2H)-one derivatives under microwave irradiation conditions. The synthesised catalyst was employed in Knoevenagel and Michael type reactions to synthesise novel piperazinyl-quinolinyl based acridine derivatives. Most importantly it was found that the solid acid catalyst can be recycled with only 5% loss of activity.



### Biography:

Dr. Arul Murugesan studied Chemistry at the Bharathiar University, Coimbatore and graduated as MSc in 2013. He then joined the research group of Prof. R M Gengan at the Durban University of Technology, organic Chemistry research group. He received his PhD degree in 2018 at the same institution. After one year postdoctoral fellowship supervised by Prof. R M Gengan at the Catalysis and organic Chemistry research group, He has published 8 research articles in SCI (E) journals.

## Influence of oxygen containing functional groups on the deposition of Pd on the activated carbon surface as catalyst carrier

Marek Wojnicki\*, Magdalena Luty Błocho

AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Mickiewicza 30 Av, 30-059 Krakow, Poland

Carbon supported palladium catalyst is frequently used in chemical synthesis. The goal of the work is to shed light on the process of Pd(II) ions adsorption from aqueous solution on the activated carbon and role of oxygen-containing functional groups on the process. It is well known that the carbon is hydrophobic, and thanks to the presence of oxygen-containing functional groups its hydrophilic properties can be controlled.

For activated carbon oxidation modified Hummers' method was applied. Additionally, comparative studies were performed with the application of reduced activated carbon. The elimination of oxygen-containing groups was possible thanks to the annealing of the activated carbon in a hydrogen atmosphere. It was found that the adsorption process strongly depends on the nature of activated carbon.

Electronic state of palladium after adsorption strongly depends on the method how the activated carbon was prepared. In case of adsorption onto oxidized activated carbon, palladium after adsorption was found on +2 and 4+ oxidation state, where else after adsorption onto reduced activated carbon palladium was found on 0 and 2+ oxidation state. Moreover adsorption capacity of activated carbon depends on the method how the activated carbon was prepared.

This clearly confirms, that there is a strong influence of oxygen-containing functional groups on the adsorption process as well as on catalyst synthesis.

### Audience Take Away:

- Activated carbon is still most commonly used as absorbent and catalyst support because of its large surface area and low costs
- The efficiency of the impregnation (adsorption) process strongly depends on the activated carbon properties, such as porosity, surface area and content of functional groups.
- Moreover, the role of palladium complex structure is crucial

### Biography:

PhD Marek Wojnicki studied Metallurgy at the University of Science and Technology in Poland and graduated as MS in 2008. He received his PhD degree in 2014 at the same institution. He has published more than 40 research articles in SCI journals. The main research topics of these works are nanomaterials and adsorption phenomenon.

## Oxyhydride perovskites: From characterization to reactivity study

Quang-Nguyen Tran<sup>a,b\*</sup>, Monica Ceretti<sup>b</sup>, Dariusz Świerczyński<sup>a</sup>, Prof. Werner Paulus<sup>c</sup>, Prof. Barbara Bonelli<sup>b</sup>,  
Dr. Ing., PhD. Francesco Di Renzo<sup>a</sup>

<sup>a</sup> Institut Charles Gerhardt Montpellier, École nationale supérieure de chimie de Montpellier, Montpellier, France

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<sup>c</sup> Université de Montpellier, Montpellier, France

Oxyhydride perovskites adapt to either conventional  $ABX_3$  or Ruddlesden-Popper  $A_2BX_4$  structures where both anions  $H^-$  and  $O^{2-}$  are accommodated in one framework. In  $ABX_3$ , hydride anions can substitute  $O^{2-}$  in any sites of the  $BO_6$  octahedron, while the figure for  $A_2BO_4$  is slightly different. Hydride partially occupies the axial positions of octahedral  $O^{2-}$  sites only along b-direction of the  $BO_2$  planar square, which may result in the filling of anionic sites by  $H^-$ ,  $O^{2-}$  or vacancies. The presence of hydride species in the structures result in intriguing characteristics: high Neel temperature observed in Cr- and Co-based oxyhydride perovskites; lability of hydrides in  $BaTi(OH)_3$  allows to synthesis oxynitrides at significantly milder conditions; hydride intercalation may alter crystallinity or unusual oxidation states of transition metals in the oxyhydride perovskites. Moreover, hydride mobility in the structures was evidenced, which lead to potential applications of oxyhydrides in catalysis.

In the presentation, two oxyhydride perovskites  $LaSrCoO_{3.5-x}H_y$  ( $y-x \leq 0.5$ ) and  $BaTiO_{3-x}H_x$  bearing Ruddlesden-Popper  $A_2BX_4$  and  $ABX_3$  structures, respectively, will be discussed in terms of their topochemical synthesis, perovskite structures and properties. Moreover, various techniques of oxyhydride perovskites characterizations will be deeply mentioned. For example, X-Ray diffraction, magnetic measurements, Fourier-transform infrared spectroscopy (FT-IR), thermogravimetric mass spectroscopic (TGA-MS), X-ray photoelectron spectroscopy (XPS) and  $H_2$ -temperature programmed reduction ( $H_2$ -TPR). The work will also show different levels of thermal stability of these oxyhydride under oxidative/reducing conditions, which were studied by *in situ* XRD and  $H_2$ -TPR techniques. Interactions of hydrides with supports lead to questions about possible reactivity of oxyhydrides towards hydro-related reactions. Reactivity of the oxyhydrides  $LaSrCoO_{3.5-x}H_y$  and  $BaTiO_{3-x}H_x$  towards hydrogenation reactions will be also discussed. The work may open some the reactive potentiality of oxyhydrides for other reactions and applications.

### Audience Take Away:

- History of oxyhydride perovskites and topochemical synthesis
- Different techniques for oxyhydrides' characterizations
- Stability under different conditions and reducibility
- Potential catalytic activity for future catalysis
- Promising applications of oxyhydrides in other fields such as electrocatalysis

### Biography:

2016-now: Erasmus Mundus PhD student, Sustainable Industrial Chemistry (Sinchem Program), École Nationale Supérieure de Chimie de Montpellier | Politecnico di Torino.

2012-2016: Senior Field Engineer, Wireline Division, Baker Hughes Inc.

2010-2012: European Master in Advanced Spectroscopy in Chemistry (ASC), Erasmus Mundus Master Program, University of Bologna (Italy) and University of Lille 1 (France)

2008-2010: Researcher, Vietnam Petroleum Institute

2003-2008: Engineer Diploma, Irkutsk State Technical University, Russia.

## Stability behaviour of Ce promoted Ni catalysts supported on modified ZrO<sub>2</sub> with La<sub>2</sub>O<sub>3</sub>, PO<sub>4</sub> & WO<sub>3</sub>, for dry reforming of methane

Ahmed S. Al-Fatesh<sup>1\*</sup>, Ahmed A. Ibrahim<sup>1</sup>, Yasir Arafat<sup>1</sup>, Samsudeen O. Kasim<sup>1</sup>, Abdulrahman Alharthi<sup>2</sup>, Francesco Frusteri<sup>3</sup>, Anis H. Fakeeha<sup>1</sup>, Ahmed E. Abasaed<sup>1</sup>

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The dry reforming of methane reaction into a valuable synthesis gas (H<sub>2</sub> and CO), is a potential candidate dealing with the dwindling energy resources and global warming challenges simultaneously. Syngas is known as the building block for petrochemical industry for the production of hydrogen and liquid fuels like methanol, paraffin, olefins, oxygenates and aromatic through Fischer-Tropsch synthesis process. An incipient wet impregnation method was used to prepare Ni supported on high surface area ZrO<sub>2</sub> and modified ZrO<sub>2</sub> catalysts. The support modifiers are La<sub>2</sub>O<sub>3</sub>, PO<sub>4</sub> and WO<sub>3</sub>. Dry reforming of CH<sub>4</sub> experiments over Ni/ZrO<sub>2</sub> catalysts, subjected to calcination at 550 °C for 3 hr, were performed at 700°C for 400 min and at atmospheric pressure in a vertical stainless steel fixed-bed tubular (9.1 mm i.d. and 0.3 m long). Prior to each test, the catalysts were activated under a continuous flow of H<sub>2</sub> (20 ml/min) for 1 hr at the 600°C temperature. Experiments were done using a feed gas mixture (CH<sub>4</sub>, CO<sub>2</sub>, and N<sub>2</sub>) at ratio 6/6/1 and the overall gas flow rate of 65ml/min (space velocity: 39000 ml (h.g<sub>cat</sub>)<sup>-1</sup>). It is well known that dry reforming reactions is negatively affected by some side reactions, for instance, Boudouard reaction, water gas shift reaction, and methane decomposition, which are mainly responsible for the deactivation of catalysts due to coke deposition. The physicochemical properties of various obtained catalysts were assessed using XRD, TPD, TPR, BET, TGA and TEM techniques. The support modification resulted in a substantial increase of the Lewis basicity of modified catalysts. La<sub>2</sub>O<sub>3</sub> incorporation produced the stable t-ZrO<sub>2</sub> phase, consequently, Ni/La-ZrO<sub>2</sub> catalyst, displayed the best performance among all the catalysts in terms of both CH<sub>4</sub> and CO<sub>2</sub> conversions. When La<sub>2</sub>O<sub>3</sub> was incorporated into ZrO<sub>2</sub>, microscopic study displayed the formation of carbon nanotubes (MWCNTs) with an average external diameter of 28 nm, while the metallic species were located both inside as well as on the external surface of MWCNTs ( the majority of metal particles were positioned on the external side). The size of metal particles was as large as 6nm. Ni/Zr had a very low CH<sub>4</sub> conversion and the activity declined rapidly, while La doping had overwhelmingly improved the catalytic activity. Compared with Ni/Zr, the percent rise in CH<sub>4</sub> conversion was 91% and CO<sub>2</sub> conversion was 48%.

TGA analysis of spent catalysts was performed to evaluate the anti-coking ability of pure and La-modified catalysts. La-modified catalyst had a weight loss of about 90% and combusting at relatively higher temperature (800°C) depicting the formation of stable carbon in the form of encapsulated or filamentous carbon. When the catalysts were promoted using 1% CeO<sub>2</sub>, monoclinic ZrO<sub>2</sub> phase transformed to tetragonal ZrO<sub>2</sub> phase. After the CeO<sub>2</sub> promotion, the amount of carbonaceous materials accumulated on the surface of catalysts significantly reduced and weight loss amounted about 50%. Furthermore, the corresponding peaks shifted to the lower temperature, which implies that the less stable carbon material had formed which burnt at relatively lower temperature. The 1% CeO<sub>2</sub> promoter enhanced the stability of the Ni/La-ZrO<sub>2</sub> catalyst.

### Audience Take Away:

- In this experimental work an incipient wet-impregnation technique was used to prepare the desired catalysts for the dry reforming of methane.
- The audience will learn how to carry out catalyst preparation in a systematic way. The research was expanded by considering different element and different operating conditions. The present work provides a practical solution to minimize the carbon deposition on the catalyst that deactivates it.
- The research work that is being presented will improve the activity and stability of the process of dry reforming of methane by reducing the greenhouse gases and therefore contributing to pollution control.
- It supports the utilization of existing resources, which leads to the production of synthesis gas.
- The synthesis gas has versatile benefits in producing various chemicals.

### Biography:

Dr. Ahmed S. Al-Fatesh: Associate Professor of Chemical Engineering, King Saud University, Riyadh, Saudi Arabia. He has three USA registered patents and over 100 publications in International journals and conferences. He has theoretical and experimental capabilities and he also gained first hand research experience on several state of the art catalyst characterization techniques. He has been involved in a number of research projects which focus on catalyst development, syngas/hydrogen production and utilization of greenhouse gases through reforming processes like dry reforming, steam reforming and catalytic decomposition of methane. Currently, the research's interests include: heterogeneous catalysis, nano-material synthesis, chemical reaction engineering, petrochemical industries.

## Green synthesis of $\text{Ni}_{0.5}\text{Zn}_{0.5}\text{AlFeO}_4$ magnetic nanoparticles by tragacanth gel and its application as a photocatalyst for degradation of reactive blue 21 dye

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<sup>1</sup>Department of Chemistry, University of Zanjan, P O Box 45195-313, Zanjan, Iran

<sup>2</sup>Research Institute of Modern Biological Techniques (RIMBT), P O Box 45195-313, University of Zanjan, Zanjan, Iran

In the last decade, preparing the nano catalyst via photocatalytic capability by using the green synthesis methods has been a favorite of researchers. Plant extracts for the biological synthesis of nanoparticles have received more attention because it is inexpensive, simple, environmentally benign and non-toxic. Further, the plant extracts are fortified by the variety of biomolecules like alkaloids, phenols, terpenoids, flavonoids and etc. In this paper, magnetic nanoparticle was synthesized using tragacanth gel as a biotemplate by the novel sol-gel method and its photocatalytic dye degradation ability from aqueous solution was studied. This method has many advantages such as nontoxic, economic viability, ease to scale up, less time consuming and environmental friendly approach for the synthesis of  $\text{Ni}_{0.5}\text{Zn}_{0.5}\text{AlFeO}_4$  magnetic nanoparticle without using any harmful chemicals. The characteristics of magnetic nanoparticles were investigated using powder X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), vibrating sample magnetometer (VSM), scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDX). The X-ray powder diffraction (XRD) analysis revealed the formation of Cubic phase MNPs with average crystallite size of 10 nm. Photocatalytic dye degradation by  $\text{Ni}_{0.5}\text{Zn}_{0.5}\text{AlFeO}_4$  magnetic nanoparticles were evaluated by UV-Vis spectrophotometer. The effects of catalyst dosage, initial dye concentration and visible light irradiation on dye degradation were investigated. The results demonstrated that the catalyst can degrade ca. 94% of the reactive blue 21 dye. The catalyst can be easily recovered by a simple magnetic separation and can be recycled six times with no significant loss of photocatalytic activity.

### Biography:

Ali Ramazani has completed his Ph.D under the supervision of Professor IssaYavari in the Department of Chemistry at the TarbiatModares University (TMU) in the Tehran-Iran. He currently works as a full professor in Chemistry at the University of Zanjan in the Zanjan-Iran. His studies focused on organic synthesis and nanochemistry and he has published more than 450 papers. He is an Editorial Board Member of the international Journal Nanochemistry Research. He has received several national and international awards, including the 2013 khwarizmi international award, several top-cited author awards and best-paper awards from leading ISI Journals, Best Researcher Awards, and the Best Lecturer Awards at the University of Zanjan.

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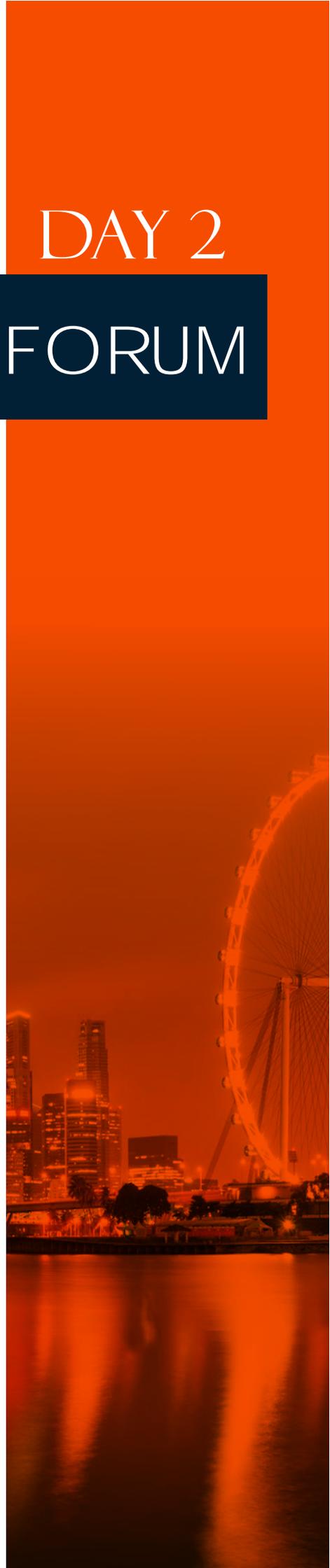
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#### Biography:

Carolina Belver is Associate Professor in Chemical Engineering Section at Autonomous University of Madrid, Spain since 2011. She received the Ph.D. in 2004 at University of Salamanca (Spain). Her specialization and current researches are related to design, processing and evaluation of novel heterostructures for applications in environmental remediation, mainly focused on heterogeneous catalysis and photocatalysis. Before the current position, she enjoyed competitive postdoctoral contracts at Catalysis and Petrochemistry Institute (2005-2007), and Material Science Institute of Madrid (2008-2011), Spain. She is associate editor of the Chemical Engineering Journal, co-author of more than 50 publications and eight chapter-books, and received in 2013 a Fulbright Fellowship. She has national and international collaborations mainly focused on synthesis of novel catalysts and adsorbents, and removal of pollutants by advanced oxidation technologies.

## Heterostructures for emerging pollutants degradation under sunlight irradiation

**Carolina Belver, Ph. D.**

Autonoma University of Madrid, Spain

This presentation deals with the synthesis of novel heterostructures for the degradation of emerging pollutants by photocatalysis using sunlight. It will be discussed the properties of those heterostructures based on metal oxide semiconductors assembled over several supports. In order to provide a global vision clays and carbon-based materials have been used as porous supports.

The discussion includes the comparison among different synthesis approaches, including sol-gel, microwave-assisted synthesis and solvothermal ways.

The main aim of this presentation is the design and optimization of novel photocatalysts able to remove emerging pollutants in water by using sunlight irradiation. Therefore, several heterostructures will be presented based on titania and titania-modified assembled over silicates and carbon materials. The characterization of the resulting catalysts reveals the formation of oxide nanoparticles that remain anchored to the surface of the support.

The photodegradation of emerging pollutants (acetaminophen and antipyrine) will be discussed in order to evaluate the photocatalytic efficiency of these heterostructures. Several parameters have been considered to design the best photocatalyst, taking in mind the physical-chemical properties of both oxide and support. In some cases, the synergic effect of oxide nanoparticles and support allowed the photodegradation after a few hours of irradiation. A complete study of both effects will be necessary to design optimum sunlight photocatalysts, pointing out the relevance of their efficiency and stability.

#### Audience Take Away:

- The audience can acquire a global vision about the current trends on a promising technology for water remediation.
- Photocatalysis is a technology under study along the world. Many researches are looking for novel catalysts active under sunlight, thus they can use this presentation to expand their research.
- The presentation will provide information about the synthesis and characterization of photocatalysts. Audience can use the information as reference for their work.
- Photocatalysis can be implemented in rural and suburban regions as water remediation technology with a low cost.



### Biography:

Prof. Holger Braunschweig is Chair and Head of Inorganic Chemistry at the Julius-Maximilians-Universität Würzburg, where is also member of the Senate and Founding Director of the Institute for Sustainable Chemistry & Catalysis with Boron (ICB). Braunschweig's research in the field of boron and main group chemistry has been published in over 500 publications. In 2009 Braunschweig was awarded the Gottfried Wilhelm Leibniz award of the DFG – the highest German-based research prize. He is a member of the Bavarian Academy of Sciences, the German National Academy of Sciences (Leopoldina), and the North Rhine-Westphalian Academy of Sciences.

## Borametallomimetics – Activation of small molecules by Low-valent Boron species

### Holger Braunschweig, Ph. D.

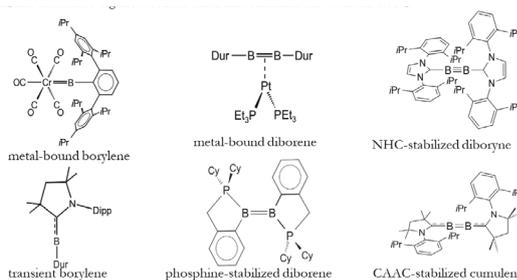
Julius-Maximilians-Universität Würzburg, Germany

The activation of small molecules is generally associated with transition metals (TM) and constitutes the basis of catalysis. It was believed that TM catalysts are required to facilitate processes such as the activation of H<sub>2</sub> and other unreactive substrates.

However, recent years have witnessed exciting developments in main group element chemistry, and the discovery of carbenes, FLPs and heavy main group species that are capable of TM-like activation reactions.

Our ongoing studies on borylenes, diborenes, and diborynes have shown that these low-valent species exhibit a very rich chemistry, which is distinctly different from that of common compounds deriving from boron in oxidation state +3.

Particularly interesting is the metal-like behavior of some borylenes and diborynes, which form CO complexes analogous to TMs, bind H<sub>2</sub> and unsaturated organic substrates under mild conditions and even activate N<sub>2</sub>.



1 a) P. P. Power, *Nature*, 2010, 463, 171; b) G. C. Welch, R. R. San Juan, J. D. Masuda, D. W. Stephan, *Science*, 2006, 314, 1124; c) G. D. Frey, B. Lavallo, B. Donnadiou, W. W. Schoeller, G. Bertrand, *Science*, 2007, 316, 439.

2 a) H. Braunschweig, R. D. Dewhurst, F. Hupp, M. Nutz, K. Radacki, C. Tate, A. Vargas, Q. Ye, *Nature*, 2015, 327; b) H. Braunschweig, K. Radacki, A. Schneider, *Science*, 2010, 328, 345; c) H. Braunschweig, R. D. Dewhurst, K. Hammond, J. Mies, A. Vargas, K. Radacki, *Science*, 2012, 336, 1420; d) M.-A. Légaré, G. Bélanger-Chabot, R. D. Dewhurst, E. Welz, I. Krummenacher, B. Engels, H. Braunschweig, *Science*, 2018, 359, 896.

### Audience Take Away:

- The history of the synthesis of reactive, electron-rich, low-valent main-group compounds.
- Techniques to prepare low-valent main-group compounds and their properties.
- How and why low-valent main-group compounds can sometimes mimic transition metal fragments in their reactivity.
- How and why low-valent boron compounds can bind and mediate the functionalization of small molecules such as CO, H<sub>2</sub>, N<sub>2</sub> and others.

SPEAKERS

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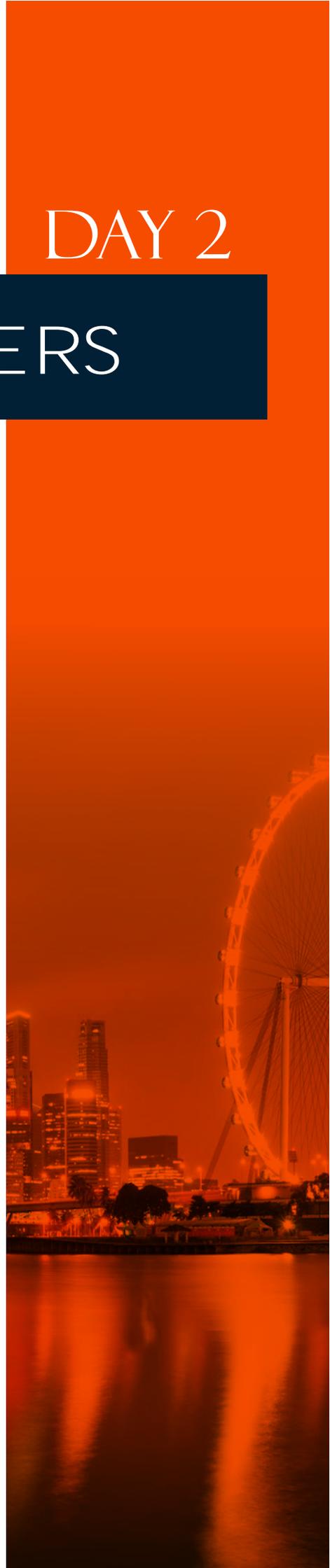
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## Recent development of Ni based composite as electrocatalysts for proton exchange membrane fuel cells

Florentina Neațu<sup>1</sup>, Mihaela M. Trandafir<sup>1</sup>, Ștefan Neațu<sup>1</sup>, Simona Somacescu<sup>2</sup>, Mihaela Florea<sup>1,3\*</sup>

<sup>1</sup>National Institute of Materials Physics, Laboratory of Condensed Matter and Physics at Nanoscale, 405A Atomistilor Street, 077125 Magurele, Romania

<sup>2</sup>"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Spl. Independentei 202, 060021 Bucharest, Romania

<sup>3</sup>University of Bucharest, Faculty of Chemistry, 4-12 Regina Elisabeta Blvd., 030016 Bucharest, Romania

The increasing worldwide energetic demands in the last decade's push humankind to seek for alternatives to the actual environmental unfriendly carbon-based energy production processes. In this regard, alkaline water electrolysis, fuel cells and metal-air batteries are nowadays among the most studied energy conversion and storage systems. Proton exchange membrane fuel cells (PEMFCs) are electrochemical devices that convert chemical energy directly into electrical energy and represent the leading candidate in the alternative energy industry. PEMFC is a two electrode system, with hydrogen evolution reaction (HER) or oxygen reduction reaction (ORR) taking place at cathode, while the anode performing oxygen evolution reaction (OER) or oxidation of chemical fuels. To increase the redox reactions rate that occur at the anode and cathode of a PEMFC, a catalyst represents a prerequisite. Currently, the most active electrocatalyst is based on Pt deposited on carbon. Nevertheless, the high cost of Pt on one side and carbon corrosion, which inherently leads to loss of catalyst, on the other side, constrain the scientific community to find alternatives. Therefore, a lot of research has been devoted for the development of new electrocatalysts with low noble metal content or even for non-noble metal systems supported on oxides.

During this presentation two case studies will be discussed: one presenting the improvement of the ORR activity by using Ni, Co, doped ZrO<sub>2</sub> self-assembled electrocatalysts and the second one describing the remarkable results obtain in OER using NiSn composite.

Both materials were prepared by cost efficient and facile hydrothermal template methods. The effect of the Ni, Co incorporation into ZrO<sub>2</sub> lattice and SnO<sub>2</sub>, respectively, on the structural, textural, surface chemistry and their activity on ORR and OER will be emphasized.

The synergetic effect induced by the incorporation of Ni and Co to stabilize zirconia as well as the presence on the surface of a large percentage of hydrous species significantly enhanced the electrocatalytic activity towards ORR, while the best material used in OER that exhibit a very good catalytic activity (more than 24 mA cm<sup>-2</sup> at an overpotential value of approx. +0.33 V vs. RHE at extremely low quantities (approx. 3.78 ng Ni species) is 5NiSn200.

### Audience Take Away:

- New facile and cost efficient preparation techniques will be well described
- Exhaustive characterization techniques will be presented
- Correlations between the characterization data and the electrochemical activity in order to understand the behavior of the best systems

### Biography:

Mihaela Florea received her Bachelor's degree in Chemistry from the University of Bucharest in 1997 and from the same university she received the Master degree in 1999. The PhD was done under the supervision of Professor Paul Grange in the field of Catalysis at the Universite Catholique de Louvain la Neuve, Belgium and she graduated in 2003 with Suma Cum Laude. In February 2004, she joined the group of Catalysis at the Faculty of Chemistry, University of Bucharest where she began her research on heterogenous catalysis, especially on catalytic selective oxidation. From 2018 she is Senior Researcher at the National Institute of Materials Physics. Her current research focuses on the synthesis and characterization of sustainable catalytic materials for selective oxidation and energy applications. She is the author of >75 publications in the field of heterogeneous catalysis and green chemistry, with a Hirsh factor of 19.

## Hydrogen generation in microgravity environments using nanostructured photoelectrodes

Ömer Akay<sup>1\*</sup>, Katharina Brinkert<sup>2</sup>, Lucia Nascimento<sup>3</sup>, Joachim Lewerenz<sup>4</sup>, Michael Giersig<sup>5</sup>

<sup>1</sup>Department of Physics, Freie Universität Berlin, Berlin, Germany

<sup>2</sup>Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California, USA

<sup>3</sup>Department of Physics, Freie Universität Berlin, Berlin, Germany

<sup>4</sup>Division of Engineering and Applied Science, California Institute of Technology, Pasadena, California, USA

<sup>5</sup>Department of Physics, Freie Universität Berlin, Berlin

Photoelectrochemical cells (PEC), which employ semiconductor-systems enable light-induced water splitting into oxygen and hydrogen. Microgravity experiments are crucial to understand the effects of gas bubble formation in these photoelectrochemical reactions. Drop tower experiments at the ZARM (Zentrum für Angewandte Raumfahrt und Mikrogravitation) simulate microgravity environments for 9.2 seconds. Herein, we show the possibility to realize efficient artificial photosynthesis in microgravity environments for deep space missions. The photosystem is based on III-V semiconductor absorbers that are coupled to nanostructured electrocatalyst layers. Drop tower experiments at ZARM showed that we could circumvent the problems of gas bubble froth layer formation in the absence of buoyancy.

Nanosphere lithography (NSL) was used as a reliable and cost-efficient tool to fabricate a three-dimensional nanostructured catalyst layer (here rhodium) on a semiconductor (p-type Indium Phosphide) photoelectrode by controlling its morphology. Our results demonstrate the photoelectrochemical production of hydrogen by measuring the photocurrent-voltage behavior of the combined half-cell p-InP/Rh/electrolyte. Size and shape modifications used in the NSL process enable nanostructured topographies to increase the catalytic activity and provide large short circuit currents up to  $>15 \text{ mA/cm}^2$  at illumination levels of white light between 70 and  $100 \text{ mW/cm}^2$ . Structural analysis including SEM, AFM, XPS for varied catalyst topography and simulations using a kinetic transport model support and complement the photoelectrochemical observations.

### Audience Take Away:

- Audience will learn about terrestrial light-induced water-splitting, wet chemistry, and water splitting in microgravity environment
- How to increase the detachment of bubbles from nanostructured surface areas in microgravity
- Dependence of catalytic activity by increased active surface areas by nanostructures
- Solution to build life-sustaining solar fueled systems for long deep-space mission

### Biography:

Ömer Akay studied Physics at the Freie Universität Berlin and graduated as Master of Science in 2016 under the supervision of Prof. Dr. Giersig. He then continued in the research group of Prof. M. Giersig working on nanostructured and plasmon active biosensing chips for pathogen detection in the biochemical and pharmaceutical institute of the same University. In 2018, he expanded his research to study on nanostructured (photo-)electrodes in microgravity environments as a doctoral student.

## Microscopic insights on fabrication and properties of catalysts using synchrotron-based methods

M. Kiskinova<sup>1\*</sup>, L. Gregoratti<sup>1</sup>, A. Gianoncelli<sup>1</sup>, G. Kourousias<sup>1</sup>, B. Bozzini<sup>2</sup>

<sup>1</sup>Elettra-Sincrotrone Trieste, Area Science Park, 34149 Trieste-Basovizza, Italy

<sup>2</sup>Dipartimento di Ingegneria dell'Innovazione, Università del Salento, via Monteroni, 73100 Lecce, Italy

**H**eterogeneous catalysis, one of the crucial technologies employed within the chemical and energy industries and electrochemical devices, is exclusively controlled by the processes occurring at the catalyst surfaces in contact with gas or liquid phase. However, the knowledge guided fabrication of efficient and long-lasting catalysts is still hindered by 'material' problems that require issues of complexity at various microscopic length scales to be faced and understood. In this respect the complementary capabilities of synchrotron-based methods in terms of imaging, spectroscopy, spatial and time resolution and variable probing depths have opened unique opportunities to explore the structure and chemical composition of morphologically complex catalyst materials at relevant length and time scales and correlate them to the actual fabrication or operating conditions. The topics that will be addressed and discussed in the talk are the events occurring with metal, alloy and composite catalysts under growth and reaction conditions uncovered by monitoring the evolution in lateral inhomogeneity in the composition and chemical state at sub-micrometer length scales. The talk will include selected results illustrating (i) compositional complexity of metal catalysts developed under reaction conditions and correlation of the spatial variations in the chemical composition to the morphology; (ii) the effect of growth conditions on the chemical state and space distribution of electrodeposited hybrid metal/polypyrrole electrocatalysts for oxygen reduction reaction in electrochemical devices – fuel cells and metal/air batteries; (iii) aging of composite metal/polypyrrole electrocatalysts cycled in O<sub>2</sub> saturated acidic or alkaline electrolyte (iv) monitoring in-situ the lateral evolution of the chemical state and local potential at the electrode/electrolyte interface in solid oxide fuel cells.

Ongoing efforts for development and implementing in-operando photoelectron microscopy experimental set-ups will be outlined and briefly discussed at the end of the talk.

### Audience Take Away:

- Benefit from the use of synchrotron radiation facilities for characterization of catalysts by implementation of multitechnique strategy.
- New information via shedding light on the missing chains in composition-structure-function relationships that define catalyst performance.
- Recent advances for overcoming the present limits in operando investigation.

### Biography:

Maya Kiskinova graduated from Sofia State University, received Ph.D in 1977 and Sc. D. in 1989. She was a senior scientist in Bulgarian Academy of Science before moving to Elettra Laboratory in 1990 where is presently the Research Coordinator. She worked at NBS, now NIST (USA) in 1980, IGF-KFA, now FZJ (Germany) in 1982-1984 and University of Pittsburgh (USA) in 1987-1988. In 2002 she received Italian citizenship for scientific merits and in 2005 was awarded Distinguished AvH Grant. She has more than 300 articles, 14 invited reviews and one book. H-index 48.

Web-page: <http://www.elettra.trieste.it/PEOPLE/index.php?n=MayaKiskinova.HomePage>

## Electrocatalytic materials for fuel oxidation and oxygen reduction reactions

Virginija Kepeniene\*, Raminta Stagniunaite, Loreta Tamasauskaitė-Tamasiunaite Jurate Vaiciuniene, Eugenijus Norkus

Department of Catalysis, Center for Physical Sciences and Technology, Vilnius, Lithuania

Improvements in the design and function of catalytic materials are crucial in solving a host of current problems including developing cleaner fuel technologies and removing environmentally harmful processes in the pharmaceutical or chemical industries. By far the most extensive industrial usage of composite materials relates to polymeric matrices reinforced with glass or carbon fibres. These form the mainstay of many important application areas in aerospace, land transport, marine, sports goods and a number of other industrial sectors. In general, these materials are mature and highly-developed, however researchers tend to focus on the composites, designed for more specialised applications. Catalytic materials are those solids that allow the chemical reaction to occur efficiently and cost-effectively. In recent years, many different catalytic materials are being studied for various catalytic processes. Porous materials consisting of organic linkers connected by metal ions provide framework scaffolds for heterogeneous catalysis, which is based on the organic, or inorganic components. Composite materials prepared by the combination of two or more different materials with distinct chemical or physical characteristics for fuel cell reactions. Various metals' containing coatings and thin solid films for corrosion resistance analysis and for investigation of others electrochemical reactions.

This work presents investigation of various carbon based catalytic materials containing noble and non-noble metals and their oxides for fuel cell reactions. Various Au, Pd, Co and  $\text{Co}_3\text{O}_4$ ,  $\text{CeO}_2$ ,  $\text{Nb}_2\text{O}_5$  supported materials using different fabrication methods such as microwave irradiation heating, electroless deposition and adsorption were prepared. Electrocatalytic properties of obtained  $\text{AuCo}_3\text{O}_4/\text{C}$ ,  $\text{PdCo}_3\text{O}_4/\text{C}$ ,  $\text{AuCeO}_2$ ,  $\text{AuNb}_2\text{O}_4$ ,  $\text{CoCo}_3\text{O}_4/\text{C}$  materials were investigated towards fuel (methanol, ethanol, ethylene glycol) oxidation and oxygen reduction reactions and discussed on the basis of electrochemical data.

### Audience Take Away:

- The audience will learn basic knowledge about the fabrication and application of electrocatalytic materials for fuel cell.
- There will be discussed and compared nano-scale materials prepared by different methods as microwave irradiation heating, electroless deposition and adsorption.
- There will be discussed specific details on particular processes: fuel (methanol, ethanol, ethylene glycol) oxidation reaction; oxygen reduction reaction.
- There will be presented opportunities of exchange of scientists and collaboration.

### Biography:

Dr. Virginija Kepeniene got her PhD degree in 2012 at the Department of Catalysis of Center for Physical Sciences and Technology. After a post-doctoral internship related to the investigation of catalysts for alkaline fuel cells she continued her work as a researcher at the same Department in relation to the various nano-scale materials formation and investigation. She has been working as a senior researcher since 2017. Virginija Kepeniene actively participates in scientific activity. She is co-author of 21 publications, among them 16 keynote author. 52 contributions to conferences, of which 28 is the keynote speaker. Co-author of the Lithuanian patent.

## Design and optimization for environmental application of TiO<sub>2</sub> photocatalysts

Tsuyoshi Ochiai<sup>1,2,3\*</sup>, Mio Hayashi<sup>1</sup>, Shoko Tago<sup>1</sup>, Akira Fujishima<sup>1,3</sup>

<sup>1</sup>Photocatalyst Group, Research and Development Department, Local Independent Administrative Agency Kanagawa Institute of Industrial Science and Technology (KISTEC), 407 East Wing, KSP, 3-2-1 Sakado, Takatsu-ku, Kawasaki City, Kanagawa 213-0012, Japan

<sup>2</sup>Materials Analysis Group, Kawasaki Technical Support Department, KISTEC, Japan

<sup>3</sup>Photocatalysis International Research Center, Tokyo University of Science, Japan

In view of the situation that environmental issues become more serious day by day, application of the strong oxidation ability of photo-excited TiO<sub>2</sub> for environmental purification has received growing attention. Under this circumstance, we summarized several key requirements for an effective photocatalytic environmental purification: (1) catalyst immobilization strategy for a cost-effective solid-liquid separation, (2) integrated or coupling system for enhanced photo mineralization or photo-disinfection kinetics, and (3) effective design of photocatalytic reactor system especially enlargement of reactive surface area and improvement of mass transfer. Based on these insights, recent achievements for development of photocatalytic environmental purification system with our contribution in each aspect and future research directions are discussed. For examples, combination of non-thermal plasma treatment and TiO<sub>2</sub>-deposited Ti-mesh filter for practical air-purifier, advanced oxidation processes (AOPs) with O<sub>3</sub> treatment for water purification, and solar-driven electrochemical and photo catalytic water treatment system with boron-doped diamond electrodes. We can expect that the continuous improvements of the material property and the reactor design would create a large number of effective environmental purification systems. Finally, we feel that, photocatalysis can realize a healthy and comfortable living environment.

### Audience Take Away:

- Photoelectrochemical properties of TiO<sub>2</sub> photocatalyst and its applications for environmental purification.
- Effective design of the photocatalytic reactors for environmental applications.
- Multidisciplinary collaboration for development of synergistic environmental purifiers.

### Biography:

T. Ochiai completed a doctoral course at the Nagoya Institute of Technology Graduate School of Engineering, Department of Materials. Many of his current research and development projects are related to environmental purification. Already many products such as photocatalytic filter materials and air-purifiers have been released by fruitful cooperation with the companies. He has published more than 70 research articles (for more details: [https://www.researchgate.net/profile/Tsuyoshi\\_Ochiai](https://www.researchgate.net/profile/Tsuyoshi_Ochiai)).

## Atomically dispersed catalysts for energy-related catalysis

**Xiaoqian Wang**

School of Chemistry and Materials Science, University of Science and Technology of China, Hefei, Anhui, China

This presentation includes three works on atomically dispersed catalysts for energy-related catalysis. In the first one, a series of atomically dispersed Co catalysts with different nitrogen coordination numbers are prepared and their CO<sub>2</sub> electroreduction catalytic performance is explored. The best catalyst, atomically dispersed Co with two-coordinate nitrogen atoms, achieves both high selectivity and superior activity with 94% CO formation Faradaic efficiency and a current density of 18.1 mA cm<sup>-2</sup> at an overpotential of 520 mV. The CO formation turnover frequency reaches a record value of 18,200 h<sup>-1</sup>, surpassing most reported metal-based catalysts under comparable conditions. Our experimental and theoretical results demonstrate that lower a coordination number facilitates activation of CO<sub>2</sub> to the \*CO<sub>2</sub><sup>-</sup> intermediate and hence enhances CO<sub>2</sub> electroreduction activity.

In the second one, we prepare atomically dispersed Au on carbon nitride (Au<sub>1</sub>/C<sub>3</sub>N<sub>4</sub>) and investigate its catalytic performance towards N<sub>2</sub> electro-reduction to ammonium ions (NH<sub>4</sub><sup>+</sup>) in sulfuric acid aqueous solution. Au<sub>1</sub>/C<sub>3</sub>N<sub>4</sub> exhibits outstanding NH<sub>4</sub><sup>+</sup> formation Faradaic efficiency which achieves 11.1% at -0.10 V vs. RHE (reversible hydrogen electrode), outperforming most of the reported catalysts. We then assemble a full electrolytic cell with Au<sub>1</sub>/C<sub>3</sub>N<sub>4</sub> as cathode to reduce N<sub>2</sub> into NH<sub>4</sub><sup>+</sup> and a platinum foil as anode to catalyze hydrogen oxidation reaction. Our experimental results demonstrate that such an electrolytic cell allows us to synthesize NH<sub>4</sub><sup>+</sup> directly from N<sub>2</sub> and H<sub>2</sub> with an energy utilization rate of 4.01 mmol kJ<sup>-1</sup>.

In the third work, we investigate the performance of CH<sub>4</sub> oxidation on atomically dispersed Ag catalyst. At a temperature of only 323 K, a methanol productivity of 0.44 mmol g<sup>-1</sup> h<sup>-1</sup> is achieved along with high selectivity, which allows us efficiently convert CH<sub>4</sub> into upgraded chemicals.

Our works underline the significant role of atomically dispersed catalysts in energy-related catalysis.

### Audience Take Away:

- Atomically dispersed catalysts may exhibit superior catalytic performance than counterparts.
- Coordination environment of atomically dispersed catalysts serves as a vital role in both catalytic activity and selectivity.
- Atomically dispersed catalysts have great potentials in energy-related catalysis.

### Biography:

Xiaoqian Wang received his B.Sc. in materials physics from University of Science and Technology of China in 2016. He is now pursuing his Ph.D. degree under supervision of Prof. Yuen Wu at iChEM (Collaborative Innovation Center of Chemistry for Energy Materials), University of Science and Technology of China. His current research interests focus on the application of nanomaterials in energy conversion and storage.)

## State-of-the-art Anion Exchange Membrane Fuel Cells

**Dario R. Dekel, Ph. D.**

Technion – Israel Institute of Technology, Israel

**A**fter a few years of intensive research, recent studies of Anion Exchange Membrane Fuel Cells (AEMFCs) finally show cell performance at the required levels for automotive applications. This achievement was mainly due to the successful development of anion exchange membranes (AEMs) with considerable high hydroxide conductivity ( $100 \text{ mS cm}^{-1}$  and above). Based on these high performance membranes, AEMFCs with power densities and limiting current densities higher than  $1 \text{ W cm}^{-2}$  and  $4 \text{ A cm}^{-2}$  have been recently achieved, which only a couple of years ago seemed far from possible. In order to achieve the next breakthrough in AEMFC technology, the following challenges need to be addressed: (A) the need for Pt-free (and PGM-free) catalysts highly active in alkaline medium, and (B) barriers in cell performance stability. Latest achievements in AEMFCs, as well as recent research on the above mentioned challenges will be presented and discussed during the talk.

### Audience Take Away:

- The audience will be able to learn about the AEMFC technology, the state-of-the-art of the technology, and the main advantages that the technology offer.
- The audience will be able to learn what are the main challenges the technology currently faces in order to reach its final research goals prior application in the field.
- This talk will allow the audience and the research community interested in this promising technology, to focus their research efforts on the main research challenges.
- Solving the challenges that will be presented and discussed during the talk, the audience will have a first-hand information on the latest advances of this technology, and know the main directions that still need further research.

### Biography:

B.Sc. in Chemical Engineering from UTN (Argentina), M.Sc. in Chemical Engineering and PhD and MBA from Technion I.I.T. (Israel). In 1998 he joined Rafael Ltd., where he led 50 researchers in the area of high temperature batteries. In 2007 Prof. Dekel co-found CellEra, where as VP for R&D he led 15 researchers to develop the Anion Exchange Membrane Fuel Cell technology. In 2015 Prof. Dekel joined the Technion, where he heads the TEEM Lab (Technion Electrochemical Energy based on Membranes), leading the largest worldwide research group on AEMFCs. Prof. Dekel hold more than 50 patents and papers on battery and FC technologies. He currently holds about \$4M government and company research grants from Israel, Europe and USA.

## Carbon-encapsulated Cu@GO catalysts and its application in ethylene carbonate hydrogenation

Chanjuan Zhang<sup>1,2,3\*</sup>, Ligu Wang<sup>1,2,3</sup>, Jiachen Li<sup>1,2,3</sup>, Yan Cao<sup>1</sup>, Peng He<sup>1</sup>, Huiquan Li<sup>1,2,3</sup>

<sup>1</sup>CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China

<sup>2</sup>Sino-Danish College, University of Chinese Academy of Sciences, Beijing, China.

<sup>3</sup>Sino-Danish center for Education and Research, University of Chinese Academy of Sciences, Beijing, China

Increasing CO<sub>2</sub> emission attracts much interest and attention on CO<sub>2</sub> hydrogenation to methanol. Ding et al found a process for indirect hydrogenation of CO<sub>2</sub> via ethylene carbonate (EC) intermediate to yield methanol with ethylene glycol as the co-product, and meanwhile the obvious advantage of the aim reaction is the high atom economy. In our previous study, Cu@SiO<sub>2</sub> has exhibited relatively high activity with the excellent stability, while the stable mechanism needs to be studied further. Therefore, it is highly desirable to develop more effective and stable heterogeneous catalysts for EC hydrogenation and its stable mechanism.

In this work, the stable carbon-encapsulated Cu@GO catalysts with disorder nanoporous network of graphite oxide were prepared by a facile, novel and brief ultrasonic hydrolysis method and the corresponding TEM image was shown in Figure 1a. The as-prepared Cu@GO catalyst was successfully employed in the hydrogenation of ethylene carbonate derived from CO<sub>2</sub>. The evaluation results of Cu@GO catalytic reusability verified that the catalytic activity was promoted obviously. Especially, the mentioned method was verified an effective method for fabricating the high dispersity carbon-encapsulated Cu@C catalysts with 20-130 nm Cu particles. Moreover, the TG/DTG result shown in Figure 1b suggested that the special amount residual carbon in Cu@GO catalysts.

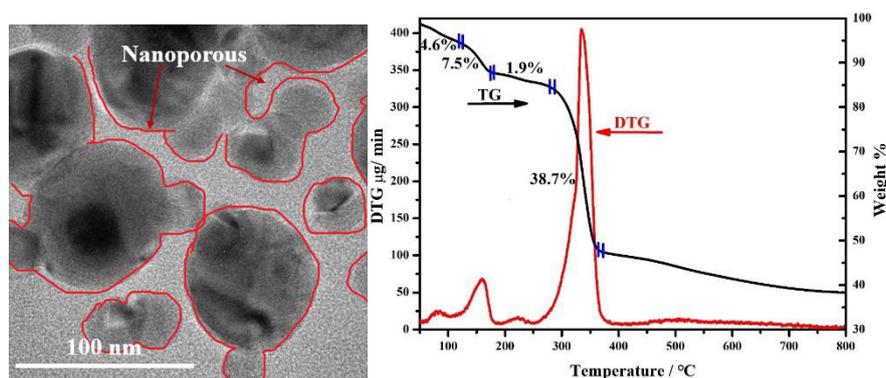


Figure 1 a) TEM image of Cu@GO catalyst, b) TG/DTG curve of the dried precursor of Cu@GO catalyst under pure nitrogen atmosphere.

The evaluation results of catalytic performance suggested that the disorder nanoporous network of graphite oxide promoted the catalytic activities in some extent, with a higher methanol selectivity of 80%, and enhanced the stability of copper-based catalysts. Furthermore, the synergistic effect between the Cu<sup>+</sup> and metallic Cu<sup>0</sup> species was considered to be the crucial for attaining catalysts with better catalytic activity.

### Audience Take Away:

- This presentation will introduce the newest research via the proposal and the development process of the mentioned method, of which will provide useful research method.
- The novel preparation method for carbon-modified copper-based catalysts will be introduced.
- The mechanism of the catalytic system for ethylene carbonate hydrogenation will be analyzed in this time.
- The special research method for studying the catalytic structure will be demonstrated.

### Biography:

Chan-Juan Zhang received her BSc degree in Sichuan University in 2016 and her MSc degree in Technical University of Denmark in 2018. She was admitted to Institute of Process Engineering, Chinese Academy of Sciences for master degree under the supervision of Prof. Hui-Quan Li and Dr. Li-Guo Wang. Her research interest is converting esters derived from CO<sub>2</sub> into commodity chemicals, e.g. methanol and ethylene glycol, and atomically-precise design of stable heterogeneous catalyst. She has published 2 research articles in SCI journals.

## Mechanistic study of Olefin/CO<sub>2</sub> coupling to form Acrylic acid: A DFT Study

**Farhan A Pasha**

CRD-SABIC, King Abdullah University of Science and Technology (KAUST) Thuwal – 23955 Saudi Arabia

CO<sub>2</sub>/Olefin copolymerization for the formation of acrylic acid is important in terms of scientific and industrial interest. There are continuous effort within framework of catalysis reduce the CO<sub>2</sub> activation energy. Recently Ni based catalyst 1,2-bis (diphenylphosphino) ethane (DCPE) in conjunction of lewis acid and base reported significant activity however, the mechanism of overall reaction is still under debate. We explored the mechanism of CO<sub>2</sub>/Olefin copolymerization using DFT calculations and studied the impact of lewis acid and base to this reaction. The study revealed that CO<sub>2</sub>/Olefin undergo oxidative coupling for metallolactone. The metallolactone show a lewis base assisted ketoenol transformation while a lewis acid helps weakening the metal-oxygen bond and a new olefin coordination to the metal helping acrylate elimination.

### Biography:

Dr. F. A Pasha, Lead Scientist SABIC corporate research and development at King Abdullah University of Science and Technology-KSA. His interest includes quantum chemical molecular interactions and finding new applications of Density functional theory. He worked (2006-2007) at Korea Institute of Science and Technology (KIST), Seoul South Korea. In January 2008, he moved to CEA Grenoble France as a Research Engineer with Dr. Martin Field to work for FP-7 Marie curie project. Later in November 2009 Dr. Pasha joined IFP energies Nouvelles (IFP) Rueil Malmaison, Paris. He worked as visiting scientist with Prof. Herve Toulhoat for the olefin oligomerization chemistry. In November 2010 Dr. Pasha Joined KAUST Catalysis Center under special agreement between KAUST and European ICE consortium where he worked extensively in close collaboration with Prof. Jean Marie Basset. In May 2014, Dr. Pasha moved to SABIC and started industrial career, currently engaged in computational chemistry efforts to wide range of industrial problems. His work encompasses the theoretical and computational exploration of structure and properties of inorganic and organic compounds, polymers and catalysts and separation technologies. However, the focus is to utilize CO<sub>2</sub> as feedstock and transforming into valuable products using inexpensive technologies. He has published over 50 articles and several patents applications.

## HPA modified clays: A remarkable green catalysts in organic synthesis

Chandra Mohan<sup>1\*</sup>, Sarla Kumari<sup>2</sup>

<sup>1</sup>Asst. Prof., School of Basic & Applied Sciences, K. R. Mangalam University, Gurugram-122103, India

<sup>2</sup>Assoc. Prof., Department of Chemistry, S. P. C. Government College, Ajmer 305001, Raj., India

Clays modified with Heteropoly acids (HPAs) have attracted much interest as green catalysts for organic synthesis. Heteropoly acids (HPAs) have several advantages over liquid acid catalysts such as noncorrosive, environmentally benign and due to their strong acidity HPAs have attracted much interest as the catalyst when used with montmorillonite and bentonite clays. Green chemistry focuses on advancement in techniques to prevent pollution and reduce consumption of hazardous chemicals. The development in this area may involve clean synthesis, ecofriendly methods, solvent free synthesis, green catalysts and avoiding the use of hazardous reagents in chemical methods.

For the the present study, heteropoly acid (HPA) modified montmorillonite & bentonite clays have been synthesized by swelling and pillaring of clays. Modified clays possess qualities such as good thermal stability, high acidity and high oxidising ability. These modified clays can be used as solid acid catalysts in reactions such as Deoxygenation of oximes of aldehydes and ketones, synthesis of acetal derivatives of aldehydes and ketones, synthesis of coumarin derivatives etc. For coumarin synthesis, these clays have been found to be efficient and reusable catalysts.

### Audience Take Away:

- One will be able to synthesize modified clays.
- Using modified clays as catalysts in organic synthesis.
- Use of green solid acid catalysts and how to reuse it.
- The clay can be modified by various methods by using different modifiers.
- This clay has wide applications as catalysts, adsorbent and for water treatment process for the removal of metal ions in problem.
- Future research can be done on these modified clays for their efficient use in microwave synthesis and for other organic reactions.

### Biography:

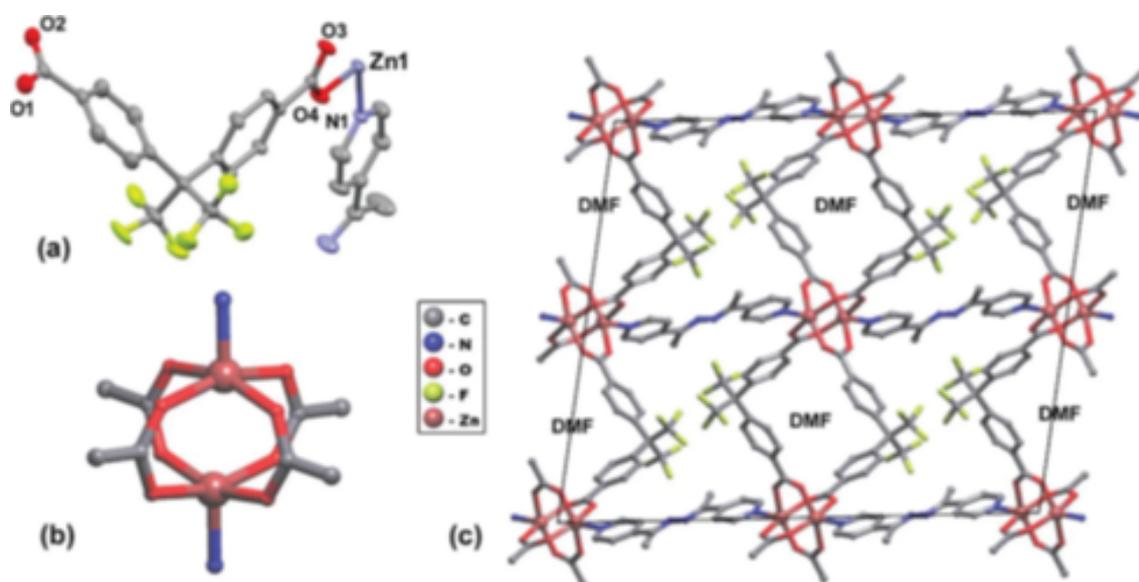
Dr. Chandra Mohan obtained his Ph.D degree in the field of "Schiff based metal complexes and their applications as Chemical Sensors" from Guru Gobind Singh Indraprastha University, Delhi, India in 2017. He has done M.Phil in Inorganic Chemistry from Delhi University and performed his research work on "Heteropoly acid intercalated clays as catalysts" in 2009. He has keen interest in research and development activities. He has 6+ years of teaching experience and about 8 years of research experience. He has published 10 research papers in reputed journals and has presented 10 research papers in various conferences and workshops held in India. He is an awardee of a national fellowship from University Grant Commission Delhi for his Ph.D. degree. He was also invited for a lecture from Sensor Lab, University of the Western Cape, Bellville, South Africa in May 2015 and as keynote speaker in the International conference at Imperial College London, UK in September 2018. Presently he is a reviewer & editorial member of 7 International Journals and 8 scientific bodies in India and abroad.

## Green Catalysis Application of some new Metal-organic frameworks

Ali Morsali

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Among continuing investigations in solid state chemistry, metal-organic frameworks (MOFs) are the class of promising materials which attracted tremendous amount of attention in the past two decades. MOFs are regarded as a subclass of coordination polymers (CP) which are constructed by self-assembly of metal ions or metal clusters linked together by organic ligands containing multiple binding sites oriented with specific angularity generating structures with permanent porosity, high specific surface area and tunable topology that can be used in different fields such as gas adsorption, separation, catalysis, sensing and drug delivery. As both parts, organic (linkers) and inorganic (metals or clusters) are able to act as catalyst in many different and important reactions, so in this presentation, the catalytic applications of these new highly porous compounds are presented compressively. Besides, Some reports are available so far regarding to the usage of MOFs as green catalyses.



### Biography:

Ali Morsali was born and raised in the Hidaj, Zanjan, Iran. He attended Tarbiat Moallem University, Tehran and earned a B.S. degree in Pure Chemistry. He received his Mnorganic Chemistry in Zanjan University, Zanjan. He then attended graduate school at the University of Tarbiat Modares, Tehran and earned his Ph.D. under the guidance of Prof. Ali Reza Mahjoub. After completing his Ph.D., he began his independent career at the University of Tarbiat Modares, Tehran, where he is a Professor in the Department of Chemistry. In 2016, he passed six months as a sabbatical period in Prof. Hupp group, Northwestern University. He also passed the other six months as a sabbatical period in Prof. Omar Yaghi group, Berkeley in 2017. His research interests are primarily in the area of inorganic chemistry, Coordination polymers and Metal-Organic Frameworks.

## Microwave catalysis by Nano-ferrites

Sandhya Mishra<sup>1\*</sup>, Sujoy Kumar Samanta<sup>1</sup> and Prashant Kumar<sup>2</sup>

<sup>1</sup>Department of Chemical and Biochemical Engineering,

<sup>2</sup>Department of Physics,

<sup>1,2</sup>Indian Institute of Technology Patna, Bihta, Patna-801106.

Synthetic dyes are used highly in many industries such as textile, paper-making, printing and dye manufacturing. The dye effluents of these industries are extremely colored and the discard of these toxic wastes into collected waters can affect the environment. Mostly, dyes are considerably toxic in nature and their presence in effluents may cause serious issues due to their potential negative effect on the aquatic life as well as human life. Moreover, dyes generally have complex aromatic structures and most of them are very difficult to degrade by physical, chemical and biological treatments. Many technologies are used such as adsorption, ultrasonic degradation, catalytic oxidation, photo catalytic degradation and microwave (MW)-enhanced advanced oxidation processes. Recently, MW-induced catalytic degradation has become a very promising technology in chemical applications due to its superior activity, short reaction time and especially when coupled with suitable MW absorbent. MW absorbing material spinel nickel ferrite, which used to degrade organic dyes under MW irradiation, was prepared by co-precipitation method of the mixed solution of ferric nitrate and nickel sulphate. The catalyst was characterized by field emission scanning electron microscopy-energy dispersive X-ray analysis (FESEM-EDX), nanoparticle tracking analysis (NTA), X-ray diffraction (XRD), UV-vis diffuse reflectance spectroscopy (DRS), thermal gravimetric analysis (TGA) and Fourier transform infrared spectroscopy (FTIR) to study the morphology and structural properties. NiFe<sub>2</sub>O<sub>4</sub> exhibits high catalytic activity for organic dyes such as Congo Red. The influence of catalyst dosage, initial dye concentration for dye degradation were also investigated. This work showed a high potential of NiFe<sub>2</sub>O<sub>4</sub> nanoparticles for environmental purification of organic pollutants.

### Audience Take Away:

- Since this work relates to wastewater treatment and has strong potential to cope with global water pollution. So the audience could easily correlate this work to their own research and also understand the importance of work.
- Microwave technique is very promising and emerging technology for the researcher in recent times. Yes, the researcher could expand their research or teaching for this potential work.

### Benefits:

Retrieval of magnetic catalyst

Short reaction time

Thermal stability

### Biography:

Sandhya Mishra is pursuing PhD at the Department of Chemical & Biochemical Engineering, Indian Institute of Technology Patna, India. She has received her B.Tech.(UPTU) and M.Tech (IIT BHU) degrees in Chemical Engineering. She is working on nanoferrites' synthesis, characterization and their application. She is also studying the interactions of different inorganic catalysts with organic dyes and antibiotics.

## On the structural changes of zeolite Y upon interaction with Alumina binder

Ubong Etim\*, Peng Bai, Zifeng Yan

State Key Laboratory of Heavy Oil Processing, Key Laboratory of Catalysis, CNPC, China University of Petroleum, No. 66 Changjiang West Road, Qingdao, 266580, East China

**Z** zeolite Y is one of the most important solid acid catalysts that find immense applications in catalytic processes such as fluid catalytic cracking (FCC), acylation and cumene cracking. The technical grades of FCC catalysts require specifications that are met by dispersing the zeolite in amorphous binders. On contact with binders, zeolite properties in composite catalyst alter. This paper discusses the structural modification of Y zeolites caused by alumina binder incorporation. Experiments employing solid state MAS-NMR, N<sub>2</sub> adsorption and FTIR techniques reveal alumina incorporation reorganizes zeolite framework in comparison of silica binder. USY and REY are more susceptible to the attack by alumina as binder due to polarization of the framework by extra-framework species (such as Al<sup>3+</sup> and Al(OH)<sub>2</sub><sup>+</sup>), which is considered to be the operating mechanism for framework distortion by migration of aluminum atoms from the binder to the framework of zeolite and its subsequent framework structure reorientation. Compensating framework Na<sup>+</sup> cations restrain the polarization of NaY framework. However, polarizability of the zeolite's framework by extra-framework alumina species is independent of the exchanged cations (RE<sup>3+</sup> or H<sup>+</sup>). The resulting catalyst is amorphized by layers of alumina that implicates the Brønsted acidity as a function of its weight in the catalyst.

### Audience Take Away:

- Understand there is existing interaction between zeolite and binder materials in catalysts.
- Learn the effects of compensating cations in the framework of zeolite Y on binders.
- Learn how zeolite structure modification benefits catalytic reactions.
- This work will contribute to the understanding of roles of binders in bound catalysts and will help in designing more robust catalysts for specific reactions. It will also offer engaging opportunities in the area of research and opens up possibilities for collaboration.

### Biography:

Dr. Ubong Etim graduated with both a M.Sc. degree in Applied Chemistry from the University of Uyo, Nigeria, in 2013. In June 2017, he obtained a Ph.D. degree in Physical Chemistry from the China University of Petroleum, East China. He is currently working at the same institution as a postdoctoral researcher on Heterogeneous Catalysis in the State Key Laboratory of Heavy Oil Processing under the guide of Prof. Zifeng Yan. Ubong Etim has published more than 20 scientific research articles in SCI journals, with an accumulated impact factor of nearly 100.

## From Sand To Sky: The story of the first Etihad Passenger flight using Biojet fuel 100% produced and refined in the UAE

Paco Laveille<sup>1\*</sup>, Ph. D. Michael Brodeur-Campbell<sup>2</sup>, Nilesh R. Chandak<sup>1</sup>, Abraham George<sup>1</sup>, Stephane Morin<sup>1</sup>,  
Alejandro Rios Galvan<sup>3</sup> and Mikael Berthod<sup>1</sup>

<sup>1</sup>Research Centre Division, ADNOC Refining, Abu Dhabi, United Arab Emirates

<sup>2</sup>Honeywell UOP, Des Plaines, IL, USA

<sup>3</sup>Department of Industrial and Systems Engineering, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates

**T**he 15th of January 2019, Etihad Airways flew the first commercial passenger flight from Abu Dhabi to Amsterdam partially fueled with a sustainable biojet-fuel produced locally from plants grown in the desert of the United Arab Emirates, and refined by the Abu Dhabi National Oil Company (ADNOC) using the UOP Ecofining process.

Liquid biofuels have the potential to meet the aviation industry's needs, decreasing carbon emissions, reducing the dependency on conventional fuels, as well as providing a more attractive market for biofuel producers compared to current ground transportation markets. Aviation fuel markets are less likely to be vulnerable to competition from non-liquid fuels (e.g., battery-electric or fuel-cell hydrogen-powered vehicles), because of the substantial greater energy density of liquid fuels and the physical constraints of aircraft design and performance. Some of the liquid biofuels that have been approved by ASTM for aviation use include fuels based on Fischer-Tropsch (FT) synthesis and hydroprocessed esters and fatty acids (HEFA).

The Seawater Energy and Agriculture System (SEAS) pilot-plant implementation was inaugurated in 2016 by the Sustainable Bioenergy Research Consortium (SBRC), whose members are Khalifa University of Science and Technology (KU), ADNOC, Etihad Airways, Boeing, Safran, GE and BAUER Resources. At the heart of the project is the 2 ha SEAS farm located on the KU Masdar campus in Abu Dhabi. The SEAS couples aquaculture ponds, that produce fish and shrimp, with fields of *Salicornia begelovii* and wetlands of *Avicennia Marina* (Grey mangrove), both halophyte plants, used as a natural filter to clean the waste water of the ponds.

As such, the biomass is grown using only seawater that is produced as a waste from the aquaculture ponds, reducing drastically the cost of the feedstock for biofuel production because of other income streams, and making the overall economics highly attractive.

*Salicornia* seeds are rich in vegetable oil, containing triglycerides having fatty acids with mostly 18 carbons. After pressing the seeds, the vegetable oil has been pretreated and refined at the ADNOC Refining Research Center Division (RCD). The pretreatment phase, supported by the Abu Dhabi Vegetable Oil Company (ADVOC), was aimed at removing phosphorous and other contaminants that may harm the catalyst during the downstream conversion process. To convert the clean vegetable oil to biojet-fuel, oxygen needs to be removed completely and the carbon chains must be shortened to C9-C15, within the jet fuel range. In order to do so, UOP has provided technical support to set up their 2-step Ecofining process in one of ADNOC RCD's pilot-plant. The first step, hydrodeoxygenation, removes oxygen as water and produces an oil with high green diesel yields (>C15). To increase the yields of the biojet fuel range, the deoxygenated product is then cracked and isomerized in a second reactor. Following a distillation, the biojet fuel cut has been certified through the "standard specification for aviation turbine fuel containing synthesized hydrocarbons" ASTM D 7566, before being blended with conventional jet fuel and used on an Etihad Airways Boeing 787.

The SEAS, as an integrated food and energy system paves the way to more sustainable and economically viable biofuel production using non arable lands, non-drinkable water and, at the same time, replying to food security issues of countries with large deserts or arid regions, such as UAE. The presentation will go through the main steps of the whole project, showing its sustainability and economic viability and highlighting the strong collaboration between the different partners.

### Audience Take Away:

- Successful example of academic and industrial collaboration
- The presentation show that the success of such project needs the involvement of the right stakeholders
- Details of all technical aspects to prepare a sustainable biojetfuel using waste seawater in the desert, up to the certification and utilization in an aircraft.

**Biography:**

Paco Laveille joined ADNOC Refining Research Center, Abu Dhabi, UAE in 2015 as a Senior Scientist in Catalysis. He leads conventional oil hydro processing projects to support Abu Dhabi refineries catalyst management and biomass to fuels R&D. He received an MS degrees in biological engineering from La Rochelle University of Science and Technology, France and, in 2009, and a PhD in Materials Chemistry from Ecole Nationale Supérieure de Chimie de Montpellier, France. After a post-doc at IFPEN, he joined KAUST Catalysis Center, Saudi Arabia in 2010 as a Research Engineer. His field of expertise is the design, synthesis, characterization and testing of various Nano-structured heterogeneous catalysts applied to energy and environmental topics.

## On the catalytic mechanisms of Snake venom thrombin-like enzymes

**Anwar Ullah, Ph. D.**

Department of Biosciences COMSATS University Islamabad, Park Road 45550 Islamabad Pakistan

Snake venom thrombin-like enzymes (SVTLEs) constitute the major portion (10-24%) of snake venom and these are the second most abundant enzymes present in the crude venom. During envenomation, these enzymes had shown prominently the various pathological effects, such as disturbance in hemostatic system, fibrinogenolysis, fibrinolysis, platelet aggregation, thrombosis, neurologic disorders, activation of coagulation factors, coagulant, procoagulant etc. These enzymes also been used as a therapeutic agent for the treatment of various diseases such as congestive heart failure, ischemic stroke, thrombotic disorders etc. Although the crystal structures of five SVTLEs are available in the Protein Data Bank (PDB), there is no single article present in the literature that has described all of them. The current work describes the structural aspects, structure-based mechanism of action, processing and inhibition of these enzymes. The sequence analysis indicates that these enzymes show a high sequence identity (57-85%) with each other and low sequence identity with trypsin (36-43%), human alpha-thrombin (29-36%) and other snake venom serine proteinases (57-85%). Three-dimensional structural analysis indicates that the loops surrounding the active site are variable both in amino acids composition and length that may convey variable substrate specificity to these enzymes. The surface charge distributions also vary in these enzymes. Docking analysis with suramin shows that this inhibitor preferably binds to the C-terminal region of these enzymes and causes the destabilization of their three-dimensional structure.

### **Audience Take Away:**

- Explain the catalytic mechanisms of SVTLEs
- Substrate specificity of SVTLEs
- Structure base mechanisms of catalysis

### **Biography:**

Prof. Dr. Anwar Ullah has completed his PhD at the age of 25 years from Sao Paulo State University, Brazil and postdoctoral studies from the same University. He is working as Professor, a in COMSATS University Islamabad-Pakistan. He has published more than 30 papers in reputed journals and has been serving as an editorial board member of repute.

## Effects of partial amorphization of TiO<sub>2</sub> photocatalyst

**Heechae Choi**

Institute of Inorganic Chemistry, University of Cologne, Cologne, Germany

Separation of photo excited electron-hole pair in a photocatalytic material, is well-known as the most important factor that determines the activity. For better carrier separations and photocatalysis, heterojunction formations and/or noble-metal cocatalysts have been suggested, and huge progresses in photocatalytic activities have been accomplished. However, such approaches make synthesis processes more complex and raise the production costs. In this study, we report that partial amorphization of anatase TiO<sub>2</sub> greatly improves photocatalytic water splitting performances by inducing strong charge separations, using through density functional theory calculations and photocatalysis experiments.

### Audience Take Away:

- How to utilize atomic-scale simulation to design photocatalytic material efficiently
- Advantage and effects of charge carrier separation for photoelectrochemical reaction even with loss of active reaction area
- Lifetime and reactivity relation

### Biography:

Dr.Heechae Choi received his Ph.D degree in 2012 in Hanyang University (Seoul, Korea). After 4-year postdoctoral researcher period at Korea Institute of Science & Technology (KIST), he founded two companies, Virtual Lab Inc. and Materials Data Corp., which provide materials simulation software and materials processing consulting service, respectively. From September of 2018, Dr.Choi works in University of Cologne as a research group leader.

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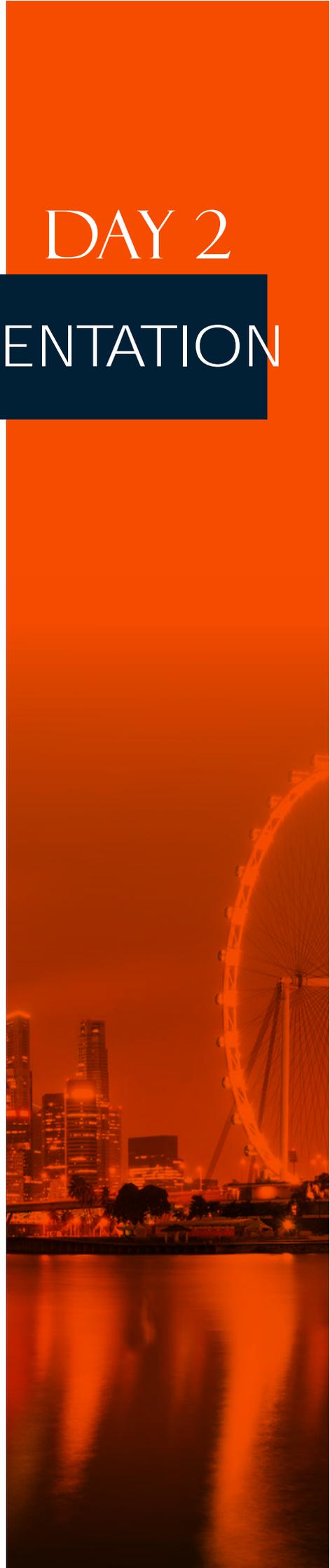
CATALYSIS AND  
CHEMICAL  
SCIENCE

MARCH

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## A new approach to modeling and simulation the catalytic processes in column apparatuses

**Christo Boyadjiev, Ph. D.**

Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. St. Angelov str., Bl. 103, 1113 Sofia, Bulgaria

The industrial column catalytic reactors are possible to be modeled, using the new approach on the base of the physical approximations of the mechanics of continua. As a result, a convection-diffusion type model (for qualitative analysis) and an average-concentration type model (for quantitative analysis) are possible to be used for the catalytic processes modeling in column apparatuses, in the cases of physical and chemical adsorption mechanism. A numerical analysis shows, that average concentration model, where the radial velocity component is equal to zero (in the cases of a constant velocity radial non-uniformity along the column height), is possible to be used in the cases of an axial modification of the radial non-uniformity of the axial velocity component. The use of experimental data, for the average concentration at the column end, for a concrete process and column, permits to be obtained the model parameters, related with the radial non-uniformity of the velocity. These parameter values permits to be used the average concentration model for modeling of different processes in the cases of different values of the column height, average velocity, reagent diffusivity, chemical reaction rate constant, etc. This possibility will be used for modeling of the catalytic processes in a gas-solid column apparatus.

### Audience Take Away:

- The heterogeneous gas-solid catalytic process will be considered in the cases of physical and chemical adsorption mechanism. The interphase mass transfer theory is not applicable for the heterogeneous catalytic processes modeling in the column apparatuses, because the interphase surface and velocity distribution in the column are unknown. This problem is circumvented in the book Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, "Modeling of Column Apparatus Processes" (Second edition), Springer-Verlag, Berlin Heidelberg, 2018, 456 pp., where new convection-diffusion and average-concentration models are used, where the surface effects (interphase mass transfer, adsorption and heterogeneous catalytic reaction) are replaced with volume sources (sinks) of the reagents and the average velocity is used.
- The new approach for the catalytic processes modeling in column apparatuses, permits to be simulated the industrial catalytic processes.

### Biography:

**Education and degrees:** 1. Education (1954 – 1960) - Higher Institute of Chemical Technology (Sofia, Bulgaria); 2. PhD (1968) – USSR, Moscow Institute of Chemical Mechanical Engineering; 3. Doctor of Technical Sciences (1978), Higher Institute of Chemical Technology (Sofia, Bulgaria).  
**Awards:** Bulgarian Order of Cyril and Methodius (first class); Russian Federation Order of Mihailo Lomonosow (National Committee for Public Prizes).

**Employment:** Institute of Chemical Engineering, Bulgarian Academy of Science, since 1962; Professor in Chemical Engineering, since 1981; Foreign Member of the Russian Academy of Natural Science – 2008.

**International activity:** Editor-in-Chief of the "Transactions of Academenergo" (Scientific journal of the Russian Academy of Science); Member of the Editorial Board for the "British Journal of Engineering & Technology"; Editorial Advisory Board Member of the "Recent Innovations in Chemical Engineering"; Chairman of the Scientific Council of the International Scientific Centre for Power and Chemical Engineering Problems (<http://www.int-sci-center.bas.bg>); Chairman of the Organizing Committee of the Workshop on "Transport Phenomena in Two-Phase Flows" (No.1 - 15).

**Publications:** Scientific papers 218.

**Monographies** 9 ([www.iche.bas.bg/Books\\_BG.htm](http://www.iche.bas.bg/Books_BG.htm)).

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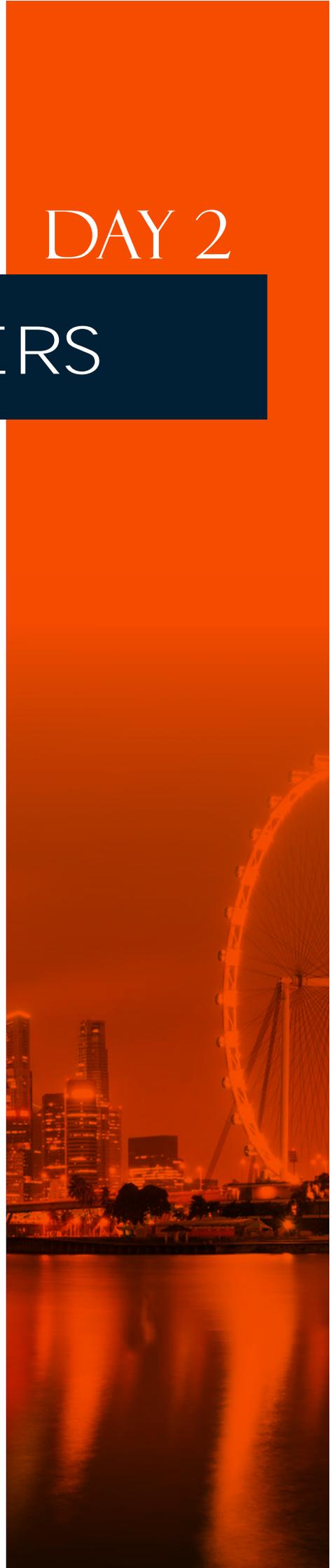
CATALYSIS AND  
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## Pt/Al<sub>2</sub>O<sub>3</sub> as NO<sub>x</sub> reduction catalyst - laboratory test results versus activity in low-power boiler fueled with biomass

Marek Kułażyński, Łukasz Świątek, Katarzyna Pstrowska<sup>\*</sup>, Jerzy Walendziewski

Wrocław University of Technology, Faculty of Chemistry, Division of Fuels Chemistry and Technology, Poland

Nitrogen oxides are among the most pervasive and difficult emissions to control. Currently, there are no commercial catalytic processes decomposing NO<sub>x</sub> without a reducing gas. Selective catalytic reduction (SCR) systems for NO<sub>x</sub> reduction use ammonia as the reducing agent. Ammonia SCR requires the handling of large quantities of toxic gases, tight temperature control, high reaction temperatures. Also effective NO<sub>x</sub> reduction requires large amount of catalyst because of the relatively low reaction rate. Lowering the cost of the reduction process by increase in the process efficiency and limiting the difficulty of handling the reducing agent would reduce the catalyst cost and decrease the operating temperature. Due to the above-mentioned arguments, the improvement of NO<sub>x</sub> reduction with ammonia SCR is important. It is also important because of the biomass use intensification (mainly due to the fact, that it is renewable energy source). Considering biomass chemical composition, NO<sub>x</sub> emission is much higher in the combustion processes comparing to the coal combustion.

The aim of this study was to compare ammonia SCR laboratory test results performed with the Pt/Al<sub>2</sub>O<sub>3</sub> catalyst with the 10kW energetic boiler SCR process effectiveness conducted under similar process parameters. The analysis of catalyst activity results under the reference gas conditions (laboratory tests) was compared with the catalyst efficiency analysis in the low power (10kW) boiler supplied by biomass. In the case of boiler conditions, the variable parameter was the type of raw material subjected to the combustion process and test conditions (presence of the catalyst/ presence of the active phase/ presence of the ammonia). Conducting this analysis allowed to determine the discrepancy between the results of laboratory analysis and results of the ammonia SCR with Pt/Al<sub>2</sub>O<sub>3</sub> catalyst in blow power boiler. Knowledge of these differences will allow for effective modification of the catalyst to improve the efficiency of the commercial SCR process.

### Audience Take Away:

- The results of laboratory SCR tests conducted under reference gas conditions strongly differ from the 10 kW boiler SCR test results due to the presence of the incomplete biomass combustion products in the boiler chamber
- The efficiency of NO<sub>x</sub> ammonia SCR process in an 10 kW energetic boiler strongly depends on the feed type
- SCR efficiency of NO reduction with Pt/Al<sub>2</sub>O<sub>3</sub> catalyst supported by NH<sub>3</sub> reductant in 10kW boiler supplied with straw pellets is 10% higher than in a boiler fed with a corn pellet

### Biography:

Katarzyna Pstrowska, Ph.D. Eng. studied Chemical Technology at Wrocław University of Technology, Poland and graduated in 2009. She joined the research group of Prof. Walendziewski and received her Ph.D. degree in 2013. Now Katarzyna Pstrowska is working on photo-electro catalytic reduction of CO<sub>2</sub> and she is continuing research connected to the biomass as a source of energy – environmental impact of the biomass use as a fuel.

## The effect of substituents bonded to silicon on the efficiency of the hydrosilylation of polybutadiene

Rafał Januszewski<sup>1,2\*</sup>, Ireneusz Kownacki<sup>1,2</sup>, Hieronim Maciejewski<sup>1</sup>, Bogdan Marciniec<sup>2</sup>

<sup>1</sup>Adam Mickiewicz University in Poznań, Umultowska 89B, Poznań, Poland

<sup>2</sup>Centre for Advanced Technologies, Adam Mickiewicz University in Poznań, Umultowska 89C, Poznań, Poland

Chemical modification of polymers has recently emerged as a topic of increasing importance in macromolecular chemistry and can often lead to novel materials with desirable functional groups which are otherwise inaccessible, difficult or too expensive to prepare by conventional polymerization techniques. Unsaturated polymers, especially diene-based polymers, are excellent polymers which can be exploited in addition reactions due to the technological importance associated with the parent materials and the reactivity of the carbon-carbon double bonds in the polymer chain. Polybutadiene (PB) is a versatile starting material due to its relatively low costs and high content of easily accessible double bonds, which enable the polymer to be modified using a wide range of chemical reactions. From the wide gamut of catalytic and non-catalytic transformations, hydrosilylation reaction seems to be very useful synthetic tool for obtaining functionalized polymers, thanks to its high selectivity and tolerance for a wide range of functional groups.

Herein we present the results of our studies on the hydrosilylation of polybutadiene with alkyl, aryl and alkoxy silanes in the presence of platinum and rhodium complexes. In order to select the most efficient catalytic system, which, under optimal conditions, smoothly promotes the incorporation of the above-mentioned organosilicon modifiers into polybutadienes of various structure via hydrosilylation, real-time in situ FT-IR spectroscopy was used. The silyl-functionalized polymeric products were characterized by NMR analysis and gel permeation chromatography (GPC). It was demonstrated that the stereo-electronic properties of substituents directly bonded to the silicon atom containing the SiH moiety play a crucial role in the formation of the desired products, as well as affecting the time required for total conversion of organosilicon reagents. Partially modified polymers containing pendant alkoxy groups can be applied as additives for rubber compounds to enhance dispersion of inorganic particles in the polymer matrix, as well as promoting the formation of organic-inorganic hybrid materials.

### Audience Take Away:

- Presented results significantly extend the knowledge about the TM-catalyzed post-polymerization process of polybutadiene
- Correlations between the electronic and steric properties on the reactivity and selectivity are presented in this work
- For the first time hydrosilylation of polybutadiene in presence of various catalysts is presented (comparison of activity)

### Biography:

Rafał Januszewski studied Chemistry at the Adam Mickiewicz University in Poznań, Poland and graduated as MS in 2014. At the same year he started PhD studies in research group of Prof. Bogdan Marciniec at the same institution. He carries out his doctoral dissertation in cooperation with the Synthos S.A. In PhD thesis he studies effects of the inert and functional groups bonded to the silicon on the hydrosilylation of polyene materials in presence of transition metal complexes. He is interested in homogeneous catalysis, hybrid materials, flame retardants and polymer chemistry. He has published 13 articles in international scientific journals.

## Catalytic reactions as a tool for modification of polysiloxanes with silsesquioxanes

Katarzyna Mituła<sup>\*1,2</sup>, Beata Dudzic<sup>1,2</sup>

<sup>1</sup>Faculty of Chemistry, Adam Mickiewicz University in Poznan, Umultowska 89B, 61-614 Poznan, Poland

<sup>2</sup>Centre for Advanced Technologies, Adam Mickiewicz University in Poznan, Umultowska 89C, 61-614 Poznan, Poland

**P**OSS- Polyhedral Oligomeric Silsesquioxanes are a family of worldwide known organosilicon, three-dimensional, nanosized compounds of the general  $[\text{RSiO}_{3/2}]_n$  formula, a topological analogues of the sphere. The most popular, not only because of their construction, but mainly because of their unique properties (solubility, non-flammability, oxidation resistance, non-toxicity) are cage silsesquioxanes, especially cubic  $T_8$  type (number eight represents the number of  $\text{SiO}_{3/2}$  units) that might possess from one to eight functional groups (R). The research on POSS compounds has influenced almost all branches of science which is well reflected in the enormous number of papers and patents published each year. Another important group of silsesquioxane family with increasing popularity, are double-decker silsesquioxanes that were discovered more than a decade ago. As the name suggests they consist of two cyclosiloxane rings (“decks”) with four inert phenyl groups each, stacked on top of one another and joined by Si-O-Si bridges. There are two types of double-decker silsesquioxane structures- with an ‘open’ or ‘closed’ core, with four or two functional groups respectively. The studies in the matter of DDSQ derivatives are quite new, therefore the number of papers considering their potential application is limited in comparison to POSS.

PS – polysiloxanes are polymers consisting of an inorganic Si-O-Si backbone chain with organic side groups attached to the silicon atoms. Thanks to their unique properties (low glass transition temperature and high thermal stability, high gas permeability, hydrophobicity), they have an enormous quantity of applications in almost every branch of chemistry as well as in everyday life, *i.e.* in space and solar applications, optoelectronics (OLED), drug delivery systems, food industries, surface modification, cosmetics and many more. The important aspect of polysiloxanes is the possibility of their modification when they contain functional groups in the structure, *e.g.* H – poly(hydro)siloxanes or vinyl – poly(vinyl)siloxanes.

Bearing in mind that reports on the modification of polysiloxanes and silsesquioxanes incorporation into their matrix are still limited in the literature, our aim was to contribute to this issue. The synthetic procedures that are presented in this presentation are based on transition metal (especially Pt) catalyzed processes, *e.g.* hydrosilylation. The decisive feature of this studies lies in the wide range of functional silsesquioxanes differing in the structure that are planned to be used for the PS modification. The crucial aspect of project presented in this presentation is to investigate the influence of the silsesquioxane frameworks incorporated into the resulting hybrid materials structures on their physical and chemical properties.

### Audience Take Away:

- The project fits into the ambitious challenges of catalysis, silsesquioxanes and material chemistry.
- Synthesized compounds as well as their derived materials along with their interesting properties will be a breakthrough in the chemistry polysiloxanes as scaffolds and precursors of hybrid polymeric materials.
- The results presented in this communication will contribute to the extension of knowledge on the methodology for functionalization of polysiloxanes with silsesquioxanes.
- The advantages of presented synthetic procedures lies not only in exploitation of new silsesquioxanes but also in the elaboration of appropriate catalytic systems (*i.e.* reaction type and its catalyst). It might give answer which catalyst is preferable (with best selectivity and efficiency) in polysiloxanes modification via hydrosilylation reaction.

### Biography:

MSc Katarzyna Mituła studied Chemistry at Adam Mickiewicz University in Poznan and graduated as MSc in 2016. Then She joined the research group of Prof. Bogdan Marciniec and Dr Beata Dudzic at the Centre for Advanced Technologies in Poznan and started hers PhD work. She has published 6 research articles in international SCI(E) journals. She was a contractor in three research grants and now she is participating in another three projects. Since 2018 She has been a Principal Investigator of her own research grant funded by the National Science Centre.

## Europium-doped $\text{CH}_3\text{NH}_3\text{Pb}_{1-x}\text{Eu}_x\text{I}_3$ for perovskite based solar cell application

Sarah Derbali<sup>1</sup>, Florentina Neațu<sup>2</sup>, Stefan Neațu<sup>2</sup>, Aurelian C. Galca, Lucia N. Leonat<sup>2</sup>, Andrei G. Tomulescu<sup>2</sup>, Viorica Stancu<sup>2</sup>, Vasilica Toma<sup>2</sup>, Ioana Pintilie<sup>2</sup>, Mihaela Florea<sup>2,3\*</sup>

<sup>1</sup>Ibn Tofail University, Av. de L'Université, Kénitra, Morocco

<sup>2</sup>Institute for Materials Physics, Department of Multifunctional Materials and Structures, Atomiștilor Str., No. 405A, PO Box MG 7, 077125, Măgurele, Romania

<sup>3</sup>University of Bucharest, Faculty of Chemistry, Bdul M. Kogalniceanu 36-46, Bucharest, Romania

The doping process, the controlled insertion of impurities into an extremely pure crystal, represents a strategic approach to improve optical and electrical properties of a device. Hybrid perovskite based solar cells have achieved high efficiency on photovoltaic applications tuning the perovskite composition by variation of the chemical composition or by doping. Inspired by the improvements of optical properties of certain materials by doping with  $\text{Eu}^{2+}$  europium could constitute a potential candidate to completely replace lead in order to reduce the defects formation and therefore to improve the stability of the hybrid perovskite solar cells. The choice is based also on their comparable ion radii ( $\text{Eu}^{2+}$ , 117 pm and  $\text{Pb}^{2+}$ , 119 pm), which according to the Goldschmidt factor, should induce the formation of a perovskite structure.

Perovskite films were fabricated by spin coating in ambient atmosphere. The crystallinity, morphology, optical absorption and photoluminescence properties, of  $\text{CH}_3\text{NH}_3\text{Pb}_{1-x}\text{Eu}_x\text{I}_3$  ( $x=0, 0.01; 0.03$  and  $0.05$ ) are studied.

The X-ray diffraction data indicate that the presence of Eu in small concentrations induces the formation of a perovskite crystalline structure. AFM images reveal an increase in roughness with the increase in Eu content. This points to the formation of a crystalline structure on the vertical direction rather than a complete surface coverage. 1% Eu content is the optimum addition for perovskite composition ensuring better crystallization as well as complete surface coverage. This work reveals Eu as a promising candidate to improve the stability in perovskite solar cells.

### Biography:

Mihaela Florea received her Bachelor's degree in Chemistry from the University of Bucharest in 1997 and from the same university she received the Master degree in 1999. The PhD was done under the supervision of Professor Paul Grange in the field of Catalysis at the Université Catholique de Louvain la Neuve, Belgium and she graduated in 2003 with Summa Cum Laude. In February 2004, she joined the group of Catalysis at the Faculty of Chemistry, University of Bucharest where she began her research on heterogeneous catalysis, especially on catalytic selective oxidation. From 2018 she is Senior Researcher at the National Institute of Materials Physics. Her current research focuses on the synthesis and characterization of sustainable catalytic materials for selective oxidation and energy applications. She is the author of >75 publications in the field of heterogeneous catalysis and green chemistry, with a Hirsh factor of 19.

## Investigation of mechanism on electrolytic Ozone generation using Pt/Ti electrode prepared by the multiple electrostrike method

Mio Hayashi<sup>1</sup>, Tsuyoshi Ochiai<sup>1,2,4</sup>, Shoko Tago<sup>1</sup>, Tsukahō Yahagi<sup>3</sup>, Akira Fujishima<sup>1,4</sup>

<sup>1</sup>Photocatalyst Group, Research and Development Department, Local Independent Administrative Agency Kanagawa Institute of Industrial Science and Technology (KISTEC), 407 East Wing, KSP, 3-2-1 Sakado, Takatsu-ku, Kawasaki City, Kanagawa 213-0012, Japan

<sup>2</sup>Materials Analysis Group, Kawasaki Technical Support Department, KISTEC, Japan

<sup>3</sup>Nanostructure Analysis Group, Kawasaki Technical Support Department, KISTEC, Japan

<sup>4</sup>Photocatalysis International Research Center, Tokyo University of Science, Japan

There are several electrodes for electrochemical ozone generation, for example, boron-doped diamond (BDD) electrode and tantalum oxide–platinum composite electrode. However, these electrodes are not inexpensive, cannot be achieved having large area, and cannot be prepared with simple methods. In this work, electrochemical ozone generation at an easily prepared platinum-modified titanium (Pt/Ti) electrode was investigated in comparison with a BDD or a Pt electrode. The Pt/Ti electrode was prepared by our original method, multiple electrostrike (ME) method as follows. A vibrating Pt wire (cathode) was rubbed over a surface of a titanium plate (anode) with a potential of 7.5 V. Subsequently, ozone generation activities of the electrodes were evaluated in acryl sealed 36 L box. Ozone gas was generated potentiostatically (5 V) in 100 mL of 0.5 M H<sub>2</sub>SO<sub>4</sub> and dispersed by the fan. Ozone generation activity of the Pt/Ti electrode was found to be much higher than that of the BDD or the Pt electrode. In addition, ozone generation was confirmed in other electrolytes including NaHCO<sub>3</sub>. From SEM observations, it was observed that molten Pt cluster on the Ti surface ranging from several nanometers to submicrometers were broken after the electrolysis. The result was expected to contribute to a better understanding of why the ozone generation increases with electrodes prepared by ME method. This research is attractive to development practical units for inexpensive and effective ozone generator.

### Audience Take Away:

- Our original method for preparing platinum-modified titanium (Pt/Ti) electrode.
- The characteristic of a Pt/Ti electrode and the superiority of a Pt/Ti electrode over high ozone generation activity.
- Application examples for the Pt/Ti electrodes.

### Biography:

Mio Hayashi received her BSc and MSc from Saitama University. After having engaged in an environmental consultant company, she has worked for the Photocatalyst Group at the Kanagawa Institute of Industrial Science and Technology (KISTEC) since 2008. In recent years, she has researched photocatalytic environmental purification units and electrolysis ozone generation electrodes.

## Catalytic materials of cobalt alloys for hydrogen generation

Zita Sukackienė\*, Ph. D. Kornelija Antanavičiūtė, Jūratė Vaičiūnienė, Arnas Naujokaitis, Loreta Tamšauskaitė  
Tamašiūnaitė, Eugenijus Norkus

Department of Catalysis, Center for Physical Sciences and Technology, Vilnius, Sauletekio ave. 3, Lithuania

It is well known that noble metals catalysts like gold, platinum and other its alloys effectively catalyze the catalytic hydrolysis of sodium borohydride. However, such catalysts are very expensive and its application is not viable. In this study we present noble metals free, low-cost, different compositions cobalt catalysts which have been successfully prepared by the electroless plating method on the copper surface using morpholine borane as a reducing agent in the glycine solutions. The cobalt coatings were deposited with small amounts of different metals such as iron, manganese, molybdenum, cerium and zinc. The catalytic activity of the different cobalt alloys catalysts towards the hydrolysis of alkaline sodium borohydride solution has been investigated under different conditions by measuring the amount of hydrogen generated. The volume and the rate of hydrogen generated in the presence of catalysts were measured by using a water-displacement method. In order to make comparison activity of the catalysts, the activation energy of the hydrolysis reaction of  $\text{NaBH}_4$  was determined by using the Arrhenius equation. It was found that the all prepared catalysts show promising catalytic activities for hydrogen generation from the sodium borohydride solution, however the highest hydrogen evolution rate and the lowest activation energy were obtained on the cobalt alloy doped molybdenum catalyst compared with other as-prepared catalysts. The as-prepared cobalt-molybdenum catalyst shows higher catalytic activity for hydrogen generation from sodium borohydride solution compared to catalytic activity of other catalysts obtained by the authors which is given in the literature.

### Audience Take Away:

- The audience will learn the formation and the characterization of new cobalt alloys catalysts.
- The audience will learn the simple and low-cost formation of the catalysts but at the same time an effective catalyst for hydrogen generation
- There will be discussed the electroless deposition method for catalysts formation and their investigation for borohydride hydrolysis reaction.
- We will discuss about the application of prepared catalysts for fuel cell and we will look for opportunities for cooperation with other institutions that would help us to work successfully.

### Biography:

Dr. Zita Sukackiene got her PhD degree in 2014 at the Department of Catalysis of Center for Physical Sciences and Technology. After PhD study she continued her work as a researcher at the same Department. She has been working as a senior researcher since 2017. Zita Sukackiene actively participates in scientific activity. She is supervisor of bachelor, master and PhD studies. She is co-author for 13 publications, 34 contributions to conferences and Co-author of the USA patent.

## Using X-ray absorption spectroscopy (XAS) to probe single atom catalysts in carbon nanotubes

Yi Cheng<sup>1</sup>, Shiyong Zhao<sup>1</sup>, Bernt Johannessen<sup>2\*</sup>, Jean-Pierre Veder<sup>3</sup>, Martin Saunders<sup>4</sup>, Matthew R. Rowles<sup>3</sup>, Min Cheng<sup>5</sup>, Chang Liu<sup>5</sup>, Matthew F. Chisholm<sup>6</sup>, Roland De Marco<sup>1</sup>, Hui-Ming Cheng<sup>5</sup>, Shi-Ze Yang<sup>6</sup>, San Ping Jiang<sup>1</sup>

<sup>1</sup>Fuels and Energy Technology Institute and Department of Chemical Engineering, Curtin University, Perth, Western Australia 6102, Australia

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<sup>5</sup>Advanced Carbon Division, Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, Liaoning 110016, China

<sup>6</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA

Single-atom catalysts (SACs) are the smallest entities for catalytic reactions with high atomic efficiency, activity, and selectivity. However, practical applications of SACs are limited by single atom loading of less than 2 wt.% or alternatively aggregation of the SACs to form larger particles, e.g. nanoparticles. In our research we have developed a class of SACs based strictly on atomically dispersed transition metals on nitrogen-doped carbon nanotubes and characterised these using a variety of complementary methods, including X-ray absorption spectroscopy (XAS) at the Australian Synchrotron in Melbourne. This material contains up to 20 wt.% SACs [Yi Cheng *et al.*, *Adv. Mater.* 30 (2018) 1706287]. In our presentation we will focus on the characterization aspect of the material with particular emphasis on XAS; sample preparation, data collection, and interpretation.

### Audience Take Away:

- Learn what X-ray Absorption Spectroscopy (XAS) is, and how it can be used to complement lab based techniques.
- Learn how to prepare samples and collect XAS data.
- Learn how to interpret XAS data.

### Biography:

Dr. Bernt Johannessen studied at Auckland University in New Zealand and then at the Australian National University graduating in 2007 with a PhD. He then worked as a beamline scientist at the Australian National Beamline Facility at the time located at the Photon Factory in Tsukuba, Japan, for two years. Following this appointment, he joined the team at the X-ray Absorption Spectroscopy beamline at the Australian Synchrotron, ANSTO, where he is now a Senior Scientist in the team. He has co-authored more than 70 peer-reviewed research articles in international journals.

## Continuous-flow asymmetric hydrogenation of diethyl itaconate by supported Ru-BINAP catalysts

Akiko Murakami\*, Y. Ikutake<sup>1</sup>, H. Nakashima<sup>1</sup>, H. Murayama<sup>1</sup>, T. Honma<sup>2</sup>, E. Yamamoto<sup>1</sup>, M. Tokunaga<sup>1</sup>

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Asymmetric hydrogenation is one of the most important reactions to synthesize optically active compounds which are synthetic intermediates for pharmaceuticals, pesticides, and perfumes. In particular, heterogeneous catalysts have advantages in terms of practical fine chemical synthesis because of their easy separation and recyclability. In addition, continuous-flow systems for synthesis of complex molecules such as optically active compounds have attracted a great deal of attention over the past few years. Flow systems have advantages over batch systems in productivity, heat and mixing efficiency and safety.

In this work, we report asymmetric hydrogenation of olefins by metal oxide supported ruthenium catalysts with chiral phosphines in batch and continuous-flow systems. The supported ruthenium catalysts were prepared by impregnation method. ZrO<sub>2</sub> was impregnated with RuCl<sub>3</sub>·3H<sub>2</sub>O in H<sub>2</sub>O and then calcinated at 550 °C. Enantioselective hydrogenation of diethyl itaconate proceeded in 99% yield and 93% ee in the presence of 1 wt% Ru/ZrO<sub>2</sub> (1.0 mol%) with (*S*)-BINAP (1.1 mol%) as a chiral ligand in a batch system. The reaction using Ru/CeO<sub>2</sub> catalyst also proceeded in good yield and high selectivity. However, the reaction hardly proceeded when Ru/Al<sub>2</sub>O<sub>3</sub> catalyst was used. The supported ruthenium catalysts were characterized and investigated for reactive species by Ru K-edge XAFS measurements. The XANES spectrum of the 1 wt% Ru/ZrO<sub>2</sub> catalyst suggested that octahedrally coordinated ruthenium oxides highly dispersed on ZrO<sub>2</sub>. On the other hand, the spectrums of Ru/Al<sub>2</sub>O<sub>3</sub> suggested that the ruthenium oxides were sintered. Under the reaction conditions, reductions of the ruthenium species were observed by in situ XANES spectra. The average oxidation state of the ruthenium species was reduced from +3.3 to +2.4 during the reaction. The reaction also proceeded under a continuous-flow system in good yield and selectivity.

### Audience Take Away:

- Asymmetric hydrogenation of olefins using metal oxide supported ruthenium catalysts with BINAP.
- Preparation of highly dispersed supported ruthenium catalysts by the impregnation method.
- In situ XANES analyses for reduced ruthenium species during the reaction.
- Asymmetric hydrogenation with heterogeneous catalysts in continuous-flow systems.

### Biography:

Ms. Murakami studied Chemistry at Kochi University, Japan and graduated B.S. in 2015. She then joined the research group of Prof. Tokunaga at Department of Chemistry, Kyushu University, Japan. She received her M.S. degree in 2017, and now, she is a Ph.D. student at the same department. She had joined the research group of Prof. Lin at Department of Chemistry, University of Chicago, USA for 8 months in 2017.

## Multifunctional silsesquioxane derivatives - synthesis and characterization

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**P**olyhedral oligomeric silsesquioxanes (POSS) are among the most intriguing examples of well-defined, nanostructured, functionalized building blocks, which find applications in academia and industry. They have been used in the synthesis of an enormous number of hybrid (co)polymers and nanocomposites characterized by complex composition, different functionalization, and architecture. Recently, much interest has arisen in silsesquioxanes bearing conjugated groups which are often called alkenyl-silsesquioxanes. Up to date, they have been used in the synthesis of porous and biomaterials, liquid crystals, fuel cells, semiconductors, as well as organic (OLED) or polymer electronics (PLED).

One of the most versatile synthetic methods for the preparation of such systems is the hydrosilylation reaction. The process gives the possibility for selective formation of specific isomer during the Si-H addition. Moreover, the hydrosilylation can be performed in the wide range of temperatures, in different types of solvents, under air atmosphere, using easily available reagents, in the presence of stable and tolerable for many reactive functionalities or impurities catalysts. All of that makes it powerful tool which appropriately used can easily provide a wide spectrum of silsesquioxanes bearing various types of functionalities.

In the communication we report studies on the hydrosilylation of a wide spectrum of terminal and internal alkynes with octafunctional spherosilicate (HSiMe<sub>2</sub>O)<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>, as well as 1,4-disubstituted-1,3-butadiynes, with monofunctional silsesquioxane (HSiMe<sub>2</sub>O)(*i*-Bu)<sub>7</sub>Si<sub>8</sub>O<sub>12</sub>). This method permitted to obtain a series of new alkenyl-substituted spherosilicates, 3-en-1-yne and 1,3-dienes with silsesquioxane moiety in high yields. The products were characterized by <sup>1</sup>H, <sup>13</sup>C, <sup>29</sup>Si NMR, FT-IR spectroscopy, ESI HR-MS spectrometry and X-ray crystallography. The influence of the reaction conditions (alkyne structure, type of the catalyst, solvent, temperature) on the process rate, its efficiency and selectivity will be presented.

### Audience Take Away:

- The developed simple, highly efficient and selective method for the synthesis of the new multifunctionalized silsesquioxane derivatives is a breakthrough in the silsesquioxane chemistry, allowing for designing new materials with tailored properties.
- Application of a wide spectrum of functionalized reagents with different structures, chemical, and physical properties permitted for a comprehensive examination of the hydrosilylation process of the C≡C bonds, optimize its conditions and identify factors having the influence on the reaction course. Moreover, in the presented syntheses, commercially available reagents and catalysts were used, making this method easily accessible, and rapid for scale up or industrial application.
- The hydrosilylation of the 1,4-disubstituted-1,3-butadiynes with monofunctional silsesquioxane (HSiMe<sub>2</sub>O)(*i*-Bu)<sub>7</sub>Si<sub>8</sub>O<sub>12</sub>) was performed for the first time.

### Biography:

Kinga Stefanowska received her MSc in Chemistry from Adam Mickiewicz University in 2015. Presently, she is pursuing PhD studies at the same institution under the supervision of Prof. dr. Piotr Pawluć and Dr. Jędrzej Walkowiak. She was chosen as the recipient of Polish grant for Young Researchers – Grant PRELUDIUM financed by National Centre of Science in Poland. She has completed 4-months (from July to October 2018) internship in Prof. dr. W. Leinter's group (RWTH Aachen, Germany) as part of the Short Term Research Grant funded by German Academic Exchange Service (DAAD). She is a co-author of 7 publications in prestigious chemical journals.

## Metallic nanoparticles supported onto TiO<sub>2</sub> nanotubes as catalysts for selective hydrogenation of nitroarenes

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Aniline and its derivatives are important chemical intermediates for the syntheses of dyes, pigments, pharmaceuticals, polymers, agrochemicals and other fine chemicals. Heterogeneous selective hydrogenation of the NO<sub>2</sub> functional group by hydrogen is a promising method to produce amino groups. In this work, we have synthesized various metal nanoparticles (Pt, Au and Ag) supported on titanium dioxide nanotubes (TiO<sub>2</sub> NTs) for the chemoselective hydrogenation of nitrobenzene. The synthesized materials were characterized by N<sub>2</sub> adsorption-desorption isotherms, X-ray diffraction, transmission electron microscopy and FT-IR measurements. The catalytic properties of these materials were tested using nitrobenzene as model compound for the hydrogenation to the corresponding anilines. All catalytic experiments were performed in batch regimen using Parr<sup>®</sup> type reactor and optimized operation conditions ensuring only a chemical control in the reaction's kinetics. To compare the selectivity of the prepared catalysts, all the substrate was hydrogenated using both metal-NPs supported on commercial TiO<sub>2</sub> carriers. These results are valuable to design novel efficient strategies for the selective hydrogenation of nitrocompounds.

### Audience Take Away:

- The audience will learn how to synthesize and characterize of Au-, Ag-, Pt-NPs supported on TiO<sub>2</sub> nanotubes as catalysts.
- The audience will learn the hydrogenation of nitrobenzene in liquid phase using various metal supported catalysts.
- The scope of the methodology presented can be extended to hydrogenation of other nitroarenes.

### Biography:

Dr. Shanmugaraj Krishnamoorthy is working as a Fondecyt Post-Doctoral Researcher in Department of Physical Chemistry, University of Concepcion, Concepcion, Chile, South America. He received his M.Phil., degree from Bharathiar University in 2011. He received his Ph.D, degree in 2017 from Bharathiar University, Tamil Nadu, India. He worked as a SERB-National postdoctoral fellow in Department of Chemistry, Gandhigram Rural Institute- Gandhigram in 2017 to 2018. He has published more than 10 research papers in reputed international journals. His current research interests are the heterogeneous catalysis for the reduction of nitroarenes and fluorescence sensing for toxic chemicals and biomolecules.

## Synthesis Na-[Al]-BEA (Beta) Zeolite by Dry-Gel conversiona (DCG) and hydrothermal (HTS) Methods: Effect of silica alumina ratio, synthesis times and synthesis methods

**Pusparatu**

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The synthesis Beta zeolite was studied by DGC and HTS methods. Beta Zeolite were compared by different synthesis methods using hydrothermal synthesis (HTS), dry gel conversion technique (DGC) with various silica to alumina ratios using structure directing agents at synthesis condition. Effect of synthesis gel composition, structure directing agent (template) and its concentration, synthesis time and synthesis method was studied in detail. The Beta was characterized by powder XRD, FT-IR, SEM, N<sub>2</sub> adsorption, NH<sub>3</sub>-TPD and solid state NMR. The TEOAH content in the starting gel influenced the phase selection, and the optimum range was found to be less than 0.1 < TEOAH/SiO<sub>2</sub> ratio is < 0.5 for Beta phase. The steaming time for crystallization of synthesis Beta zeolite with dry-gel conversion method and hydrothermal method has been studied. The steaming time for crystallization of synthesis Beta zeolite with dry-gel conversion method was faster than hydrothermal method. The product yield increased with increased the steaming time until 5 days for hydrothermal method and 24 hours for dry-gel conversion method. The particle size increased when the concentration of TEOAH was decreased. It is clear that small crystal size of Beta can synthesize by DGC method.

### Audience Take Away:

- When the large-scale synthesis was attempted at 175oC, only a Beta crystallized within 3 days . Accordingly, the gel with small-scale synthesis was initially heated at 175oC for 14 – 72 hours.
- This procedure was reproducible Beta was synthesized by this method on large scale with varying silica to alumina ratio.
- Following this procedure, pure Beta was synthesized with silica to alumina ratio input of 20, 30, 50, 75, 100, 150, 400,500 and 600.
- ICP analysis of these samples showed output ratios of 31, 33, 67, 109, 103, 209 and 208, respectively. However at silica to alumina ratio < 500, the crystallinity reduced, amorphous phase with Beta phase was observed.

### Biography:

Dr. Pusparatu studied Chemistry at the Gifu University, Japan and graduated as M.Eng in 2000. She then joined the research group of Prof. Yoshihiro Sugi at the Gifu University of Catalysts and their Applications, Japan. She received her Ph.D degree in 2005 at the same University. After that She joint in the Reseach and Development Center for Oil and Gas Technology as reseacher. After eight years She Moved to Oil dan Gas Academy Cepu, Indonesia as A Lecturer.

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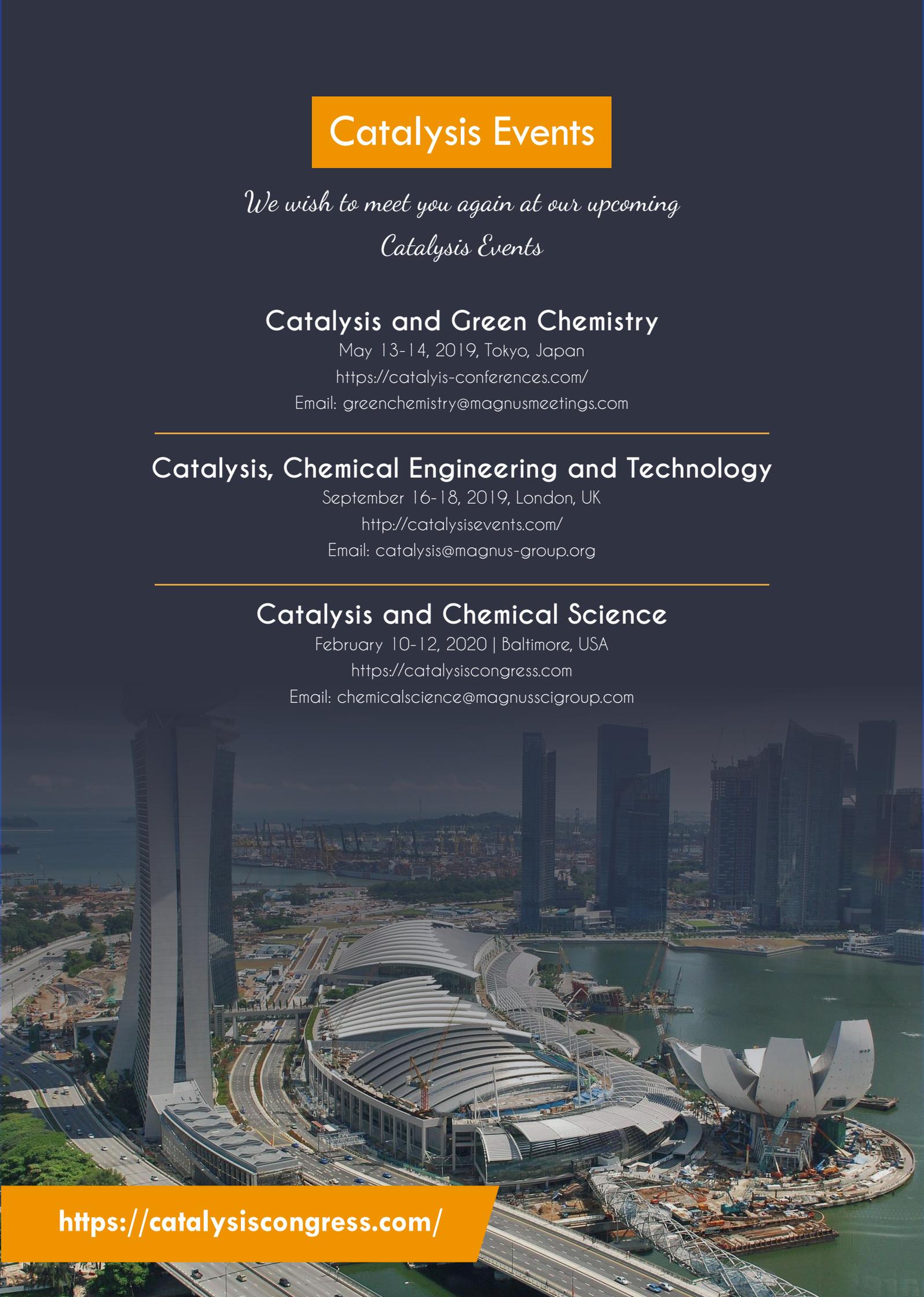
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## Catalysis and Chemical Science

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An aerial photograph of Singapore, showing the modern skyline with several tall skyscrapers. In the foreground, the distinctive white, lotus-like architecture of the Gardens by the Bay is visible, surrounded by greenery and water. The city extends to the water's edge with various buildings and infrastructure.

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