magnus
Group

Global Conference on

CATALYSIS & REACTION ENGINEERING

2017
OCT 19 TO OCT 21

GCR
2017

Venue
Hampton Inn Tropicana and Event Center
4975 Dean Martin Drive |
Las Vegas, NV 89118

http://catalysis-conferences.magnusgroup.org/

Index

Welcome Message

Dear ConferenceVisitors and Colleagues,

It is an honor and pleasure to welcome you to this wonderful conferences. As we all know, one method of accelerating the rate of a reaction is to low the activation energy of the reaction by utilizing a catalyst. The production of most industrially important chemicals requires the presence of catalysts. Therefore, research on catalysis is one of the most important and most exciting research area now. During this conference and today's presentation, we are going to hear the design and synthesis of single-site zeolite catalysts, photosynthesis, cobalt nanocatalysts, water-soluble platinum; catalysts for producing polymers, fuels, and many other industrially important chemicals; and chemicals for improving our environment. Based on these high quality of researches, we are optimistic that the breakthrough in catalysis will occur in the near future.

Buchang Shi

Dr. Buchang Shi

Eastern Kentucky University

USA

Welcome Message

Dear Congress Delegates,

I am delighted to welcome you all here to the Global Conference on Catalysis and Reaction Engineering, 2017. The breadth of the scientific program is impressive, covering new and important advances across 14 different, yet cohesive disciplines. Catalysis underpins our daily lives, from medicines to clothes, to food and energy. The major catalytic discovery a century ago by Haber and Bosch allowed the population of the planet to boom, due to the abundance of food harvested using ammonia from artificially fixed N_2. This increase in population brings with it issues regarding sustainability, rising CO_2 levels from increased reliance on fossil fuels, key issues which can be directly tackled using catalysis. Fundamental breakthroughs often lie on the intersection of different disciplines; the marriage of new catalyst innovations with advances in reactor design and engineering mean this scientific field can continue to address contemporary economic, social and environmental problems.

J Edwards.

Jennifer Edwards
Cardiff Catalysis Institute
UK

Welcome Message

Dear Congress Visitors,

It is my honor and great pleasure to write a few welcome notes to you. The XXI century is called “The century of new materials” because the synthesis of new materials can allow mankind to maintain the current development. Through centuries people are fascinated with the possibilities of synthesis of new materials with extraordinary properties. New materials are practically needed in all domains of life. Design and synthesis of new materials is one of the most important and interesting part of the material sciences. Particularly a synthesis of new active and selective catalysts is a very important challenge. Our main aim concentrates on the new methods of the synthesis of one-pot single-site hierarchical porous zeolite catalysts with acid-base and redox properties. Such zeolite catalysts with active sites formed by incorporation of hetero elements in their frame work are perspective as catalysts of biofeedstock conversion into valuable chemicals.

Stanislaw Dzwigaj

Stanislaw Dzwigaj
Sorbonne Universités
France

Keynote Speakers

Jennifer Edwards
Cardiff Catalysis Institute
UK

Michael Schnürch
TU Wien
Austria

Buchang Shi
Eastern Kentucky University
USA

Mohamed El-Far
Mansoura University
Egypt

Stanislaw Dzwigaj
Sorbonne Universités
France

Dennis Y.C. Leung
The University of Hong Kong
Hong Kong

Kenichi Komura
Gifu University
Japan

Dionysios (Dion) Demetriou Dionysiou
University of Cincinnati, USA

Dibakar Chandra Deka
Gauhati University
India

About Magnus Group

Magnus Group (MG) is initiated to meet a need or to pursue collective goals of scientific community, especially in exchanging the ideas which facilitates growth of research and development. We specialize in organizing conferences, meetings and workshops internationally to overcome the problem of good and direct communication between scientists, researchers working in same fields or in interdisciplinary research.

MG promotes open discussions and free exchange of ideas at the research frontiers mainly focusing on science field. Intense discussions and examination based on professional interests will be an added advantage for the scientists and helps them learn most advance aspects of their field.

It proves that these events provide a way for valuable means of disseminating information and ideas that cannot be achieved by usual channels of communications. To encourage an informal community atmosphere usually we select conference venues which are chosen partly for their scenic and often isolated nature.

About GCR 2017

Magnus Group is pleased to invite you to participate in the 'Global Conference on Catalysis and Reaction Engineering' during October 19-21, 2017 at Las Vegas, USA.

GCR 2017 will bring together a collection of investigators who are at the forefront of their field and will provide opportunities for junior scientists and graduate students to interactively present their work and exchange ideas with established senior scientists.

The Chemical Engineering conference explores the entire breadth of catalysis with earlier and contemporary work and provides a critical review of the present state of the subject. GCR 2017 provides an international forum to intensify the information exchange and is an excellent opportunity for Researchers, Technologists, Industrialists and Scientists in the domain of chemistry from around the world and to promote/present innovative ideas that will influence and foster continued research. The speakers and delegates come from academia, industries, private and government laboratories across the world.

DAY 1

Keynote Forum

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Advances in the direct synthesis of hydrogen peroxide from hydrogen and oxygen

Jennifer K Edwards, Ph.D*
Cardiff Catalysis Institute, Cardiff University School of Chemistry, UK

The field of gold catalysis has expanded rapidly since its inception in the early 1980s, when independently Professors Hutchings and Haruta demonstrated that subdivided nanoscale gold can be successfully utilised as a highly effective catalyst for the hydrochlorination of acetylene and CO oxidation. Over the last decade, it has been demonstrated by a number of research groups that the addition of Pd into Au catalysts can increase the activity of a catalyst, whilst maintaining the high selectivity achieved when using Au based catalysts. My research focuses on the development of novel AuPd nanoalloy catalysts, achieving high levels of control for particle size, shape and composition. These catalysts show exceptional activity for a number of industrially important catalytic reactions including alcohol oxidation and the direct synthesis of hydrogen peroxide.

Audience Take Away:

- During my lecture the audience will learn how to prepare PGM supported heterogeneous catalysts, the different ways the activity can be evaluated in laboratory conditions and the real word application of such materials in the chemical and water industries.

Biography

Jennifer Edwards is a senior research fellow in the Cardiff Catalysis Institute, based in the School of Chemistry at Cardiff University. She has published over 90 papers and patents, and has a particular interest in the design and application of precious metal catalysts. Her efforts in the field have been recognized by the International precious metal institute (Carol Tyler award 2011) and the German Catalysis network Unicat (Clara Immerwahr award 2013). She was a finalist in the Science category for the Women of the Future awards in 2015.

Decoration of acyclic amines via metal catalyzed C-H activation reactions

*Michael Schnurch**
TU Wien, Austria

Metal catalyzed C-H activation chemistry can be considered as the logic advancement of cross-coupling chemistry (e.g. the famous Suzuki-Miyaura reaction). Instead of using two pre-functionalized reaction partners, the C-H bond itself is used as functional group. This bears the potential for a significant improvement regarding step economic synthesis of complex compounds. C-C bond forming processes are the most important reactions for building up the skeletons of organic molecules. Alkylation and arylation reactions are frequently applied transformations in this field. Many different aryl sources have been used in metal catalyzed C-H activation reactions. Also we contributed to this field by investigating the □-arylation of aliphatic acyclic amines. Three different protocols were developed, which all proceed via distinctively different mechanisms and hence, require a specific set of reaction conditions. This allows using the transformation which reaction conditions are best compatible with a given substrate.

In the field of direct alkylation, we will report on a new type of alkyl source as alternative to the frequently applied olefins. Olefins have the drawback that the short chained representatives are gaseous at room temperature, and hence high pressure equipment has to be used in many cases. Our development makes this special equipment obsolete and alkylation reactions, including ethylations, can be carried out in standard glassware. The applied reagents are solid materials and stable at ambient conditions for a prolonged time. This leads to operationally simpler and safer alkylation reactions, which in turn will surely increase the number of applications for these processes.

Furthermore, mechanistic and kinetic studies will be presented, leading to the proposal of a reaction mechanism for all of the reported transformations.

Audience Take Away:

- The direct functionalization of aliphatic amines in alpha position will be presented.
- Methods for arylation and alkylation will be discussed.For arylation, three different aryl sources were investigated, which result also in different mechanisms operable. This allows choosing for the same reaction the type of transformation which suits best to the respective problem.
- For alkylation, a new type of alkyl source was identified, which makes the use of high pressure equipment obsolete, as opposed to the most frequently applied olefins as aryl source. This allows significantly safer and operationally simpler alkylation processes.
- Kinetic and mechanistic studies will give insight into this reaction archetype.

Biography

Assoc. Prof. Michael Schnürch studied Chemistry at TU Wien and did his Masters as well as PhD thesis under the supervision of Prof. Peter Stanetty. During his PhD thesis, he conducted a four months internship with Prof. Victor Snieckus at the Queen´s University in Kingston, Ontario, Canada. He then went on to a postdoctoral stay as Erwin Schrödinger Fellow with Prof. Dalibor Sames at the Columbia University in New York. After his return to Vienna, he started his independent career and finished his habilitation in 2013. In 2016 he was promoted to Associate Professor in the field of organometallic chemistry.

Isotope tracer studies on the mechanism of Fischer-Tropsch synthesis: Its impacts on selective catalysts developments, geoscience, planetary studies and the origin of hydrocarbons on the Earth

Buchang Shi*, Ph.D

Eastern Kentucky University, USA

The Fischer–Tropsch (FT) reaction is a non-selective process in which CO and H_2 are converted to fuels and chemicals such as n-alkanes, 1-alkenes, 2-alkenes and oxygenates as well as branched hydrocarbons. The commercial importance of this reaction is that it provides a route for the production of liquid fuel from coal or biomass via gasification to CO and H_2. With the prospect of oil supplies drying up completely in the foreseeable future and the environmental concern in desiring to have a renewable energy source, there is a great revival of interest in FT reactions. Furthermore, the theoretical significance of FTS is that it is invoked to explain the formation of abiogenic hydrocarbons in the Earth's crust, precursors of life essential building blocks, and organic matters in the solar nebula. Therefore, studying the mechanism of FT reactions is of importance both commercially and fundamentally. However, nearly 100 years of studies show that it is a challenge to propose a mechanism that can explain formation of all FT products. We conducted H_2/D_2 switching and competition FT reactions catalyzed by cobalt, iron, and ruthenium catalysts and found that all of these FT reactions showed an inverse isotope effect, the deuterium enrichments in hydrocarbons produced by these reactions, and the deuterium enrichment is a function of carbon number. These results led us to propose an alkylidene mechanism for FT reactions. By this mechanism, the carbon-carbon bond formation is through the coupling of monomer $M{\equiv}CH$ with the growing chain ($M{=}CHR$), which will show the inverse isotope effect since the sp^2 carbon of the growing chain will be changed to sp^3 hybridized carbon. This mechanism also can explain the deuterium enrichment and the enrichment is a function of the carbon number of a hydrocarbon. This mechanism predicts that if hydrocarbons were produced through a FT-like reaction, deuterium enrichments in these hydrocarbons should be observed and the enrichments would increase as the carbon number increases.

Audience Take Away:

- H_2/D_2 switching experiments can determine the paraffin/olefin ratio and the α value of an FT reaction more accurately since the possible products accumulation problems can be avoided.
- Deuterium enrichments in hydrocarbons and the deuterium contents increasing as the carbon number increases can be used as an indicator to figure out whether the hydrocarbons were produced through a FT-like reaction in geoscience or not.
- Deuterium contents and possible ^{13}C contents determinations could be used to find the origin of the hydrocarbons in other planets.
- A true selective FT catalyst will produce hydrocarbon products that are not obey the ASF distribution, which could result in irregular deuterium contents in hydrocarbons. Therefore, D_2/H_2 competition experiments could be used to develop selective FT catalysts.

Biography

After obtained his PhD from the University of Kentucky, he worked as a senior scientist at the Center for Applied Energy Research (CAER) of University of Kentucky for 14 years. Then he moved to Eastern Kentucky University as an associate Professor. His current research includes mechanistic studies of catalytic and organic reactions using isotope tracer techniques. His focus are on Fischer Tropsch synthesis, and bio-fuel related reactions.

Photodynamic Therapy (PDT) of tumors: An overview of long-term team(s) four decades experience

Mohamed El-Far*

Mansoura University, Egypt

A series of land-mark contributions were made in our laboratories in PDT of tumors by LASER as well as other invented light source(s). Lecture will cover our journey over 40 years from bench to clinical applications. It includes novel approaches as:

1) Using natural photosensitizes (PS)/materials (as Uroporphyrin or ALA) "For the first time" to identify (diagnosis) precancerous and certain malignant cells (via red florescence), followed by exposure to intense light of appropriate wavelength for PS activation leading to death of tumor cells (treatment).

2) Selective therapeutic ALA-PDT by the action of Biocatalyst and the mechanism of action.

3) Synthesis and development of photosensitizes for more selective accumulation into target cells with possible activation by straight sodium lamps.

4) Clinical applications for treatment of tumors.

5) Novel approach for removal of skin photo-toxicity. We will present basic ways for innovations related to this field.

Biography

Professor Mohamed El-Far, worked in biochemistry field for 40 years, published over 90 peer-reviewed papers. He received Fulbright and British council fellowships several times as well as German DAAD grant to establish PDT Program at Munich, also received US-AID grant to establish PDT unit in Egypt. He is serving on the editorial boards and Hon. Editor to four international journals. He acts as UNESCO expert in science and technology. Dr. El-Far served as visiting professor to University of California as well as Utah laser center also Mayo clinic for several years. He also served as a visiting professor to Cardiff and Swansea Universities, UK. He is a member of International Photodynamic Association and Royal Society of Chemistry, UK. Selected and served as expert and consultant for biochemistry in the national committee of suprime council of Universities in Egypt, which is the highest nation honor. Recently selected as a member of higher Education and Research committee for Mansoura University. Selected by the International Biographical Centre, Cambridge, England to be among top 100 scientists 2012. Received honary doctorate of letters from International Biographical Centre, Cambridge, England. Selected on list of global speakers as a keynote speaker and honorable guest for several international conferences in cancer and diabetes as well as other recent biomedical applications as stem cells and nanotechnology.

DAY 1

Speakers

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Sessions on: Environmental Catalysis and Nano Catalysis | Molecular and Heterogeneous Catalysis | Modelling in Catalytic Processes

Session Chairs

Jennifer Edwards
Cardiff Catalysis Institute, UK

Stanislaw Dzwigaj
Sorbonne Universités, France

Session Introduction

Title: **Assessment of the production of hydroxyl radical using nano zero-valent iron embedded in a meso-porous silica matrix**
Erick R. Bandala, Desert Research Institute, USA

Title: **Catalysis effects over atmospheric particles composed by H_2O, HCl, HNO_3 and H_2SO_4: Quantum analysis**
María de los Ángeles Verdes Gago, Universidad Autónoma de Madrid, Spain

Title: **Computational design of novel catalyst system**
Tadashi Ogitsu, Lawrence Livermore National Laboratory, USA

Title: **CO_2 activation and reduction catalyzed by FeS nanocatalyst: A DFT study**
Nelson Y. Dzade, Utrecht University, Netherlands

Title: **Super-capacitor characteristics based on several composite materials**
Hee-Je Kim, Pusan National University, Republic of Korea

Title: **Pt and Pd clusters confined in the bulk of fiberglass as an effective heterogeneous catalysts**
Bair S. Bal'zhinimaev, Boreskov Institute of Catalysis, Russia

Title: **Tuning the surface adsorption properties of polymer sorbents via facile methods**
Lee D. Wilson, University of Saskatchewan, Canada

Title: **Metal supported on titania for nitrate reduction**
Peter J. Miedziak, Cardiff University, UK

Title: **Fischer-Tropsch synthesis catalyzed by small TiO_2 supported cobalt nanoparticles prepared by sodium borohydride reduction**
Jorge A. Delgado Delgado, Centre Tecnològic de la Química, Spain

Title: **Inline concentration profiles in enzyme catalyzed reactive rectification using infrared spectroscopy**
Marc-Andreas Christlieb, Hamburg University of Technology, Germany

Title: **Thermal stability study of catalysts in esterification reaction processes**
Edidiong Okon, The Robert Gordon University, UK

Title: **Computational study of the Fischer-Tropsch process catalyzed on small Ru clusters: Beta-elimination versus reductive elimination**
Edward Brothers, Texas A&M University, Qatar

Title: **Cobalt(III)-supported chemically modified mesoporous silica as heterogeneous oxidation catalyst**
Purabi Sarmah, Nalbari College, India

Title: **Design of heterostructure photoelectrodes for solar fuels**
Yan-Gu Lin, National Synchrotron Radiation Research Center, Taiwan

Title: **Photocatalytic hydrogen evolution from water splitting over mixed valence tin oxide semiconductor under visible light irradiation**
Toyokazu Tanabe, Kanagawa University, Japan

Title: **Active carbons as nanoporous materials for solving of environmental problems**
Victor Mukhin, Neorganika, Elektrostal, Russia

Assessment of the production of hydroxyl radical using nano zero-valent iron embedded in a mesoporous silica matrix

Steven Huezo[1], Soroosh Dehkordi[2], Jaeyun Moon[2], Ph.D., Erick R. Bandala*[1], Ph.D
[1]Desert Research Institute, USA
[2]University of Nevada, USA

Zero-Valent Iron (Fe^0) has been shown to detoxify water by creating hydroxyl radicals through Fenton-like reactions combined with hydrogen peroxide (H_2O_2) to get rid of organic contaminants. Nano-sized zero-valent iron (n/ZVI) in combination with oxidants and UV radiation, has been reported can increase the Fenton reaction rate and make water detox more effective. In this work, the production of reactive oxygen species, particularly hydroxyl radicals, was assessed for the heterogeneous photo-assisted Fenton-like reaction using nZVI embedded in a mesoporous silica matrix, hydrogen peroxide, and UV-A radiation. The experiments consisted of preparing a 10 µM solution of N, N-dimethyl-p-nitrosoaniline (pNDA, used as $HO^•$ radical probe) in 100 mL of water and adding the silica-embedded nZVI at three different loads (21 mg/L to 24 mg/L) with or without H_2O_2, and/or UV-A radiation (λmax= 365 nm). The absorbance of the pNDA was measured and compared to that of clear, deionized water. The trials consisted of using immobilized nZVI alone, immobilized nZVI/H_2O_2, and immobilized nZVI/H_2O_2/UV. The best conditions for hydroxyl radicals production measured as pNDA bleaching were by the combination of immobilized nZVI/H_2O_2/UV despite nZVI, UV-A radiation and hydrogen peroxide alone were capable of bleaching pNDA to a certain extent. The use of the H_2O_2/UV system reached a plateau for hydroxyl radical production after 20 min of reaction. Two kinetic models were proposed to fit experimental data for the different reaction conditions tested and the obtained results were capable of fitting experimental data fairly good meaning that the proposed reaction mechanisms may occur within the reaction mixture to some extent. This novel material was found with interesting capabilities to produce reactive oxygen species, particularly hydroxyl radicals, under photoassisted conditions and high potential for further photocatalytic applications in water treatment.

Audience Take Away:

- A clear idea on the actual trend for the development of novel nanomaterials for photocatalytic applications.
- Basic knowledge on the processes occurring within the use of zero-valent iron nanoparticles in environmental restoration.
- First-hand information on novel lab scale developments.

Biography

Erick R. Bandala, Assistant Research Professor for Advanced Water Technologies at the Desert Research Institute in Las Vegas, NV. He holds PhD degree in Engineering, a Master degree in Organic Chemistry and a B.S. degree in Chemical Engineering. Dr. Bandala's research interests include A) Mechanistic aspects of the use and application of solar driven advanced oxidation processes (AOPs) for environmental restoration B) Development of advanced water and soil treatment for site restoration C) Synthesis, characterization and application of nanomaterials for Indoor Farming systems D) Development of Climate Change adaptation methodologies for water security. Dr. Bandala is author or co-author of over 100 international publication including 72 peer-reviewed papers in international journals (average impact factor 2.7, >1680 citations, h-index 23); 5 books, 25 book chapters and 65 works published in proceedings of international conferences.

Catalysis effects over atmospheric particles composed by H_2O, HCl, HNO_3 and H_2SO_4: Quantum analysis

Marian Verdes*, Ph.D
Universidad Autónoma de Madrid, Spain

Ozone depletion is closely related to HNO_3, $H2SO_4$, HCl and H_2O particles that form Polar Stratospheric Clouds (PSCs) over polar areas in the winter. Surface–catalyzed reactions on PSCs particles generate chlorine compounds that photolyze readily to yield chlorine radicals that react with HNO_3. The stratospheric H_2SO_4/H_2O aerosols absorb amounts of HNO_3 hydrates that grow to form the PSCs by condensation at several degrees above of the ice frost point. Heterogeneous atmospheric reactions have been experimentally studied at photochemistry level for different atmospheric compounds —organic and inorganic species— that taking part in aerosols as free radicals yielded by UV radiation in the Atmosphere.

Some heterogeneous reactions among these strong acids compounds were theoretically assessed by means of Density Functional Theory (DFT) to evaluate what type of dimers, trimers and hydrates are created among them with optimized geometries at different levels of theory. Initially, the optimization calculations of dimers geometries was the first step as precursors the trimer structures. The pairing was between HCl, HNO_3 and H_2SO_4 with H_2O molecule to obtain the nuclei for trimers aggregates. Later, these structures were solvated by one H_2O molecule in pairs performed by HNO_3/H_2SO_4, HCl /HNO_3 and HCl/HNO_3. The high atmospheric interest of these aggregates incited that the thermochemistry was evaluated at different stratospheric temperatures as 188K, 195K, 210 K and 298 K, to know their relative stabilities among them when decrease along the altitude.

After these calculations, the optimized structures were achieved for heterogeneous nucleation reactions suggested, as $HCl/HNO_3/H_2SO_4$, $HCl/H_2SO_4/HNO_3$, even for reactions formed with $HNO_3/H_2SO_4/H_2O$ and $H_2O/HNO_3/H_2SO_4$ that are known experimentally as Supercooled Ternary Solution (STS). These aggregates were penta-hydrated to develop the optimization of their pentahydrates at mentioned temperatures. The results accomplished to respect their optimized structures are in agreement with experimental data because generated spherical and pentagonal geometries —like in crystallizations of particles in PSCs— being a potential precursors of nucleation of the atmospheric aggregates.

The B3LYP hybrid method and aug-cc-pVTZ was the level of theory selected to develop the optimizations for all candidate structures after calibrate different methods by mean of Gaussian 09 program package.

Audience Take Away:

- The audience can apply the methodology of my presentation in their total or partial systems in study considering the available measurements or data. For instance, they can predict the geometrical shapes, inter-monomeric and intra-monomeric distances, angles, dihedral angles, IR spectra, vibrational frequencies, temperatures, concentration ratios, Gibbs free energies, Enthalpies, etc.
- As well as, the audience can predict the eventual results previous experimental investigations spending less time and economy. Moreover, they can discover physical-chemical properties about the problem in assessment as structures, shapes, IR spectra, the potential energy surfaces, temperature ranges, hydrogen bonds, thermochemistry data, kinetic reactions, etc.
- Through this methodology, the attendees can assess the cheaper manner if the problem must be treated in depth experimentally, for instance.
- This methodology will be useful to the audience in their job because they can obtain valuable data in short time and less expensive that experimental laboratory probes, even these results can help them to make measurements (altitude, temperature, physical chemical properties, concentration ratios...) in the different atmospheric layers, or different chemical catalytic system... for instance.

- Moreover, this computational methodology can expand and adapt to their/other systems in assessment to obtain efficient results briefly. Also, it is possible to teach for to manage the atmospheric, catalytic, photochemical, etc. researches, hetero and homogeneous reactions, or aggregations of compounds, spectra (shifting of Hydrogen Bonds, for instance), thermodynamic properties... conveniently.
- The results predicted —applying this theoretical methodology— are clear, faster, accurate and efficient that permits to research team improve their works successfully.
- The accuracy of these theoretical methods is high to resolve the problem designed. Other benefits are:

  -Accurate of results
  -Efficiency (results/computational time) -Comfortable to work
  -Faster results than experimental data
  -Agreement results yielded to respect experimental data -Cheaper economic cost than experiments
  -Clean – only use processors-
  -Adaptable to systems to assess –high or low level--Optional possibilities of efficiency
  -Diversity of systems to evaluate
  -Working from two to thousands of atoms is possible
  -Many levels of theories – low, high, very high level- to develop the works -It is possible working anywhere: university, home, office...
  -It is possible develop various systems simultaneously
  -It is possible establish collaborations with institutions anywhere -Flexible respect to approaches
  -Independent of number of workers and economy

Biography

Marian Verdes received her Bachelor's degree in Physical Chemistry and developed her minor thesis at University of Basque Country at Leioa (Biscay). She obtained her Diploma of Advanced Studies at University Complutense of Madrid in the inter-university doctorate program in Physical Applied Chemistry. She achieved her Doctorate in Physical Applied Chemistry at University Autonomous of Madrid (UAM) in 2015. Nowadays, she carries out her theoretical investigations (Physical-Chemistry properties) about atmospheric aggregates at UAM.

Computational design of novel catalyst system

Tadashi Ogitsu*
Lawrence Livermore National Laboratory, USA

Recent progresses in theory of catalytic reactions led to successful computationally guided discoveries of novel catalyst systems. However, simultaneously, it also disclosed presence of intimate relation between energetics and kinetic of elemental catalytic reaction processes for multi-step catalytic reactions such as oxygen evolution, CO_2 reduction, ammonia synthesis, a part of which has been known as Evans-Polanyi relation. Presence of such a relation suggests that catalytic system consisting of a homogeneous and a single component catalyst material will likely to face a great challenge in improving catalytic performance compared to known conventional catalysts since substituting the catalyst material in hope of improving kinetics of rate limiting step will likely to lead to a worse kinetics of the other steps, one of which may turn into the rate limiting step. This relation also poses a challenge in controlling selectivity since the kinetics of branching reactions are also likely to be correlated in a linear fashion. At the presentation, we will first discuss about underlying concepts based on our research experiences about computational design of novel catalyst [Choi et al. JCPC 117, 21772 (2013); Choi et al. Adv. Ener. Matt. 1501423 (2015)] as well as about transport properties of reaction intermediate at solid-liquid interfaces [Wood et al. JACS 135, 15774 (2013)]. We will then discuss about the factors that need to be further studied in order to overcome the challenge implied by the scaling relation. This work was performed under the auspices of the U.S. Department of Energy under contract No. DE-AC52-07NA27344, and supported by DOE Fuel Cell Technology Office.

Audience Take Away:

- Basics of catalytic reaction processes
- The known obstacles for novel catalyst development
- I would like to share what I have learned about the success and the limitation in computationally aided novel catalyst design and further discuss candidate approaches that may lead to a solution for overcoming the known obstacles.

Biography

Tadashi Ogitsu is a deputy group leader of Quantum Simulation Group at Lawrence Livermore National Laboratory and is the point of contact for DOE/EERE HydroGEN consortium, which is designed to facilitate sustainable hydrogen production R&D.

CO_2 activation and reduction catalyzed by FeS nanocatalyst: A DFT study

Nelson Y. Dzade*[1], Ph.D., Nora H. de Leeuw[2]
[1]Utrecht University, Netherlands
[2]Cardiff University, UK

Iron sulfide minerals are relevant in origin of life theories, due to their potential catalytic activity towards the activation and conversion of carbon dioxide (CO_2) to small organic molecules, which may be applicable to the production of liquid fuels and commodity chemicals.The mechanistic details of the catalytic reactions between CO_2 and H_2 at iron sulfide surfaces however, remain poorly understood, although this information is critical to the development of improved iron sulfide catalysts for the conversion of CO_2 into fuels and chemicals. Herein, we perform high quality periodic density functional theory (DFT) calculations of the reaction mechanisms associated with the direct and hydrogen-assisted CO_2 reduction reactions on the prefect and defective surfaces of layered iron monosulfide (mackinawite). The low-index Miler surface of FeS are systematically characterized and based on the calculated surfaces energies, we have simulated the thermodynamic crystal morphology using Wulff construction. The fundamental aspects of CO_2 adsorption, including the registries of the adsorption complexes, adsorption energies, electronic properties, and structural parameters are presented. It is demonstrated that the CO_2 molecule physisorbs on the most stable (001) surface, but chemisorbs relatively strongly on the (011) and (111) FeS surfaces, preferentially at Fe sites. We have also examined the creation of sulfur vacancies on the FeS(001) surface and their impact on CO_2 adsorption and found that the exposed Fe sites on the defective FeS(001) surface are catalytically active towards the adsorption and activation the CO_2 molecule due to reduced work function. Compared to the perfect surface (001), the adsorption of the CO_2 on the defective FeS(001) surface is shown to be characterized by significant charge transfer from the interacting surface Fe ions into the π-antibonding of the CO_2 molecule, which induced a large structural transformation in the molecule (i.e., forming a negatively charged bent $CO_2^{-\delta}$ specie, with weaker C−O confirmed via vibrational frequency analyses). The thermodynamics and kinetics of the direct versus hydrogen-assisted CO_2 reduction pathways on the defective FeS(001) and on the perfect (011) and (111) FeS surfaces were also systematically analyzed and will be discussed.

Audience Take Away:

The main take home message from the presentation will include the following:

- Activation of carbon dioxide is the most important step in its conversion into valuable chemicals.
- The catalytic activities of solid-state catalyst surfaces differ significantly depending on the surface structure and electronic properties, with the surfaces exhibiting low work functions more promising for CO_2 activation as they favor electron transfer.
- Defective FeS(001) surface represents a promising catalyst for CO_2 activation and conversion.
- Theoretical methods can be used to accurately describe surface chemical reactions in detail and to understand variations in catalytic activity from one catalyst to another.
- Explain how the audience will be able to use what they learn?
- The information provided will useful to the audience for the understanding and interpretation of their own research results. The information may also stimulate more research activities into the design of more active solid-state catalyst for CO_2 activation and conversion. Information on the characterization of the surface stability of the different FeS surface, Wulff construction, and work function calculations and their impact on CO_2 activation may be useful for faculties to expand their research or teaching.

Biography

Dr. Nelson Dzade is a computational materials scientist with broad experience in the application of state-of-the-art computer simulation and modelling techniques, including density functional theory (DFT) and interatomic potential-based simulations to (a) design and predict new materials with tailored and improved functionalities and (b) describe interface phenomena such as adsorption, surface chemical reactions, and heterogeneous catalysis. He gained his PhD from University College London (UCL), UK, before moving to the Utrecht University in the Netherlands as a postdoctoral researcher.

Super-capacitor characteristics based on several composite materials

Hee-Je kim*, Ph.D., B. Balamuralitharan, Ph.D., S. Selvam, Ph.D., Chandu V. V. M. Gopi, Ph.D
Pusan National University, South Korea

This paper demonstrates, reduced graphene oxide/Manganese selenide and CNT/NiS composite electrodes have been sucessfully synthesized by convenient hydrothermal methode for supercapacitor applications. The hydrothermal reaction carried out with sodium borohydride ($NaBH_4$) as a reductant and $MnCl_2.4H_2O$ and SeO_2 as precursors, and then used as electrode material for supercapacitor applications. The synthesized composite material were characterized by X-ray diffraction, scanning electron microscopy and X-ray photoelectron spectroscopy. The material was subject to electrochemical characterize like cyclic voltammetry, galvanostatic charge–discharge and electrochemical impedance spectroscopy tests was carried out in two-electrode supercapacitors were performed. In comparison with pure RGO/CNT and $MnSe_2$, NiS based supercapacitor, the RGO/MnSe and CNT/NiS based composite electrodes have been better performnce because the electrical conducivity and specific surface area were increased due to RGO. This composite electrode exibits the areal specific capacitance of 20.86 mF cm^{-2} at 25 mV s^{-1}. And CNT/NiS composite material exibits the maximum power density of 35.39 Wh kg^{-1} which is very high compare to pure MnSe/RGO and CNT/CoS, PbS, CuS. As well as, the supercapacitor exhibits high rate capability and long cyclic life. The results showed that the composite is a suitable electrode material for supercapacitor applications such as EV, ESS, UPS, Emergency power supply and so on.

Audience Take Away:

- Recently, super-capacitor is very important to save energy with fast charging and discharging. Especially, there are many applications such as EV, ESS, UPS, Emergency power supply, and so on. So it is very helpful for the audience to understand how to make the excellent super-capacitor.
- We made a new concept power supply that is three parallel connected by super-capacitor, Li ion battery and electro-chemical battery. So this presentation will provide a practical solution to a problem that could simplify or make a designer's job more efficient. It provides new information for fast charging and discharging about various applications.

Biography

Prof. Hee-Je kim obtained Ph.D. degree of Engineering from Energy Conversion Engineering, Kyushu University, Fukuoka, Japan 1990, march and Master degree of Engineering in Electrical Engineering, Pusan National University, Jangjeon-Dong, Geumjeong-Gu, Busan, 46241, Korea 1982. February. He done his Bachelor degree of Engineering in Electrical Engineering, Pusan National University, Jangjeon-Dong, Geumjeong-Gu, Busan, 46241, Korea 1980, February. He worked as Predecessor researcher at Korea Electrotechnology Research Institute, Changwon, Gyoungnam 641-120, Korea 1983, August – 1995, November and as Professor of Department of Electronics and Electrical Engineering, Pusan National University, Jangjeon-Dong, Geumjeong-Gu, Busan, 46241, South Korea 1995, November - Present.

Pt and Pd clusters confined in the bulk of fiberglass as an effective heterogeneous catalysts

Bair S. Bal'zhinimaev*
Boreskov Institute of Catalysis, Russia

Non-porous fiberglass (FG) textile materials of silicate origin (the BET surface area of ca 0.5 m^2/g) are produced for a long time in industry and are widely used as perfect heat and electric insulators. However, these microfiber materials are much less known in catalysis in spite of their obvious advantages, in particular, high thermal stability and improved hydrodynamics. In spite of extremely low metal content (0.01-0.02% wt.), the FG based catalysts showed high performance in many reactions due to their ability to confine highly dispersed transient metals species in the bulk of glass. In this paper we present the NMR and FTIR study of the molecular structure of these glasses as well as the features of Pd/FG and Pt/FG catalysts synthesis, size and charge of Pd and Pt clusters and their location obtained by HAADF-STEM, XPS with ion etching, and UV-Vis DRS. Both catalysts were tested in the VOC and CVOC abatement, and in the selective hydrogenation of acetylene in ethylene feedstock, respectively. SSITKA studies with the use of double labelled $^{13}C_2H_2$ and $^{18}O_2$ molecules allowed us to elucidate the main features of both reaction mechanisms.

The glass structure is characterized by the short range ordering and presents alternating chains of randomly bound silicon-oxygen tetrahedra (dense spaces) with low density spaces where the hydroxyl groups are localized, the ratio between different phases being defined from chemical glass composition. The key stages of FG catalyst synthesis are i) ion exchange of Pt and Pd cations with the strong glass protons; ii) redox treatments to form and to stabilize in the bulk of the glass (at a depth of 10-20 nm) the highly dispersed Pd-, and Pt clusters of 1 nm in size.

The Pd/FG-Al catalyst shows high performance in acetylene hydrogenation, so that a 100% conversion (residual C_2H_2 concentration ≤ 3 ppm) is reached at a temperature of ca 70°C. At high conversion (99%+) the selectivity is higher compared to commercial bimetallic catalyst due to ability of glass to absorb predominantly the polarizable molecules like acetylene (but not ethylene).Indeed,as follows from the SSITKA study, the ethane as the main by-product is produced mainly from acetylene but not from ethylene in spite of very high ethylene/acetylene ratio.

FG-Zr is a more preferable catalyst support for VOC and CVOC abatement, including dioxins since this material has a higher thermal stability (up to 1000°C). It is remarkable that Pt./FG-Zr reveals a higher activity in the deep oxidation of different volatile hydrocarbons (paraffins, aromatics, ethers etc) as compared with commercial one, although its Pt content is 1-2 orders lower. The isotopic studies with the use of ^{18}O showed the main reason is the formation of more reactive molecular oxygen species. High performance of this catalyst was successfully confirmed on industrial level in the abatement of waste gases from synthetic rubber plant (JSC Nizhnekamskneftekhim, Russia), when the catalyst showed purification efficiency 99%+ for more than 4 years.

Audience Take Away:

- First, the audience will understand how the ordinary material like glass can be converted into advanced functional one like catalyst. Second, the audience really will see how all platinum atoms are engaged in the chemical conversion. The presentation on fiberglass based catalysts will extend our knowledge in area of environmental catalysis, show the effective and relatively cheap ways on destruction of very hazardous emissions. Finally, the lab findings were demonstrated on the industrial level.

Biography

Dr. Bal'zhinimaev completed his doctorate at the Boreskov Institute of Catalysis in 1978. Then, he studied successfully the light olefin epoxidation and SO_2 oxidation. Starting from 1991 as a head of research group he performed a number R&D projects related to light paraffins activation, acid catalysis, application of novel materials like glass fiber in oxidative and environmental catalysis. Dr. Bal'zhinimaev was Member of Editorial Board of Green Chemistry, Journal of Natural Gas Chemistry, Journal of Energy Chemistry. He is member of Russian Mendeleev Chemical Society, ACS, Scientific Counsil on Catalysis of Russian Academy of Sciences.

Tuning the surface adsorption properties of polymer sorbents via facile methods

Lee D. Wilson*, Ph.D.,Mohamed H. Mohamed, Ph.D
Department of Chemistry, University of Saskatchewan, Canada

Cross-linked polymers were prepared by coupling β-cyclodextrin (β-CD) with two different types of diisocyanates, respectively. Materials with diverse structural and textural properties were obtained by varying the rate of diisocyanate addition: rapid (R) or drop-wise (D; 0.1 mL/min). Characterization of the structural and textural properties was investigated by spectroscopic (^{1}H NMR in solution, solid state ^{13}C CP-MAS solids NMR, dynamic light scattering, UV-vis, and IR), thermogravimetric analysis, powder x-ray diffraction, and scanning electron microscopy. The accessibility of the β-CD inclusion sites of the polymers was independently evaluated using an equilibrium dye adsorption method at equilibrium and in parallel with a kinetic dye-based uptake method. The characterization methods strong support that drop-wise additions affords materials with greater cross-linking relative to the rapid addition method. Herein, we report a first example of such cross-linked polymers with tunable structure and physicochemical properties, according to the mode of cross-linker addition (R versus D) to control the reaction conditions. The resulting physicochemical properties of these polymers are shown to play a significant role in catalytic transformations and controlled-release carrier systems.

Audience Take Away:

- New approaches to materials design with tunable properties
- The role of morphology and surface adsorption properties in catalysis
- The use of self-assembly and cross-linking for surface modification
- Adsorption based processes are ubiquitous in catalysis and the ability to design improved catalyst materials is a topic of ongoing research. This research will contribute to facile strategies on how to modify the surface chemical and textural properties of polymer materials for a range of organocatalysis and materials science & engineering applications.

Biography

Dr. Lee D. Wilson (PhD) is an Associate professor in the department of chemistry at the University of Saskatchewan with research interests in physical chemistry and macromolecular systems in aqueous media. Wilson's research is in the area of Physical Chemistry, Materials & Environmental Science where current efforts are being directed at the development of new types of macromolecular materials and their structure-function relationships that relate to adsorption phenomena. Modified biopolymer materials will have a tremendous impact on areas such as green catalysis, aquatic environments, biotechnology, medicine, chemical delivery/separation systems, and sorbent materials for water purification.

Metal supported on titania for nitrate reduction

Peter J. Miedziak*, Ph.D., Thomas Caswell, Stuart H. Taylor, Graham J. Hutchings
Cardiff University, UK

The contamination of ground water with nitrates from highly soluble nitrogen based fertilizers is a major problem. Nitrate and nitrite, which is formed by reduction of nitrate, are toxic to the human body, particularly for infants. Photocatalysis provides a method for removing these nitrates which is simple, when compared to existing methods, and therefore would enable the transfer of the technology to the required point of use, where more complicated technology, such as such as ion-exchange, biodegradation and reverse osmosis may not be available.Previous work has focused on the use of titania (P25) for this photocatalytic reaction, and has shown the beneficial effect of supporting gold nanoparticles on the titania. In this presentation I will focus on optimizing the preparation procedure of various precious metals supported on titania including gold, silver, platinum and palladium. Gold catalysts gave the best selectivity to nitrogen whereas Silver and Platinum showed some selectivity to nitrite. Different preparation methods (incipient wetness, wet impregnation, deposition precipitation and sol-immobilization) were used and the differences in the activity and the characteristics of the formed metal particles will be discussed. Taking an optimized catalyst I will discuss the effect of sieving the catalyst, drying the catalyst, the nature of the gas in the heat treatment, the temperature of this heat treatment and the ramp rate. The most significant factor was the total metal loading of the catalyst, with low loadings of metal found to give the optimum activity. All these catalysts have been characterized by TEM, XRD and XPS and the results of this characterization will be discussed.

Audience Take Away:

- Introduction to Photocatalysis.
- Knowledge of different catalyst preparation methodologies.
- A demonstration of the sensitivity of these methods to minor changes and how these affect the final catalyst.

Biography

Peter Miedziak received his MChem and PhD in Heterogeneous Catalysis from Cardiff University. The focus of his PhD thesis was on the preparation of supported gold and palladium bimetallic catalysts and their application for selective oxidation reactions. He has remained in Cardiff as a post-doctoral researcher working on biomass valorization and subsequently working for the U.K. Catalysis Hub, as part of the environmental theme, focused on photocatalysis. He has co-authored over 60 publications with a h-index of 17.

Fischer–Tropsch synthesis catalyzed by small TiO_2 supported cobalt nanoparticles prepared by sodium borohydride reduction

J. A. Delgado*[1], C. Claver[1,2], S. Castillon[2], D. Curulla Ferre[3], C. Godard[2]
[1]Centre Tecnològic de la Química (CTQ), C/ Marcel.li Domingo, Spain
[2]Universitat Rovira I Virgili, C/ Marcel.li Domingo s/n, Spain
[3]Total Research and Technology Feluy, Zone Industrielle Feluy C, Belgium

Fischer-Tropsch Synthesis (FTS) is considered a key process of the XTL technologies (biomass-to-liquid, BTL, gas-to-liquid, GTL, and solid-to-liquid, STL) since through this catalytic reaction, syngas (a mixture of H_2 and CO) can be transformed into clean fuels. One of the main challenges in Fischer-Tropsch is the design of highly active catalysts and for this purpose, the particle size of the active phase is probably one of the most relevant parameters for the optimization of the catalyst productivity.

In the present work, the synthesis of well-defined small cobalt nanoparticles and its catalytic evaluation in the Fischer-Topsch synthesis is described. Cobalt nanoparticles in the range of 1.7–7 nm were synthesized in water using sodium borohydride as reducing agent and subsequently immobilized on TiO_2. Both colloidal and TiO_2 supported NPs were characterized by TEM, XRD, HRTEM, XPS, TGA, ICP techniques and their catalytic performance of the supported catalysts evaluated in the Fischer–Tropsch synthesis. As a general trend, an increase in activity and TOF was observed when the particle size decreased. These results were rationalized by the higher reducibility of the catalysts bearing the smaller nanoparticles. The unconventional stability of these relatively small CoNPs in FTS was attributed to the promoting effect of boron on the stability of the cobalt nanocrystals.

Audience Take Away:

- Small cobalt nanoparticles (1.7 nm) supported on TiO2 resulted very active and stable in the FTS.
- CoNPs in the range of 1.7–7 nm were synthesized using NaBH4 and immobilized on TiO2.
- The stability of the small CoNPs was attributed to the promoting effect of boron.

Biography

Jorge A. Delgado was born in Bogotá, Colombia in 1987. In 2009, he completed his undergraduate studies in chemistry at the Universidad Nacional de Colombia and subsequently he moved to Spain to conduct postgraduate studies. In 2014, he concluded his PhD thesis at the Universitat Rovira i Virgili in Tarrragona (Spain) which dealt on the development of novel cobalt nanocatalysts for the Fischer-Tropsch synthesis. Since 2015 he has a postdoctoral position at the Centre Tecnologic de la Química (CTQ) working in an industrial project sponsored by Total S.A. His research interests lie in the areas of transition metal nanoparticles for catalytic transformations with particular focus on synthetic fuels and energy technologies.

Inline concentration profiles in enzyme catalyzed reactive rectification using infrared spectroscopy

Marc-Andreas Christlieb*[1], Steffen Kühn[1], Robert Hiessl[1], Joscha Kleber[1], Anne Stöbener[1], Irina Smirnova[1], Andreas Liese[1]
[1]Institute of Technical Biocatalysis, Hamburg University of Technology, Germany
[2]Institute of Thermal Separation Processes, Hamburg University of Technology, Germany

Enantiopure compounds are of high value to the pharmaceutical industry and enzymes such as the lipase B from Candida antarctica (CalB) can perform highly enantioselective reactions. On the contrary enzyme catalyzed reactions are often inhibited by a reaction product or thermodynamically limited. This can be avoided by using a reactive rectification column (RRC) setup to remove selectively a product in situ.

The integration of enzymes in a reactive rectification process requires a detailed optimization which is enabled by inline analytical tools. In order to acquire precise data to correctly determine local concentration profiles Fourier Transform Infrared (FTIR) spectroscopy with multiple attenuated total reflection (ATR) probes is used. Omitting the time to take and analyze offline samples abbreviates the time required for process optimization. Furthermore ATR-FTIR spectroscopy can be applied without the knowledge of compound properties like vapor liquid equilibrium.

The racemic resolution of (R/S)-3-hydroxy ethyl butyrate is used as a model reaction system which is catalyzed by CalB in a solvent free environment. (S)-3-hydroxy ethyl butyrate is a precursor in the production of antibiotics. Along the height of the RRC a temperature difference up to 40 °C is observed during the course of the reaction under vacuum conditions. First chemometric models were established using the partial least squares method. To circumvent the temperature dependency of the IR spectra a chemometric model was calibrated by means of indirect hard modeling. First results indicate excellent agreement between offline gas chromatographic and inline FTIR analytics. Future experiments will focus on enzyme deactivation and obtaining a pure product over the top of the RRC.

Biography

Marc-Andreas Christlieb was born on 15th April 1986 in Hamburg, Germany. Since July 2014 he is doing Ph. D thesis in the group of Prof. Dr. rer. nat. Andreas Liese, Institute of Technical Biocatalysis, Hamburg University of Technology (TUHH), Hamburg, Germany. During September 2013 – April 2014, he done his Diploma Thesis in the group of Prof. Dr.-Ing. Schlüter, Institute of Multiphase Flows, Hamburg University of Technology (TUHH), Hamburg, Germany

Topic: “Experimental Investigation and Modelling of Hydrodynamic Parameters in Industrial Bubble Columns.”

September 2011 – February 2012: Studies abroad: Czech Technical University (CTU), Department of Mechanical Engineering, Prague, Czech Republic.

October 2006 – April 2014: Academic Studies: Process Engineering, Hamburg University of Technology (TUHH), Hamburg, Germany

Professional Experience:

September 2013 – December 2013: Diplomate at Evonik Industries in Marl, Department of Reaction Engineering

November 2012 – April 2013: Internship at Evonik Industries in Marl, Department of Computer Aided Process Engineering

Thermal stability study of catalysts in Esterification reaction processes

Edidiong Okon*, Habiba Shehu, Ifeyinwa Orakwe, Edward Gobina
The Robert Gordon University Aberdeen, United Kingdom

In this study, the esterification of lactic acid with ethanol catalysed by cation-exchange resin catalyst to produced ethyl lactate also known as a petrochemical chemical solvent was carried used in a batch wise mode. The different catalysts used for the esterification process was amberlyst 36, amberlyst 15, dowex 50w8x and amberlyst 15. The surface of the resin catalysts was characterised using different analytical methods including gas chromatography coupled with mass spectrometry, FTIR-ATR, Liquid nitrogen isothermal adsorption method and scanning electron microscopy coupled with energy dispersive x-ray analyser was also used. Langmuir Hinshel wood model was used to describe the component with the most adsorption on the surface of the resin catalysts. The carrier gas used for the analysis of the esterification product was tested with silica membrane before employing the gases for the analysis of the ester product with gas chromatography. The experiment was performed at the gauge pressure range of 0.10 – 1.00 bar at the temperature of 353 K. The EDXA of the membrane support show that the membrane was initially coated with TiO_3 and subsequently with SiO_2 and ZrO_2. The SEM of the support show a crack free surface indicating that membrane was defect free. The different gases tested were helium, nitrogen, argon and carbon dioxide. The gas permeance was found to decrease with an increase in temperature indicating Knudsen flow mechanism of gas transport. From the FTIR result of the resin catalyst, different structural bond were observed on the surface of the spectra of the resin catalysts including C=O, C-H, -O-C=O- and C-O bonds. The BET surface area of the resin catalyst was found to be high after the esterification process. The BJH pore size of the catalyst exhibited a typical type IV isotherm which was in accordance with the mesoporous classification of such material. In conclusion, amberlyst 36 and amberlyst 16 catalyst were found to be stable at higher temperatures and could withstand the effect of higher concentration of the reactant solvents.

Biography

Edidiong Okon is a Doctoral researcher/Research assistant at the School of Engineering, Robert Gordon University, Aberdeen, United Kingdom, having previously obtained her Bachelor and Master of Science degrees in Applied Chemistry and Instrumental Analytical Sciences respectively. She is currently working on ''Esterification of Lactic acid with Ethanol using cation-exchange resins impregnated metallic membrane reactor''. She has previously published and co-authored a number of academic papers in international journals. Her research interests are in the area of heterogeneous catalysis and metallic membrane reactor for ethyl lactate separation. She is a member of various Professional bodies including Royal Society of Chemistry and International Association of Engineers. She has also made several oral/poster conference presentations in the United State of America and United Kingdom.

Computational study of the Fischer-Tropsch process catalyzed on small Ru clusters: Beta-elimination versus reductive elimination

Edward Brothers*[1], Salvador Moncho[1], Benjamin G. Janesko[2]
[1]Texas A&M University at Qatar, Qatar
[2]Texas Christian University, USA

The Fischer-Tropsch (FT) process is a key step in the production of hydrocarbons from natural gas, coal or biomass. In particular, the FT process generates a mixture of liquid hydrocarbons from synthesis gas (i.e. CO and H_2), obtained via steam reforming. The composition of this product mixture determines its properties and utility. The content of the product mixture follows a distribution which is mainly dependent on the catalyst used. Most FT catalysts are based on metallic cobalt and ruthenium surfaces, doped with additional "promoter" atoms. However, catalyst research is an active field, because both the activity of the process and the selectivity toward particular mixtures of hydrocarbons can be significantly improved. For example, by modifying the catalyst, the output can be modified from traditional fuel products to various light olefins with a higher economic value.

In this study, density functional methods known to work well in catalytic, we study the Fischer-Tropsch process on small ruthenium clusters.In particular, we analyzed the case of pure four-atom ruthenium metal clusters, Ru_4. Different geometries and spin-states of the cluster were compared and compared in our reactivity studied. The effect of "promoter" atoms altering the electron density of the metal is studied by including extra charged points around the cluster. We studied the reaction mechanism for several of the steps involved in the FT process; such as the breaking of the C-O bond, the growth of the C-C chain and the release of both saturated and unsaturated hydrocarbons. The termination reactions (beta elimination and reductive elimination) determine if the released product is an olefin or a paraffin. Thus, depending on the relative energies a catalyst can be tuned to obtain an olefin-rich or paraffin-rich hydrocarbon mixture.

Audience Take Away:

- How modern electronic structure can be used to model catalysis.
- How the selection between reaction routes (rate determining steps, etc.) and hence products occurs in FT.
- How simple promoters can be used to modify the catalyst's chemistry, which then can be mapped to real promoters, greatly aiding catalyst optimization.

Biography

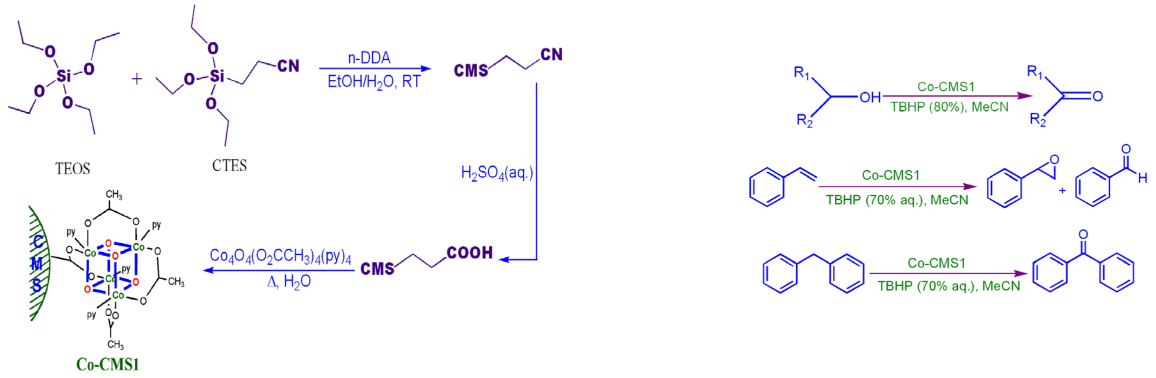
Edward N. Brothers is an associate professor of chemistry and the chair of the science department at Texas A&M University at Qatar. His active research program, funded by The Qatar National Research Fund and involving both academic and industrial partners, centers around the elucidation and optimization of catalysts via modelling reaction processes using modern electronic structure theory.

Cobalt(III)- supported chemically modified mesoporous silica as heterogeneous oxidation catalyst

Purabi Sarmah*[1], Ph.D., Birinchi Kumar Das[2], Ph.D
[1]Nalbari College, India
[2]Gauhati University, India

The catalytic activity of a heterogeneous oxidation catalyst, named as Co-CMS1based on a cubane-like Co(III) oxo cluster which is immobilised on a porous organomodified silica, will be described. The heterogeneous Co(III) supported chemically modified silica (CMS) system (Co-CMS1) has been well characterized by powder XRD, SEM, TEM, BET analysis, IR, solid UV-Vis-NIR and XPS techniques. The catalyst has been found to promote the efficient and selective oxidation of benzylic alcohols and cyclohexanols with TBHP as the oxidant which can be reused without any significant loss of activity. The Co-CMS1 catalyst has also been found to catalyse efficiently the oxidation of both styrene and diphenylmethane using aqueous TBHP as the oxidant.

Graphical abstract:



Audience Take Away:

- I think the audience will surely get benefited by the work presented herein as the methodology developed is quite simple, advantageous and easy to handle.
- The presenter has reported an excellent heterogeneous catalytic system which definitely will be able to draw attention of the audience and also it may help in exploring its further utility and possibly might be able to extend its applicability to some other reaction system.
- Hopefully, share and exchange of ideas between the audience and the presenter will lead to a fruitful influence in the future course of research which may help in designing much more advanced as well as improved catalytic system.

Biography

Dr.Purabi Sarmah is an Assistant Professor in Chemistry, Nalbari College, Nalbari, Assam, India. She completed her Ph. D in Gauhati University, Guwahati in 2011.She done her M. Sc. (Organic Chemistry), 2002 Gauhati University and BSc (Chemistry), 1999, Gauhati University. Other qualifications include CSIR-UGC National Eligibility Test (NET), CSIR-JRF, June- 2005 and CSIR-SRF, 2008.

Research Experience and Expertise:

- Eight years of research experience under the supervision of Dr. Birinchi K Das, Professor, Department of Chemistry, Gauhati University in the field of Catalytic Chemistry.
- Research experience as a guest worker in the National Chemical Laboratory (NCL), Pune under the guidance of Dr. A. P. Singh, Scientist F, Catalysis Division which involves the synthesis of chiral complexes and their immobilization over solid supports.

Design of heterostructure photoelectrodes for solar fuels

Yan-Gu Lin*, Ph.D
National Synchrotron Radiation Research Center, Taiwan

Global climate warming and environment pollution have spurred scientists to develop new high-efficient and environmental-friendly energy technologies.Sunlight is a clean, renewable and abundant energy source on the earth. Its conversion to hydrogen has been considered an ideal solution to counter the depletion and environmental problems of fossil fuels.Hydrogen is an ideal fuel for fuel cell applications. Hydrogen has to be produced from renewable and carbon-free resources using nature energies such as sunlight if one thinks of clean energy and environmental issues. In this regard, a photoelectrochemical cell consisting of semiconductor photoelectrodes that can harvest light and use this energy directly for splitting water is a more promising way for hydrogen generation.Photocatalysis utilizes the energy delivered by light and enables chemical reactions that otherwise cannot take place. When used to power thermodynamically uphill reactions, photocatalysis offers a solution to large-scale solar energy storage. Despite over four decades of intense research, however, photocatalysis remains either too expensive or too inefficient or both. Poor understanding of the mechanisms behind the low performance is a key reason that limits the progress of this important field. To address this critical challenge, and to complement existing efforts focused on discovering new materials for photocatalysis, we present here a series of experiments designed to elucidate the working principles of photocatalysis. First, we compared two co-catalyst systems, one heterogeneous and one homogeneous and found that they improve the performance of the photocatalyst by fundamentally different mechanisms. Next, we established a quantitative correlation between surface treatment and charge transfer kinetics. Lastly, we employed synchrotron X-ray spectroscopy to provide a complete picture of surface energy evolution as a function of water splitting history. The key value generated by this body of research lies in the fundamental understanding of the thermodynamics and kinetics of the photocatalyst/electrolyte interface, which is expected to serve as a foundation for future research on photocatalysis.

Biography

I received my PhD degree from Materials Science and Engineering at National Chiao-Tung University, Taiwan, in 2010. After graduation, I became a Postdoctoral Fellow in Institute of Atomic and Molecular Science at Academia Sinica, Taiwan, in 2011. Thereafter, I joined Dr. Jeffrey T. Miller's group in Chemical Sciences and Engineering Division at Argonne National Laboratory, United States, as a postdoctoral researcher from 2012 to 2013. Currently, I am the assistant research scientist in National Synchrotron Radiation Research Center, Taiwan. My major research is focused on the field of energy conversion and storage application.

Photocatalytic hydrogen evolution from water splitting over mixed valence tin oxide semiconductor under visible light irradiation

Toyokazu Tanabe*, Ph.D., Takao Gunji, Ph.D., Shingo Kaneko, Ph.D., Takeo Ohsaka, Ph.D., Futoshi Matsumoto, Ph.D
Kanagawa University, Japan

Water splitting using a particle photocatalyst with visible light has attracted interest, because this will realize efficient conversion of the solar energy to hydrogen fuels for sustainable energy managements. Many water-splitting photocatalysts, such as metal-doped oxides, metal-(oxy)nitrides, and metal-oxysulfides, exhibit water reduction and oxidation ability when absorbing visible light. However, in such water-splitting photocatalysts, solely doping and/or replacement of foreign element at host material has been attempted to prepare visible-light-driven photocatalysts. The doping and/or replacement induces defect sites and charge imbalance into photocatalyst, resulting in the formation of recombination centers between excited electron and holes, in return to create new valence state. Therefore, the development of new native visible-light-sensitive photocatalyst for water splitting without doping of foreign elements is a major challenge for photocatalyst research.

Herein, we report that an undoped metal oxide, Sn_3O_4, can efficiently catalyze Hydrogen (H_2)-evolution in the presence of a sacrifice agent and, furthermore, can split water to H_2 and O_2 under irradiation of visible light by two-step photoexcitation (Z-scheme) systems using Sn_3O_4 as H_2-evolving photocatalyst, combined with an appropriate O_2-evolving photocatalyst in the presence of iodate/iodide (IO_3^-/I^-) as an electron mediator.

We prepared nanocrystals of Sn_3O_4 by hydrothermal synthesis using sodium citrate as a ligand. The Sn_3O_4 significantly catalyzed hydrogen evolution in aqueous solution in the presence of sacrifice agent under irradiation of visible light ($\lambda>420$nm), even without Pt co-catalyst (Figure 1). Pt co-catalyst was critical for Sn_3O_4 material to exhibit higher photocatalytic activity, so far in this study. The apparent quantum yield was 0.2% for high purity Sn_3O_4 and 1.5% for Pt loaded-Sn_3O_4, competitive to that of visible-light-sensitive doped metal oxide and (oxy)nitrides photocatalyst. Simultaneous evolution of H_2 and O_2 was attempted by using Sn_3O_4 as H_2-evolving photocatalyst, combined with an appropriate O_2-evolving photocatalyst ($BiVO_4$, WO_3 etc.,). By employing the appropriate combination of Sn_3O_4 and the redox couple (IO_3^-/I^-), simultaneous evolution of H_2 and O_2 stably proceeded with higher rates.

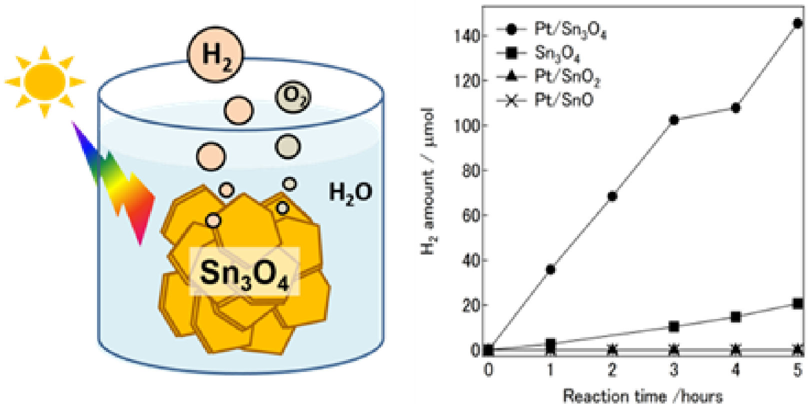


Fig1. Single phase Sn_3O_4 synthesized by optimizing hydrothermal reaction condition significantly catalyzed hydrogen evolution in aqueous methanol solution under irradiation of visible light ($\lambda>420$nm), even without Pt co-catalyst.

Audience Take Away:

- Hydrogen will play an important role in clean energy system because it is an ultimate clean energy and it can be used in fuel cells.
- Water splitting using a particle photocatalyst will realize efficient conversion of the solar energy to hydrogen fuels for sustainable energy managements.
- An oxide of abundantly available and environmentally non-toxic tin, Sn_3O_4, can efficiently catalyze the targeted water splitting in aqueous solution under irradiation of visible light.

Biography

Dr.Toyokazu Tanabe, Doctor of Engineering (Ph.D.-Engineering),now is an Assistant professor of Department of Material & Life Chemistry in Kanagawa University. Currently Dr.Toyokazu Tanabes' researches focus on the Water splitting and Organic matter decomposition using photocatalyst.

Active carbons as nanoporous materials for solving of environmental problems

Victor Mukhin*, Vasily Guryanov
"Neorganika", Elektrostal, Russia

However, up to now, the main carriers of catalytic additives have been mineral sorbents: silica gels, alumogels. This is obviously due to the fact that they consist of pure homogeneous components SiO_2 and Al_2O_3, respectively.

It is generally known that impurities, especially the ash elements, are catalytic poisons that reduce the effectiveness of the catalyst. Therefore, carbon sorbents with 5-15% by weight of ash elements in their composition are not used in the above mentioned technologies. However, in such an important field as a gas-mask technique, carbon sorbents (active carbons) are carriers of catalytic additives, providing effective protection of a person against any types of potent poisonous substances (PPS).

In ESPE "JSC "Neorganika" there has been developed the technology of unique ashless spherical carbon carrier-catalysts by the method of liquid forming of furfural copolymers with subsequent gas-vapor activation, brand PAC.

Active carbons PAC have 100% qualitative characteristics of the three main properties of carbon sorbents: strength - 100%, the proportion of sorbing pores in the pore space – 100%, purity - 100% (ash content is close to zero).

A particularly outstanding feature of active PAC carbons is their uniquely high mechanical compressive strength of 740 ± 40 MPa, which is 3-7 times larger than that of such materials as granite, quartzite, electric coal, and is comparable to the value for cast iron -400-1000 MPa. This allows the PAC to operate under severe conditions in moving and fluidized beds.

Obviously, it is time to actively develop catalysts based on PAC sorbents for oil refining, petrochemicals, gas processing and various technologies of organic synthesis.

Audience Take Away:

- The new technology of liquid shaping of the spherical carbon sorbents will be presented;
- The adsorption and strength properties of the new active carbons class PAC and its high degree of purity (low ash contamination) will be shown;
- The different applications in industry, medicine and ecology will be discussed.

Biography

Victor M. Mukhin was born in 1946 in the town of Orsk, Russia. In 1970 he graduated the Technological Institute in Leningrad. Victor M. Mukhin was directed to work to the scientific-industrial organization "Neorganika" (Elektrostal, Moscow region) where he is working during 47 years, at present as the head of the laboratory of carbon sorbents.

Victor M. Mukhin defended a Ph. D. thesis and a doctoral thesis at the Mendeleev University of Chemical Technology of Russia (in 1979 and 1997 accordingly). Professor of Mendeleev University of Chemical Technology of Russia.

Scientific interests: production, investigation and application of active carbons, technological and ecological carbon-adsorptive processes, environmental protection, production of ecologically clean food.

magnus
Group

DAY 2

Keynote Forum

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Design and application of single-site zeolite catalysts

*Stanislaw Dzwigaj**

Laboratoire de Réactivité de Surface, Sorbonne Universités, France

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

During the plenary talk the design of new single-site zeolite catalysts with transition metal species (V, Fe, Co, Ni, Ag, Cu, Ta, Nb) will be described and characterized by different physical techniques both at the macroscopic level (chemical analysis, XRD, BET, thermal methods (TPR, TPO, TPD), TEM) and molecular level (FT-IR, NMR, diffuse reflectance UV-Vis, XPS, EPR, XAFS).

The application of single-site zeolite catalysts in different catalytic processes such as oxidative dehydrogenation of propane into propene, Fischer Tropsch synthesis, selective catalytic reduction of NO_x to N_2, hydrodechlorination of chlorinated volatile organic compounds into non-toxic, environmentally friendly products, production of 1,3-butadiene or hydrogen from renewable sources, including ethanol obtained from biomass will be discussed.

This two-step postsynthesis method applied in this work allowed obtaining single sites V-, Fe-, Co-, Ni-, Ag-, Cu-, Ta- and Nb-containing zeolite catalysts with mononuclear metal species active in above mentioned processes. Their catalytic activity strongly depends on the speciation and amount of metal incorporated into zeolite structure as well as their acidity.

Takeaway Notes

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

Biography

Professor Stanislaw Dzwigaj was trained in chemistry in Institute of Catalysis and Surface Chemistry, Krakow (Poland) where he obtained his PhD in Science in 1982 in the group of Prof. Jerzy Haber. After a postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris, France) in the group of Dr Denis Barthomeuf (1987-1988) 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.

Photocatalysis for degradation of environmental pollutants under VUV irradiation

Dennis Y.C. Leung*, Ph.D

The University of Hong Kong, Hong Kong

Photocatalytic oxidation (PCO) is one of the fastest developed technologies for the control of environmental pollutants (in both gaseous and aqueous state) as well as for energy production (such as hydrogen generation and dye-sensitized solar cell). The PCO process is normally triggered by the irradiation of UV light. The most widely used UV sources in PCO are 254 nm and 365 nm UV lamp. However, conventional PCO process has disadvantages such as recombination of electron-hole pair leading to low efficiency and photocatalyst deactivation. In order to improve the efficiency and stability of the PCO process, UV lamps with partial 185 nm UV irradiation (denoted as VUV lamp) can be used to activate photocatalysts. 185 nm VUV lamps cannot only irradiate photocatalyst but also generate active oxidants such as O radicle, OH radicle, and ozone all of which enhance the oxidation of the organic components in the nearby pollutants. The VUV lamps are also facile, cheap, and energy efficient. In this paper, the results of VUV enhanced photocatalytic degradation of common VOCs (such as toluene and benzene) and water pollutants (such as methyl blue are acrylic wastewater) are presented and discussed. In addition, ozone is a byproduct generated in the process, which can enhance the oxidation but can also cause harmful effects on our health. The removal of the residue ozone using modified catalyst will also be discussed.

Takeaway Notes

- Learn the different processes of oxidation and reduction under VUV photocatalysis.
- Learn how efficient the VUV photocatalysis on degrading air and water pollutants.
- Learn how the ozone generated can help to degrade the pollutants and how the residue ozone can be totally removed.
- Enhance the research on advanced oxidation processes (AOP).

Biography

Professor Dennis Y.C. Leung is currently a full professor of the Department of Mechanical Engineering at the University of Hong Kong specializing in environmental pollution control and clean energy development. He has published more than 400 articles in this area including 220+ peer reviewed top SCI journal papers. He was invited to publish more than 20 review articles in leading journals. His current h-index is 54 with total citations more than 15,000. He is one of the top 1% highly cited scientists in the world in energy field since 2010 (Essential Science Indicators) until now. Professor Leung has delivered more than 50 keynote and invited speeches in many conferences as well as public lectures. He serves as a chief editor or editorial board member of a number of journals including Frontiers in Environmental Sciences, Applied Energy, Journal of Power & Energy, just name a few.

Mesoporous silica is a mysterious material: From viewpoints of its catalysis for direct amidation reaction of carboxylic acids and amines

Kenichi Komura*, Ph.D
Department of Materials Science and Technology, Gifu University, Japan

Mesoporous silica is a material having a uniformed mesopore, a large specific surface area and a pore volume, and a topology reflecting its bulk architectural matrix. Almost reported catalytic reactions using mesoporous silica have been relied on the Brønsted acid site by introducing Al into the framework. We found that the siliceous mesoporous silica showed the excellent catalytic activity for direct amidation using equimolar amounts of carboxylic acids (including fatty acids) and amines, and recently reported that the catalytic activity (the initial reaction rate) uniquely depended on the pore size of the catalyst SBA-15 having P6mm topology. In this reaction, the catalyst after the calcination can be recycled and reused without loss of its catalytic activity, and successfully applied in the synthesis of procainamide. In this honorable lecture, the brief background of recent heterogeneous amidations and the selected our reported characteristic feature of this reaction system will be introduced, and unique results that we are just facing on will propose to realize not only the reason why mesoporous silica is a mysterious but also the importance of pore size when you will use mesoporous silica as a catalyst.

Takeaway Notes

- Mesoporous silica is an active catalyst for direct amidation.
- The reaction only requires an equimolar amounts of acids and amines.
- Mesoporous silica catalyst can be recyclable and reusable without loss of its activity.
- The maximum catalytic activity is depended on pore size of the catalyst.

Biography

Associate Prof. K. Komura (Ph.D.) received his bachelor of Eng. at Kansai University in 1996 (Prof. T. Nishiyama) and he went to a degree of master course at Nagoya University in 1996 (Prof. M. Kitamura and Prof. R. Noyori), then moved in 1997 at Toyohashi University of Technology for earning a Ph. Dr. under Prof. S. Itsuno and received Ph. D. in 2002. His first carrier for researches of micro- and mesoporous materials began at Advanced Industrial Science and Technology (AIST) in Sendai joining with Dr. F. Mizukami's group in 2002. In 2004 he became an assistant professor at Gifu University with Prof. Y. Sugi and Y. Kubota group working on parts of shape-selective alkylation of aromatics using microporous materials. He became an associate professor in 2008 at Gifu University. His current active interests are to develop the Catalytic Reactions using micro- or mesoporous materials such as Zeolite and Mesoporous silica based on the concept of Green Sustainable Chemistry.

DAY 2

Speakers

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Sessions on: Kinetics and Catalysis | Advances in Catalysis | Chemical Reaction Engineering | Applied Catalysis

Session Chairs

Buchang Shi
Eastern Kentucky University, USA

Dibakar Chandra Deka
Gauhati University, India

Session Introduction

Title: GaN a novel catalyst material for the direct non-oxidative methane aromatization
Jan Kopyscinski, McGill University, Canada

Title: Sub-micromolar reaction screening in flow
Neal Sach, Pfizer Inc, USA

Title: Development of a new approach to study of catalytic reaction mechanisms
Irina Khalfina, Novosibirsk State University, Russia

Title: Microkinetic rate theory: Generalization, application to catalysis, prospects as basis for continuum rate theory
Michael Frederick Francis, Los Alamos National Laboratories, USA

Title: Transesterification of non-edible vegetable oils to biodiesel using a heterogeneous catalyst derived from banana plant
Md. Abdul Halim Shah, Dhanamanjuri University, India

Title: Solar water splitting by doping-treated $BiVO_4$
Won Jun Jo, Lawrence Berkeley National Lab, USA

Title: Oxidation of sulfur dioxide to sulfur trioxide over V_2O_5/TiO_2 catalyst and sulfur balance
Tingyu Zhu, Institute of Process Engineering, Chinese Academy of Sciences, China

Title: High performance catalysts for hydrogen & oxygen evolution reactions and water electrolysis
Zhifeng Ren, University of Houston, USA

Title: Photo-oxidation reaction scheme triggered by the nozzle of submerged plasma torch
Florent Lemont, Atomic Energy Commission, Marcoule, Bagnols-sur Cèze Cedex, France

Title: OsO_4 catalysed oxidation of atropine sulphate monohydrate with chloramine-T in alkaline medium: Delineation of mechanistic pathways and kinetic modelling
Nirmala Vaz, Jyoti Nivas College Autonomous, India

Title: Novel nickel-palladium catalyst for hydrogenation aromatic compound
Su Ying-Chou, National Cheng Kung University, Taiwan

Title: Silica-immobilized bifunctional L-prolinol organocatalysts: Stereoselective michael addition in heterogeneous environment
Jiri Tuma, University of Chemistry and Technology Prague, Czech Republic

Title: Nanocrystalline synthetic ferrihydrite as a catalyst for Fischer-Tropsch synthesis
Dong Hyun Chun, Korea Institute of Energy Research, Republic of Korea

Title: A novel heterogeneous catalyst from red cotton flowers and its applications
Hitesh Barman, Rangia College, India

Title: Study of the use of ceramic membranes coated with Copper and Zirconium oxides in the oxidation of Carbon monoxide
María Dolores Sosa Lucio, Escuela Politécnica Nacional, Ecuador

Title: Deactivation kinetics of Pt-Sn/Al2O3 catalyst in the dehydrogenation of light alkanes
Saeed Sahebdelfar, Petrochemical Research and Technology Co., Iran

Title: Observation of dynamic Cu redox behavior in MFI-zeolite during NH_3-SCR using in-situ XAFS
Kakuya Ueda, Nagoya University, Japan

GaN a novel catalyst material for the direct non-oxidative methane aromatization

K. Dutta, Jan Kopyscinski*
McGill University, Canada

Vast amount of shale gas and gas hydrates has been discovered, which will undoubtedly change the landscape of the chemical industry. In this context, methane is a feedstock of special interest for the production of key building blocks such as aromatic compounds. Processes that convert methane into chemicals are indirect oxidative (syngas), direct oxidative, and direct non-oxidative dehydrogenation. The syngas route with its low efficiency, high capital cost and CO_2 emissions is the dominant industrial practice. One the other hand, the direct non-oxidative methane conversion is more environmentally friendly and economical. However, this route is very challenging due to thermodynamic and kinetic constraints. The activation of the strong C-H bond requires high temperature (750-1100°C) and an efficient catalyst, of which various metal-modified zeolites have been investigated.

With this work, we present gallium nitride – a semiconductor material that has not been used as a catalyst for a high temperature process – and explore its catalytic activity towards the direct methane conversion in a flow reactor. The GaN catalyst exhibits a much higher benzene selectivity than typical Mo-containing zeolites. Commercially available GaN material has a very low surface area of less than 10 $m^2\ g^{-1}$, an increase in its surface area to more than 200 $m^2\ g^{-1}$ result in a much higher methane conversion and benzene yield. This material an interesting catalyst worth for further investigation because to date all catalysts studied for C-H activation are metal oxides. III-nitride semiconductors are highly chemically stable due to the strongly ionic character of the atomic bonds. However, the interaction between CH_4 and GaN and reaction mechanism are not known, but it is suggested that carbon from methane is attached to the lattice Ga^+ cation, whereas one hydrogen atom of the methane molecule is adsorbed by the adjacent lattice N^{3-} anion (alkyl adsorption model).

Audience Take Away:

- Metal nitrides such as GaN are an interesting catalyst material and alternative to metal oxides.
- GaN catalyst is able to convert methane to benzene with high selectivity.
- Development and optimization of GaN catalyst is at its beginning and there is considerable room for improvement.

Biography

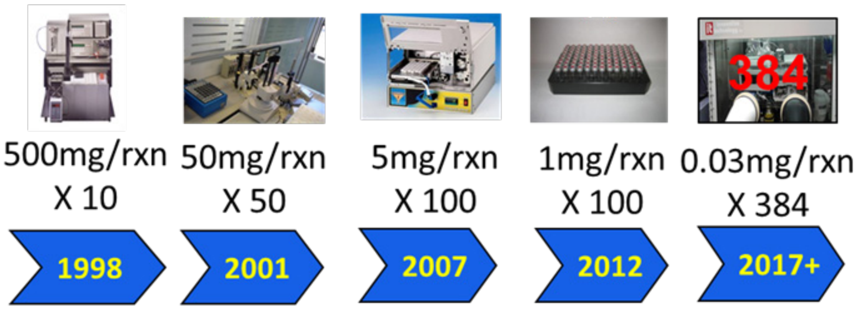
Dr. Kopyscinski obtained his doctor of sciences (Dr. Sc.) from the Swiss Federal Institute of Technology (ETH Zurich) in 2010. From 2010 to 2013 he was postdoctoral fellow at University of Calgary in the group of Dr. J.M. Hill and University of Toronto working with Dr. C. Mims on hydrodenitrogenation, catalyzed gasification and kinetic modeling. Since 2014, Dr. Kopyscinski is an Assistant Professor and leads the laboratory of Catalytic Process Engineering in the Department of Chemical Engineering at McGill University. His research group is engaged in the development and understanding of catalyzed processes and reactor engineering concepts dedicated to sustainable energy conversion technologies.Processes of special interests are direct non-oxidative methane aromatization, the production of renewable natural gas and energy storage via the power-to-gas process. Dr.Kopyscinski is specialized in reactor design with spatially resolved measurement capabilities and novel catalyst design such as gallium-nitrides and ordered mesoporous alumina.

Sub-micromolar reaction screening in flow

Neal Sach*, Shalini Brahmbhat, Ashley Chong, Bill Farrell, Chris Helal, Ph.D., Damith Perera Ph.D., Paul Richardson Ph.D., Joe Tucker Ph.D
Pfizer Inc., USA

As block-buster opportunities dwindle and personalized medicines prevail there is a strong drive to reduce drug development costs to ensure medicine discovery remains a viable proposition. One outcome of this changing landscape is the pressure to identify scalable synthetic routes at an earlier stage to minimize any delays in the transition from small scale pre-clinical work, to large scale patient studies.

Chemical technologies have played a leading role in that goal over the past two decades with batch reaction screening tools being central to that progress. In this presentation, a new and novel flow technology will be detailed that enables miniature scale chemistry optimization experiments. The technology reduces the scale of each reaction to less than 0.01mg, enabling the user the ability to screen over 1500 combinations (solvent, base, catalyst, and temperature) automatically in 24 hours using just 15mg of substrate. The presentation will demonstrate the technology through a model Suzuki coupling in which over 4500 combinations were attempted in 3 days to arrive at a scalable process suitable for scale up.



Audience Take Away:

- The audience will gain an understanding of the impact new technology and specifically reaction screening technology has had on drug discovery in the pharmaceutical community over the past two decades. Further, they will gain an appreciation of the next generation of technologies and how these could revolutionize the industry and aid personalized medicine approaches. Specifically the audience will learn how to modify common place laboratory equipment to enable rapid reaction screening that will miniaturize traditional, round-bottom flask, modes of optimization.

Biography

In 1995 Neal began his career at Rhone-Poulenc Agriculture in the UK as a school leaver training four days a week as a Discovery Synthetic Chemist whilst studying Chemistry at the University of Hertfordshire on a day-release program. In 1998 he switched fields and joined Process Chemistry at Pfizer Sandwich, becoming the first member of the high-throughput reaction optimization group. Over the next decade the application of technology to process chemistry become increasingly valuable and Neal eventually headed up a group of five scientists, before, in 2007, he switched divisions within Pfizer and moved to Discovery Chemistry in San Diego. Neal currently applies miniaturized high-throughput screening technologies, including flow technology, to solving chemical problems in the discovery portfolio.

Development of a new approach to study of catalytic reaction mechanisms

Irina Khalfina*
Departament of Natural Sciences, Novosibirsk State University, Russia

Earlier, we studied the substituent effects on the activation parameters □H≠ and □S≠ for isokinetic series of the transesterification reactions of aryl benzoates with potassium aryloxides in DMF. To explain the obtained results we proposed a new interpretation of the isokinetic effect based on the monotonic dependence of the enthalpic benefit on the entropic cost for electrostatic bonding. According with this interpretation a change from one isokinetic series to another was described as a motion of the transition state in the Tiso and □□H≠ coordinates which can be decomposed into two component vectors, one along the reaction coordinate and one perpendicular to it.

A two-dimensional reaction coordinate diagram, also known as a More O'Ferrall-Jencks diagram, is a tool for identifying changes in the free energy surface of the reacting system being responsible forthemotion of the transition state. As a result, a new four-step mechanism was suggested for the transesterification reactions of aryl benzoates.

This approach was successfully applied in the study of the solvent effect on the reactions of 2,4-dinitrophenyl benzoate with potassium aryloxides, too. Moreover, we used it to examine the nature of the base - reagent interaction for the reactions of 2,4-dinitrophenyl benzoates with potassium aryloxides and substituted phenols in the presence of the strong base K_2CO_3 and the weak base $KHCO_3$ in DMF.

The results of these investigations give hope that the suggested approach can be useful to study the catalyst effect on the free energy surface of the reacting system.

Biography

1984-1989: Novosibirsk State University, Department of Natural Science, Specialty "Chemistry"

1975-1983: High School

Scientific Degree: Candidate of Chemical Sciences

2016 – Present: Novosibirsk State University, Department of Natural Science, Assistant Professor

1989-2016: N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of Siberian Branch of Russian Academy of Sciences, Researcher (1989-2013), Academic Council Secretary (2013-2016)

Research Interests:

Mechanisms of organic reactions

Kinetics and Catalysis

Synthesis of electrochemically active compounds

Microkinetic rate theory: Generalization, application to catalysis, prospects as basis for continuum rate theory

Michael Frederick Francis*
Los Alamos National Laboratories (LANL), USA

Microkinetic Rate Theory (MRT) has been an important part of chemical kinetics, being taught in undergraduate physics and chemistry courses, and forming the basis of modern descriptor theory used widely in research. In spite of MRT's ubiquitous importance, it has remain unformalized and ungeneralized. In this talk, MRT is formalized and generalized. MRT is cast as an algebraic expansion and those matrix elements forming the coefficients of the generalization defined in terms of reaction rate constants, which are in turn connect to statistical mechanics. MRT is then applied to ammonia synthesis catalysis as a demonstration case where and a robust method of determining rate limiting steps, promotors, inhibitors is described. The current limitations of MRT and prospects as a basis for continuum rate modeling are also discussed.

Transesterification of non-edible vegetable oils to biodiesel using a heterogeneous catalyst derived from banana plant

Md. Abdul Halim Shah*[1], Ph.D., Dibakar Chandra Deka[2], Ph.D
[1]D.M. College of Science, Dhanamanjuri University, India
[2]Gauhati University, Guwahati, India

The chemical process used to convert oils and fats to biodiesel is known as transestertification. The transesterification process can be carried out either by employing an acid or a base catalyst. We have developed a heterogeneous base catalyst that has been successfully used to convert vegetable oils to biodiesel. The catalyst has been derived from post-harvest banana plant. Post-harvest banana plants are of no use, and these are usually considered waste bio-bass. Therefore, we were looking for fruitful use of post-harvest banana plants and have been successful in converting them to a strongly basic heterogeneous catalyst. The catalyst can be prepared at a nominal cost, and hence should be quite useful in biodiesel industries. Details of preparation of the catalyst, and its efficacy in transesterification reaction would be discussed.

Another aspect that would be discussed is the conversion of non-edible vegetable oils to biodiesel. Conversion of edible vegetable oils to biodiesel brings in conflicts of interest, especially in developing countries thanks to shortage of edible oils and constraints of farming lands. However, non-edible vegetable oils from wild sources can be converted to biodiesel without involving any conflict of interest. Non-edible vegetable oils available in North-Eastern part of India and their conversion to biodiesel would be reported.

Audience Take Away:

- Scientific use of waste biomass for economic benefits and employment generation.

Biography

Dr. Abdul Halim Shah is presently working as an Associate Professor in the Department Of Chemistry, D.M. College of Science, Dhanamanjuri University, Imphal, Manipur, India. After completing his school education in Air Force Central School, CBSE New Delhi in 1979, he joined D.M. College of Science, Manipur University, Imphal and received his B.Sc. (Hons) degree in Chemistry in 1984. Subsequently, he received his M.Sc. (Organic Chemistry) degree from Indore University in 1986 and Ph. D. in Chemistry under the guidance of Professor D.C. Deka, Gauhati University, Assam in 2015. Dr. Shah has been teaching both graduate and post graduate students since 1987.

Solar water splitting by Doping-treated $BiVO_4$

Won Jun Jo*[1], Ph.D., Karen K. Gleason[2], Ph.D., Jae Sung Lee[3], Ph.D
Lawrence Berkeley National Lab, South Korea

Cost-effective solar fuel generation requires suitable photocatalysts for artificial photosynthesis. To develop such appropriate photocatalysts, their atomic structure control is of primary importance since their functionalities (e.g., electronic band frame, electric properties, kinetics, etc.) are governed by their atomic structure. In this regard, $BiVO_4$'s atomic structure has been engineered via P^{5+} doping and In^{3+}/Mo^{6+} dual doping. The significantly enhanced photo-responsive characteristics of doping-treated $BiVO_4$ have been studied within experimental and theoretical domains.

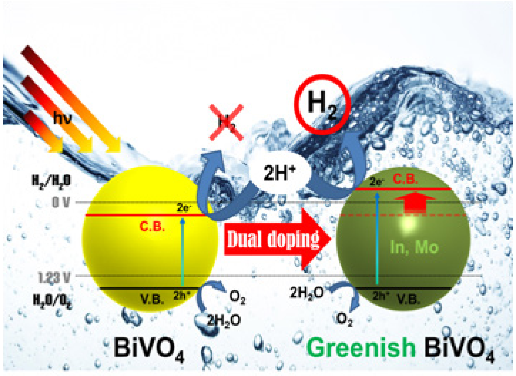


Fig. 1. Enhanced photocurrent by phosphate doping into monoclinic $BiVO_4$ under figure 1

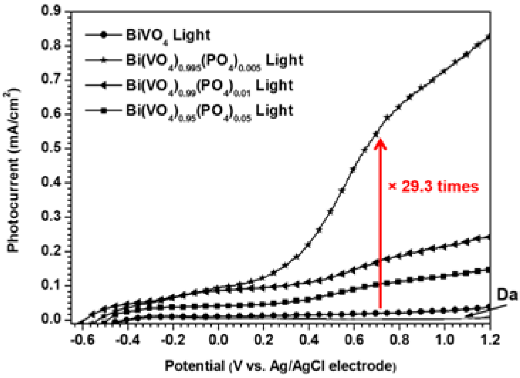


Fig.2. Overall water splitting reaction by In^{3+}/Mo^{6+} doped $BiVO_4$ under fig 2

Specifically, to reduce the charge-transfer resistance of monoclinic (m-) $BiVO_4$, phosphorous was doped into its vanadium sites for the first time through VO_4 and PO_4 oxoanion exchange. As a result, the charge-transfer resistance was significantly reduced, and thus solar-to-hydrogen efficiency was enhanced up to 29.3 times, as Figure 1 shows. Notably, this brand-new oxoanion exchange technique can be applied to other various VO_4-based semiconductors to improve their electronic, catalytic, and photochemical properties.

Thanks to the phosphorus doping study, it is possible to make m-$BiVO_4$ function as an excellent photocatalyst for water oxidation ($2H_2O(l) + 4h+ \rightarrow O_2(g) + 4H+$) under visible light. However, its conduction band is located at a more positive potential than that of proton reduction (0 VRHE at pH 7, RHE: reversible hydrogen electrode), it is still incapable of evolving H_2 ($2H+ + 2e- \rightarrow H_2(g)$). This is why overall water splitting ($2H_2O(l) + 4h+ + 4e- \rightarrow O_2(g) + 2H_2(g)$) under visible light irradiation over $BiVO_4$-based photocatalysts has never been fully achieved.

To meet this challenge, the band edges of m-$BiVO_4$ was engineered by simultaneously substituting In^{3+} for Bi^{3+} and Mo^{6+} for V^{5+} in the host lattice of monoclinic $BiVO_4$, which induced partial phase transformation from pure monoclinic $BiVO_4$ to a mixture of monoclinic $BiVO_4$ and tetragonal $BiVO_4$. This In^{3+}/Mo^{6+} doped $BiVO_4$ has a slightly larger band-gap energy (Eg ~ 2.5 eV) than usual 'yellow' monoclinic $BiVO_4$ (Eg ~ 2.4 eV), as supported by the unique color change to green, and higher (more negative) conduction band edge (− 0.1 VRHE at pH 7) than $^{H+}/H_2$ potential (0 VRHE at pH 7). Consequently, as Fig. 2 displays, the In^{3+}/Mo^{6+} doped $BiVO_4$ is able to split water into H_2 and O_2 under visible-light irradiation without using any sacrificial reagents (e.g. CH_3OH or $AgNO_3$). This outcome is the first example of a pure water-splitting photocatalyst responding to visible light without any noble-metal cocatalyst.

Audience Take Away:

- The basic principle of solar water splitting: The audience can use this for their teaching.
- How to dope phosphorus into the vanadium sites of $BiVO_4$ using the oxoanion exchange technique: The audience can expand their research via the oxoanion exchange technique.
- The underlying mechanism of In^{3+}/Mo^{6+}doping-induced domino effect from phase transition to band edge engineering: Based on my experimental and theoretical studies, the audience will figure it out how In^{3+}/Mo^{6+}doping induces crystal-structure phase transition, which triggers electronic band structure engineering. Then, they can take advantage of their understandings to improve their research as well as teaching.

Biography

Won Jun Jo received a B.Sc. and Ph.D. in chemical engineering from POSTECH and MIT, respectively. He then joined the LBNL where he is currently a postdoctoral research fellow. His research interests encompass photocatalysis, photovoltaics, and electrochemistry. His work focuses on material innovations for the establishment of renewable energy technologies, including artificial photosynthesis, solar cells, and fuel cells. He is the recipient of MRS Graduate Student Award (2016 and 2017), Dow Chemical Travel Award (2015), AIChE Doh Wonsuk Memorial Award (2014), Samsung Fellowship (2011), Talent Medal of Korea (2010), UN Peace Medal for his military peace-keeping operations in Lebanon (2009), GE and Fulbright Fellowship (2006), Korea Presidential Science Fellowship (2004), etc.

Oxidation of sulfur dioxide to sulfur trioxide over V_2O_5/TiO_2 catalyst and sulfur balance

Tingyu Zhu*, Ph.D., Yuran Li, Ph.D., Jin Xiong
National Engineering Laboratory for Cleaner Hydrometallurgical Production Technology, Institute of Process Engineering, Chinese Academy of Sciences, China.

The oxidation of sulfur dioxide (SO_2) to sulfur trioxide (SO_3) is undesirable during the selective catalytic reduction (SCR) of nitrogen oxides (NO_x) found in the flue gas of power plants. Sulfur trioxide has a toxicity over ten times than that of SO_2 and is highly corrosive, resulting in corrosion of equipment and pollution of the environment. The objectives of this research are to establish the fundamental kinetics and mechanism of SO_2 oxidation over supported V_2O_5/TiO_2 catalyst and establish sulfur balance, then, use these insights to propose a basic theory for collaboratively controlling SO_3 emissions. A series of supported V_2O_5/TiO_2 catalysts were prepared with various V_2O_5 contents: 0.5%, 1%, 1.5%, 3%, 4% and 5%. Raman spectroscopy is used to determine the coordination of surface species. Isolated vanadia species were dispersed on the TiO_2 surface as Ti-O-V bonds at VO_x coverage below the monolayer. Sulfur dioxide temperature-programmed desorption and in situ diffuse reflectance infrared Fourier transform spectroscopy were conducted to study the interaction between SO_2 and V_2O_5/TiO_2. It was found that Ti-O-V was demonstrated to play a critical role in the SO_2 adsorption and oxidation. A possible reaction mechanism of SO_2 oxidation over V_2O_5/TiO_2 catalyst was established in this study. The turnover frequency for SO_2 oxidation was very low, approximately 10^{-5} s^{-1} at 320°C. Over the range of conditions studied, the rate of SO_2 oxidation is zero-order in oxygen and first-order in SO_2, and the apparent activation energies for SO_2 oxidation was obtained. The decrease of SO_2, the gaseous SO_3 and the sulfate deposited on catalyst surface were to be quantified by Fourier transform infrared spectrometer (FTIR), PENTOL SO_3 analyzer and ion chromatography (IC), respectively. Then, the sulfur balance was established.

Audience Take Away:

- Facilitate the design of SCR DeNO$_x$ catalysts with minimal sulfur dioxide oxidation activity.
- Instruct conditioning the flue gas parameters to restrict the SO_3 formation.
- Prevent the poisoning of the catalyst caused by the deposition of ammonium sulfate.

Biography:

Professor Tingyu Zhu obtained his doctor degree in chemical engineering from the Institute of Coal Chemistry, Chinese Academy of Sciences. His research interest includes: combined removal of SO_2, SO_3, NO_x and Hg from coal-fired flue gas, collaborative control of multi-pollutants (PM/SO_2/NO_x /Dioxins) in sintering gas, multiple pollutants control technology using activated carbon for the coke-oven flue gas, et al. He is the deputy director of Beijing Engineering Research Center of Process Pollution Control, the Member of Innovation Excellence Center for Urban Atmospheric Environment of CAS. He published the monograph, Emission Control Technologies and Engineering Applications for Sintering Flue Gas, and published many peer-reviewed papers, and got several patents. He has been twice honored with the second prize of Environmental Protection Science and Technology, awarded by Ministry of Environmental Protection of The P.R. China in 2010 and 2015.

High performance catalysts for hydrogen &oxygen evolution reactions and water electrolysis

Zhifeng Ren*
Department of Physics and TcSUH, University of Houston, USA

Water electrolysis for hydrogen production is very important but not efficient due to high cost of the noble metal containing catalysts or low performance of the non noble metal based catalysts. Water electrolysis involves hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). HER catalysts are normally good only in acid and OER catalysts only in base, but none of them are good in both acid and base or bifunctional for both HER and OER, which makes the overall water electrolysis not efficient. We recently discovered some catalysts better than the noble metal containing ones in both acid and base, which made the overall water electrolysis more efficient than the noble metal containing catalysts. In this talk, I will present a few examples on our recent discovery on new catalysts to achieve water splitting for current density larger than 500 mA/cm^2 at less than 1.7 V.

Photo - oxidation reaction scheme triggered by the nozzle of submerged plasma torch

Florent Lemont*, M.Marchand, D.Milleli, L. Ruffel, T. Barral
CEA, DEN, DE2D, SEVT, LPTI, F-30207 Bagnols-sur-Cèze, France

The French Atomic Energy Commission develops innovative processes for the treatment of radioactive organic liquids. One of them, named ELIPSE, involves a thermal plasma working under a water column, which ensures the cooling, the filtration and the scrubbing of the gases coming from the degradation. Studies in progress deals with the ability of the ELIPSE process to destroy the pure organic liquids and then to reduce the amount of organic matter remaining in the aqueous solution by means of the thermal or radiative properties of plasma.

Preliminary test have shown how efficient the process is for the destruction of the organic liquids when they are directly fed in the plasma hearth. Extensive researches have been performed to assess the ability of the submerged plasma to destroy the remaining organic matters either by reinjecting them with the aqueous solution into the plasma or by using the UV ray coming from the plasma itself. A comparison of the experimental results obtained with various mechanisms proposed by the work carried out highlighted that this UV radiation could, by excitation of water molecules, produce radicals OH° which may either dimerise to produce hydrogen peroxide H_2O_2, or react with organic substances present. The calculation of an activation energy of $8.5 \pm 0.9 kJ.mol^{-1}$ during the experiments shows that these radicals OH° act directly after having been formed which explains a low H_2O_2 content stability when the solution contains organic compounds. Thus, this photo-oxidation taking place in the water column could be used to improve the destruction of residual organic matter in the solution by maintaining the plasma after processing a given amount of organic liquids. It could also be used to help the decontamination of various aqueous solutions coming from different industrial or medical activities.

Biography

HDR – Head of Innovative Processes Laboratory
Scientific expert – Processes and High Temperature Chemistry
Atomic Energy Commission
CEA – Marcoule BP 17171 30207 Bagnols-sur Cèze Cedex
Academic Title:

- HDR (Accreditation to supervise research) – February 2007 – Materials and Process Engineering – Grenoble
- Doctor of "Institut Nationale Polytechnique de Grenoble" Sciences and Materials Engineering.
- Diploma of Advanced Studies – Condensed and diluted matter – institute Nationale Polytechnique de Grenoble
- Engineering degree from "Ecole Nationale Supérieure de l'Energie et des Matériaux"

Scientific Activities:

- Head of Innovative Processes Laboratory – French Atomic Energy Commission
- Scientific expert – Processes and High Temperature Chemistry
- PhD – Thesis director
- Teacher at the Engineering school of Albi
- Teacher at the Master of Science of Pau
- Teacher at the master of Science of Marseille
- Member of "Program Advisory committee" of International Conference on Thermal Treatment   Technologies and Hazardous Waste Combustor
- Member of Scientific Committee of International Conference on Engineering for Waste and Biomass Valorization
- Member of Scientific Committee of SFGP
- Scientific Advisor CIRP (Taiyuan – Chine)
- Referee - International Journal of Hydrogen Energy
- Referee - International Journal of Environmental Engineering Science
- Referee - International Journal of High Temperature Materials and Processes
- Referee - International Journal of Hazardous Materials
- Referee – Nuclear Technology
- Session Chair in several conferences (Waste Eng, WHTC, IT-3)

OsO_4 catalysed oxidation of atropine sulphate monohydrate with chloramine-T in alkaline medium: Delineation of mechanistic pathways and kinetic modelling

Nirmala Vaz*, Ph.D
Jyoti Nivas College Autonomous, India

Atropine sulphate monohydrate(ASM) is a prominent anticholinergic drug . In the present research, osmium tetraoxide(OsO_4) catalysed oxidation of ASM with chloramine-T (CAT) in NaOH medium has been kinetically investigated at 303K. The reaction rate exhibits a first – order dependence on each [CAT] and [ASM] and fractional – order dependence on both [NaOH] and [OsO_4] . Atropine N-oxide was identified as the oxidation product of ASM by spectral data. Effects of added p-toluenesulfonamideandNaCl, varying dielectric constant and ionic strength of the medium on the rate of the reaction have been investigated. Activation parameters for the overall reaction and also with respect to OsO_4 catalyst were deduced. It was found that OsO_4 catalysed reaction is about fourteen-fold faster than the uncatalysed reaction. It clearly justifies the use of OsO_4 as a catalyst for the present redox system. Based on the experimental results detailed mechanistic pathways and kinetic modelling have been carried out.

Audience Take Away:

- The present paper on oxidation-kinetic study of Atropine sulphate monohydrate(ASM) (anticholinergic drug) will throw some light on the mechanistic pathways and the fate of the drug in the biological system
- It is also expected to give an insight into the interaction of metal ions with redox systems.
- The proposed kinetic study will give an impetus, as the substrate is a prominent anticholinergic drug
- The outcome of these work will have immense applications in pharmaceutical industries from the kinetic and mechanistic view points.

Biography

- Dr. Nirmala Vaz is a Professor & Head of Chemistry and Director of Research for IGNOU (Indira Gandhi National Open University)
- Completed her B.Sc., M.Sc., B.Ed., M.Ed, and M.Phil from the University of Pune. Ph.D. in 2004 from the Bangalore University. Recently completed her Post Graduation in Event Management from XIME.
- Member of University Grant Commission (UGC) the apex body for higher education.
- Member of Board of Studies (BOS) in Chemistry and member of the Board of Examination (BOE) for the Mysore University.
- Academic council member of Indira Gandhi National Open University.
- Member of the Indian Science Congress Association
- Member of the Association of Kineticists of India
- Member of the Indian Council of Chemists
- The Indian Congress Association, Calcutta
- Chemical Research Society of India, IISc Bangalore
- Research experience in the field of Physical and Organic chemistry for over two decades.

Awards:

- Young scientists' award was given for the innovative and novel method of preparing 3-benzylcoumarins and their derivatives with varied substitution patterns and its benzoderivatives by using the Wittig approach in 1990 by the Indian Science Congress.
- Lifetime Achievement Award in Science for the contribution and achievement in the field of Chemistry was given by the Board of Management of the Venus International Foundation based on the VIWA 2017 Expert Committee Report and Apex Committee Recommendations on 4th March, 2017.
- Published 29 papers in National and International Journals.
- Research collaborations with:
  1. Dr. A Radhakrishna, Joint Director, Shriram Institute for Industrial Research, Bangalore.
  2. Dr. Venkat, Hindustan Unilever, Bangalore,
  3. Completed Minor Research and Major Research Project from University Grant Commission (UGC).
- Presented 81 papers at National and International Conferences.

- Invited to give a talk on Oxidation of purine and pyrimidine base components of nucleic acids by bromamine-B in aqueous alkaline medium at Belgium.
- Visited several foreign Universities to name a few: University of Cambridge, Portsmoth, Manchester, University of Huddersfield, UK and Pisa University.
- Examiner for setting CET, NET and UPSC question papers for India, SET question papers for University of Jammu, Pune, Assam, Bharathiar and Osmania University.
- UGC observer for NET exam for Gujarat, Portblair, Calicut, Cochin, Thiruvananthapuram, Bangalore, Bharathiar, Chennai, Pune, Tirupathi, Mangalore, Maduri Kamraj and Osmania Universities.
- Organised several National and International Conferences.

Novel nickel-palladium catalyst for hydrogenation aromatic compound

Ying-Chou Su*, Chuh-Yung Chen, Cheng-Chien Wang
National Cheng Kung University, Taiwan

The novel hydrogenation catalysts, palladium (Pd) immobilized in nickel wire (Pd/Ni_w), were prepared via exterior magnetic field following reduction reaction in this study. Characteristic and the morphology were identified by using X-ray diffraction and scanning electron microscopy, respectively. Amount of Pd in Pd/Ni_w was in the range of 13 wt.% to 15 wt.% from inductively coupled plasma-atomic emission spectroscopy measurement. The particle size of Pd in Pd/Niw was ca. 20-100 nm via high-resolution transmission electron microscopy observation. The saturation magnetization of Pd/Ni_w catalyst was 37.25 emu/g after PPMS-16T measurement. Furthermore, as the Pd/Ni_w was acted as catalyst for the hydrogenation of bis (2-ethylhexyl) phthalate (DEHP), 100% conversion of DEHP was obtained at 180°C and 1000 psi. At the optimum condition 100% conversion of dimethyl terephthalate (DMT) and bisphenol A (BPA) were also achieved This novel hydrogenation catalysts has easy manufacture with low cost and has potential for commercialization in future.

Audience Take Away:

- We can turn some aromatic compound to saturated structure completely.
- The catalyst in this study has industrial potential.
- The synthesis method is simple.

Biography

My name is Su Ying-Chou. I'm twenty-five years old and studying in PhD program in National Cheng Kung University. I have great interest in industrial application, polymer science and catalyst especially. Riding motorcycle to travel is my favorite.

Silica-immobilized bifunctional L-prolinol organocatalysts: Stereoselective Michael addition in heterogeneous environment

Jiri Tuma*, Michal Kohout, Ph.D
University of Chemistry and Technology Prague, Czech Republic

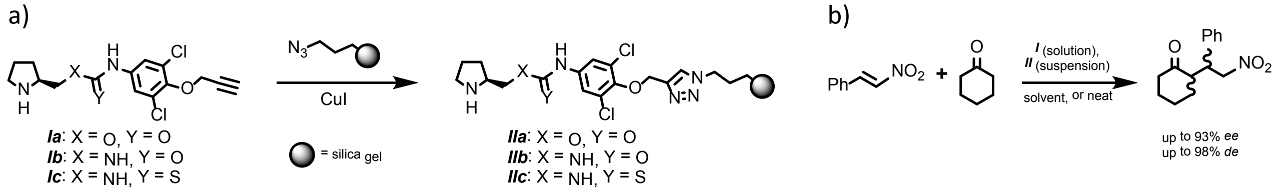
Stereoselective Michael additions represent the staple reactions in the field of organic synthesis. The stereoselectivity of the reactions is usually mediated by bifunctional catalysts, which activate both the electrophile and nucleophile at the same time. One of the many challenges in the field is to develop a suitable heterogeneous catalytic system, which provides an easy way of regeneration of the catalyst by standard filtration.

Herein we present a series of bifunctional L-prolinol based organocatalysts (Ia-c), which have also been immobilized via click-reaction to azidopropyl-modified silica solid phase yielding heterogeneous catalysts (IIa-c; Scheme 1a). The synthesis as well as the catalytic properties of both the homogeneous (Ia-c) and the heterogeneous (IIa-c) catalysts in a selected model Michael addition of cyclohexanone and β-nitrostyrene (Scheme 1b) will be discussed.

The experiments showed a very high impact of the solvent polarity on both yield and stereoselectivity. The less polar solvents used (hexane, toluene) delivered the highest conversion and stereoselectivity, whereas the polar solvents (dichloromethane, methanol) were significantly less effective. Nevertheless, the best results were achieved in neat cyclohexanone (up to 93% ee; up to 98% de).

Furthermore, the catalysts were packed in-house into stainless steel columns (150x4 mm) and tested in a continuous flow reaction setup, which does not require the filtration step during the catalyst regeneration cycle and thus enables a quick and easy regeneration by simple washing.

A general preparation strategy of silica-based heterogeneous organocatalysts, their catalytic activity, properties, easy tunability and their potential for scale-up applications will be discussed.



Scheme 1: a) Structure of the studied organocatalysts; b) Model Michael addition

Audience Take Away:

The presentation will focus on explanation of the methodology used for preparation and study of the properties of the synthesized heterogenous catalysts. The audience will be familiarized with these key points:

- Why is silica a suitable solid support for organocatalysts
- How to synthesize silica-based heterogenous organocatalysts
- How to study the properties of the catalysts and how to easily tune them
- Why are silica supported organocatalysts perfectly suitable for large scale applications

Biography

Jiri Tuma is a Ph.D. candidate currently working on his thesis in a newly established work group of Dr. Michal Kohout at the Department of Organic Chemistry, UCT Prague, Czech Republic. His research is mainly focused in the field of stereoselective organocatalysis and chiral separation. In his work he aims at design of various bifunctional compounds based on L-prolinol, resp. their derived silica-supported analogues and their applications as either heterogeneous organocatalysts, or chiral selectors for enantiomeric separation in HPLC. His interest in this topic mainly stems from his experience with the silica-supported materials gained during his stay at the University of Vienna in the group of prof. Wolfgang Lindner.

Nanocrystalline synthetic ferrihydrite as a catalyst for Fischer-Tropsch synthesis

Dong Hyun Chun*, Ph.D., Geun Bae Rhim, Ji Chan Park, Ph.D., Ho-Tae Lee, Ph.D., Jung-Il Yang, Ph.D., Heondo Jung, Ph.D., Heon Jung, Ph.D
Korea Institute of Energy Research, Republic of Korea

Fischer-Tropsch synthesis (FTS) has been considered a promising way for conversion of syngas (H_2 + CO) into synthetic liquid fuels and/or high value-added chemicals. Iron-based catalysts are highly promising for FTS due to their high activity and low cost. In general, the as-prepared iron-based catalysts are inactive for FTS and barely activated in usual FTS conditions. Therefore, they must be pre-activated in CO or low-pressure syngas ($\leq$ 0.3 MPa) to change the as-prepared catalysts into active iron carbide species prior to the reaction, which is disadvantageous considering operation efficiency and facility simplification. Ferrihydrite is a nanocrystalline iron-oxyhydroxide, which is abundantly present in nature and, also, can be synthesized in iron-containing aqueous environments. Due to its small crystallite size and high surface area, the ferrihydrite has high potential as a catalyst for iron-catalyzed reactions such as FTS. But, only few studies about ferrihydrite as a FTS catalyst has been performed. In this study, we report a novel characteristic of synthetic ferrihydrite as a catalyst for FTS. Even though no activation pre-treatment was carried out, the siliceous ferrihydrite-based catalysts promoted by Cu and K showed high catalytic performance as they were spontaneously activated during the initial period of reaction. The performance of the spontaneously activated catalysts was comparable to that of the pre-activated catalysts in terms of catalytic activity and even higher than that of the pre-activated catalysts in terms of C^{5+} selectivity. Furthermore, we successfully demonstrated the spontaneous activation of ferrihydrite-based FTS catalysts in a pilot-scale slurry bubble column reactor (5-15 bbl/d).

Audience Take Away:

- Understanding of Fischer-Tropsch synthesis and catalysis
- Facile synthesis of massive nanocrystalline catalysts based on crystallographic understanding
- Reduction and carburization behavior of ferrihydrite-based catalysts
- A story of catalysis R&D from lab-scale study to pilot-scale demonstration

Biography

Dong Hyun Chun Current position is Principal Researcher: Clean Fuel Laboratory, Korea Institute of Energy Research (Republic of Korea). He worked as Associate Professor in Department of Advanced Energy and Technology, University of Science & Technology (Republic of Korea). He completed his Doctor of Philosophy: Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (Republic of Korea), 2003–2007, Master of Science: Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (Republic of Korea), 2001–2003 and Bachelor of Science: Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (Republic of Korea), 1997–2001.

Carrier to Date:

Senior Researcher: Clean Fuel Laboratory, Korea Institute of Energy Research (Republic of Korea), 2007–2016.

Guest Scientist: Fuel Cell Materials Center, National Institute for Materials Science (Japan), 2004–2006.

A novel heterogeneous catalyst from red cotton flowers and its applications

Hitesh Barman*[1], Ph.D., Mostafa Momin[2], Ph.D., Dibakar Chandra Deka[2], Ph.D
[1]Rangia College, Rangia, Assam, India
[2]Gauhati University, Guwahati, Assam, India

Naturally fallen red cotton flowers are available in plenty in North-East of India, especially in Assam. It is known that these flowers are traditionally being used to prepare cleansing agents in some parts of the state. Our investigation focused on converting these flowers into a catalyst for industrial applications. The catalyst prepared in our laboratory has been successfully tested and used in transesterification reactions, and it is found that the catalyst is quite efficient in the process of biodiesel preparation from vegetable oils. The presentation will describe the methodology for the preparation of the catalyst, studies done on its efficiency in transesterication reations including biodiesel preparation and the reusability of the catalyst.

Audience Take Away:

- Scientific use of traditional knowledge for economic benefits of the society.

Biography

Dr. Hitesh Barman is presently working as an Associate Professor in the Department Of Chemistry, Rangia College, Rangia, Assam, India. Educated in Gauhati University for his M.Sc. and Ph.D., Dr. Barman is serving the college for the last 24 years. He is an active member of All India Association of Chemistry Teachers and The Society for Chemical Education Assam. Apart from his normal activity in the college, he is also devoting his time in popularization of Chemical Education.

Study of the use of ceramic membranes coated with Copper and Zirconium oxides in the oxidation of Carbon monoxide

María Dolores Sosa Lucio*, A. Chico
Escuela Politécnica Nacional, Ecuador

The presentation will deal with the development of ceramic membranes coated with copper oxide and zirconium (CuO and ZrO_2) oriented to the oxidation of carbon monoxide (CO) to carbon dioxide (CO_2). The ceramic membranes were prepared through the replica technique by impregnation of polyurethane matrices with slurries prepared using mixtures on dry basis of Ecuadorian clay, feldspar and quartz based on a Simplex Centroide design. The ceramic membranes were subjected to a heat treatment with three different levels of final sintering temperature and the response variables studied were porosity and compressive strength. According to an statistical analysis it was determined that the formulation of slurry and temperature that maximized these properties, with values of 91.4 % of porosity and 0.1 MPa of resistance, were the composition of 66, 5 %; 20 % and 13.5 % of clay, feldspar and quartz respectively and the temperature of 1 135 ° C. With these conditions there where prepared ceramic membranes that were coated with suspensions of CuO a/o ZrO_2 in different dry basis compositions according to a Simplex Latice design. The reduction capacity of the CuO a/o ZrO_2 oxides as coatings of the ceramic membranes was evaluated through a H_2-TPR and it was determined that loads of 6.3 % ZrO_2 and 1.7 % Cu per gram of ceramic membrane to 6.1 % Cu without ZrO_2 presented a reduction profile with a maximum temperature between 258 and 270 °C. Finally, a CO-TPR was performed on the coated membranes that presented a reduction profile and it was determined that a load of 6.1 % Cu obtained the highest CO_2 production with a value of 16,02 cm^3 CO_2/g and a reduction temperature of 236 °C. It was determined that the oxidation of CO was influenced by the amount of CuO in the coating but the presence of ZrO_2 influenced the temperature of oxidation also.

Audience Take Away:

- During the presentation it will be explained simple and economical techniques to develop structured ceramic supports applicable to catalytic processes as oxidation.
- The work on exhibition will propose an alternative to the utilization of clay materials oriented only to the development of conventional ceramics for its application in the obtaining of ceramic supports with catalytic applications. It will be explained also the properties of the support developed.
- The present work deals with the potential application of metal oxides such as CuO and ZrO_2 which are abundant materials in nature as an alternative to the unique application of platinum in the oxidation of carbon monoxide from the incomplete combustion of the engines.
- The paper explores the direct use of metal oxide coatings in ceramic supports, such as CuO and ZrO_2, rather than the traditional application of copper and zirconium salt precursors for the oxidation of carbon monoxide.
- The presentation explains the possible interactions of CuO and ZrO_2 that allows the oxidation of carbon monoxide.

Biography

Maria Sosa is a student of the Faculty of Chemical Engineering and Agroindustry of Escuela Politécnica Nacional in Quito, Ecuador, and she has been working on her thesis to obtain the title of Chemical Engineer. She has a specialization in Polymers at the Escuela Politécnica Nacional and has been working with ceramic materials and oxidation systems in automobile exhaust pipes in order to reduce the emissions of carbon monoxide. She developed her thesis based on the use of Ecuadorian raw materials from low exploited sites for its application in oxidation processes with the use of copper and zirconium oxides.

Deactivation kinetics of Pt-Sn/Al2O3 catalyst in the dehydrogenation of light alkanes

Saeed Sahebdelfar*, PhD
Petrochemical Research and Technology Co., Iran

The catalytic dehydrogenation of light alkanes (propane and isobutane) has received much attention for on-purpose production of the corresponding olefins. The rapid deactivation of the catalyst due to coke formation is a major technical problem of the reaction which complicates its industrial implementation. Consequently, catalyst deactivation is an important issue in the development of the catalyst and process for alkane dehydrogenation. In this work the kinetics of deactivation of Pt-Sn-K/Al2O3 catalyst in dehydrogenation of propane and isobutane was studied. A power-law rate was used for the forward and reverse main reactions and a concentration-dependent rate expression incorporating all the main reacting species was used for catalyst deactivation. The long-term catalyst performance test runs were performed in a fixed-bed reactor under the representative commercial operating conditions (575 and 620 °C for isobutane and propane, respectively). The reactor outlet was analyzed by an on-line GC for C1-C4 hydrocarbon products. During the first 100 h on stream, the catalyst exhibited significant deactivation in both reactions although the selectivity to the corresponding olefins remained fairly constant. The parameters of the kinetic models were estimated by non-linear least-squares method using numerical optimization. Favorable fits were observed for both propane and isobutane conversion data. According to the relative magnitudes of the rate constants of deactivation, it was concluded that the deactivation mechanism is chiefly of consecutive type for propane dehydrogenation and of parallel type for isobutane dehydrogenation. Hydrogen showed high coke removing potential thereby it could be used in relatively low concentrations to increase catalyst lifetime.

Audience Take Away:

- A concentration-dependent kinetics for deactivation of Pt-based catalysts is applicable in the dehydrogenation of light alkanes.
- The deactivation mechanisms of propane and isobutane dehydrogenation over Pt-based catalysts are of consecutive and parallel types, respectively.
- Hydrogen is an effective feed additive to extend the lifetime of Pt-based dehydrogenation catalysts.

Biography

Saeed Sahebdelfar earned his PhD degree in Chemical Engineering from Sharif University of Technology. He is currently the head of Catalysis Research Group in Petrochemical Research and Technology Company. His research interests are in the fields of natural gas conversions and environmental technologies. His main research activities are focused on catalytic oxidative coupling of methane, paraffin dehydrogenation and carbon dioxide utilization. He published more than 60 scientific papers in international journals.

Observation of dynamic Cu redox behavior in MFI-zeolite during NH_3-SCR using in-situ XAFS

Kakuya Ueda*, Junya Ohyama, Ph.D., Atsushi Satsuma, Ph.D
Nagoya University, Japan

In order to enhance the activity of selective catalytic reduction of NO_x by NH_3 (NH_3-SCR) using Cu ion-exchanged zeolite catalyst, observation of Cu species in zeolite structure during NH_3-SCR reaction have been paid attention. Several studies have been revealed the state of Cu species in equilibrium conditions using in-situ XAFS, however, dynamics of Cu species under transient conditions have not been discussed. We carried out in-situ XAFS study of the dynamics of CuII/CuI redox behavior. We measured XAFS spectra under reduction (NH_3–NO) and oxidation (NO–O_2) conditions, and estimated CuII/CuI ratio using linear combination fitting of Cu K-edge XAFS. In a flow of NH_3–NO, CuII species linearly decreased dependent on time. On the other hand, CuII species increased by two steps in a flow of NO–O_2. The first oxidation step was much faster than the second one. These results indicated the presence of two types of CuI species, which were different oxidation susceptibility, in zeolite matrix. The increase in the Cu ion-exchange ratio enhanced the ratio of easily oxidized Cu species and NOx reduction rate per Cu atom during NH_3-SCR. We concluded that the more Cu-MFI contained easily oxidized Cu species, the higher Cu-MFI exhibited the NH_3-SCR performance.

Audience Take Away:

- Cu oxidation/reduction behavior in zeolite matrix
- Reaction mechanism of NH_3-SCR
- Strategy of catalyst design to enhance NH_3-SCR performance

Biography

2014 - Bachelor of Engineering, Nagoya University, Nagoya

2016 - Master of Engineering, Nagoya University, Nagoya

2016 - Doctor course in Engineering, Nagoya University, Nagoya

Research interest:

Development of automotive and fuel cell catalysts using base-metal oxide catalysts; Investigation of reaction mechanism using in-situ and operando spectroscopies

Poster Presentations

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Supported silver nanoparticles for catalytic reduction processes

Lee D. Wilson*, Ph.D., Mohamed H. Mohamed, Ph.D
Department of Chemistry, University of Saskatchewan,Canada

Biopolymers and their composites were used as supports for the preparation of silver-based nanoparticles (Ag-NPs). The supported Ag-NPs were structurally characterized using a range of methods such as Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), NMR spectroscopy, transmission electron microscopy (TEM), thermogravimetry. The adsorption properties of the biopolymers and composites in presence and absence of Ag-NPs were evaluated using a dye-based method to assess the textural properties and surface accessibility of active adsorption sites of these materials. The catalytic properties of the supported Ag-NPs were studied by examining the reduction of 4-nitrophenol in the presence of sodium borohydride (cf. graphic abstract). A systematic study of the reaction kinetics for this process provides a detailed understanding of the kinetic pathway for the reduction of 4-nitrophenol.

Audience Take Away:

- New approaches to materials design with catalytic properties
- The role of morphology and surface adsorption properties in catalysis
- The use of biopolymers for anchoring silver nanoparticles
- Adsorption based processes are ubiquitous in catalysis and the ability to design improved catalyst materials is a topic of ongoing research. This research will contribute to facile strategies on how to modify the surface biopolymer materials for a range of organocatalysis and materials science & engineering applications.

Biography

Dr. Lee D. Wilson (PhD) is an Associate professor in the department of chemistry at the University of Saskatchewan with research interests in physical chemistry and macromolecular systems in aqueous media. Wilson's research is in the area of Physical Chemistry, Materials & Environmental Science where current efforts are being directed at the development of new types of macromolecular materials and their structure-function relationships that relate to adsorption phenomena. Modified biopolymer materials will have a tremendous impact on areas such as green catalysis, aquatic environments, biotechnology, medicine, chemical delivery/separation systems, and sorbent materials for water purification

Selective conversion of methanol to para-xylene over Zn doped core-shell zeolite catalyst

Koji Miyake*, Kaito Ono, Masahiro Nakai, Yuichiro Hirota, Yoshiaki Uchida, Norikazu Nishiyama
Osaka University, Japan

p-Xylene is the most important isomer of xylenes for chemical industries since it can be converted into terephthalic acid which is one of the precursors of polyethylene terephthalate (PET). Currently, p-xylene has been mainly produced from petroleum resources through multistep processes including reaction and separation processes.

There is a serious problem in these processes; petroleum resources will be exhausted in the future. Furthermore, there is another problem that separation of p-xylene from xylenes needs huge energy due to the repetitive adsorptive separation and isomerization. Thus, more simple processes to produce p-xylene from nonpetroleum resources is strongly desirable. Direct p-xylene synthesis from methanol is one of the most promising candidates to solve both problems.

In this study, We designed Zn ion doped ZSM-5/silicalite-1 core-shell zeolite catalyst (Zn/ZSM-5/S). We confirmed that the prepared catalyst was the Zn doped core-shell zeolite by XRD, XPS, ICP, N_2 adsorption measurements and FE-SEM observations. On methanol to para-xylene (MTpX) over the core-shell catalyst, p-xylene yield was 40.7 C-mol% and para-selectivity (para-xylene selectivity in xylene isomers) was higher than 99 C-mol% owing to suppressing the undesired isomerizations of xylenes on the acid sites on the external surfaces, which substantially exceeds the other results reported in the literature. In addition to the high yield and selectivity of p-xylene, the coke deposition rate of the fabricated core-shell catalyst was slower than conventional zeolite due to suppressing the extreme coke formation by the acid sites on the external surfaces, which leads to prolonged catalyst lifetime.

Hence, this work disclose that Zn doped core-shell zeolite catalyst showed excellent catalytic performances on MTpX, which provides the new direction for the production of p-xylene via sustainable routes.

Audience Take Away:

- Fabrication of core-shell zeolite catalyst
- Location of active sites on the zeolite
- New production route of p-xylene for the sustainable future

Biography

Mr. Koji Miyake was received the B. E degrees in engineering science from Osaka University, Osaka Japan, in 2015, he also received the M. E degrees in engineering science from Osaka University, Osaka Japan, in 2016. He is now a doctor course student of Osaka University. Due to his high quality research, he received “Award for graduate school of engineering science” which is given to the most valuable student in research activities. His research interest includes synthesis of porous materials and heterogeneous catalysts.

Reusable Cu catalysts dispersed on two types of supports and its application in the [3+2] cycloaddition in water: Revere phase silica geland thermoresponsive poly (NIPAM-co-4-VP)

Minkyung Lim*, Heejin Lee, HaKjune Rhee
Hanyang university, The republic of Korea

Two types of solid supports synthesized for the preparation of heterogeneous catalysts. 2-Pyridinecarboxaldehyde ligand was anchored on commercially available revere phase 3-aminopropyl-functionalized silica gel followed by Cu metal immobilization. Amino-functionalized reverse phase silica with alkyl end capped amino groups was used to induce hydrophobic behavior in the polar silica support. Poly(NIPAM-co-4-VP) was synthesized from N-isopropylacrylamide and 4-vinylpyridine with a 1:1 monomer ratio and followed by Cu metal immobilization. Poly(NIPAM-co-4-VP) undergoes a phase transition at the low critical solution temperature with a change from the hydrophilic to the hydrophobic core in a hydrophilic solvent. These properties of the catalysts enabled the [3+2] cycloaddition in water and showed good results. These catalysts are stable in air and reusable over several times with negligible leaching of Cu metal. Various characterization methods including XPS, ICP, DSC, SEM, BET, 1H- and 13C-NMR, solid NMR are used to verify the efficiency of the catalysts.

Audience Take Away:

- From this presentation, they will learn how to synthesis new heterogeneous catalysts and the [3+2] cycloaddition using catalysts.
- They will be able to obtain information on the organic reaction in water using reverse phase silica catalyst and polymer catalyst with LCST behavior.

Biography

Minkyung, Lim majored in organic chemistry in the department of applied chemistry at Hanyang University. She is currently a Ph.D. student in the department of bionanotechnology at Hanyang University.

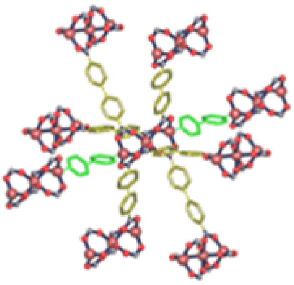
She is interested in organometallic catalyst and has published related papers. Her research is focused on the synthesis of new catalyst and the application of various organic chemical reactions in water by metals such as Pd, Au, Cu, etc.

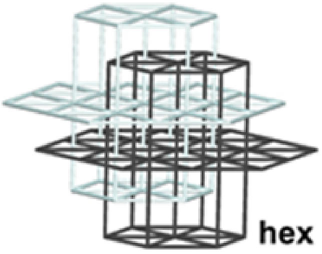
Trinuclear microporous coordination polymers as catalysts for oxidation of arylboronic acids into phenols

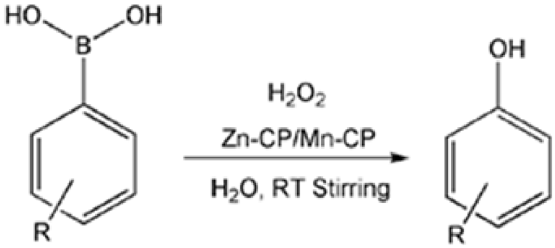
Sanchay Jyoti Bora*, Ph.D., Rima Paul
Pandu College, India

Two isostructural trinuclear coordination polymers (CPs) have been synthesized, characterized and successfully applied as robust heterogeneous catalysts for the oxidation of arylboronic acids into phenols with aqueous hydrogen peroxide (H_2O_2). The microporous CPs with formulation $[M_3(bpdc)_6(bipy)_2].2DMF.2H_2O$ [M = Zn and Mn] are analogous because these two species differ only on the basis of the metal ions present in them and may be termed as isostructural. Each structure consists of two crystallographically distinct M^{2+} (M_1 & M_2) centers that are connected via carboxylate bridges from six bpdc ligands, generating a trinuclear metal cluster, $[M_3(bpdc)_6(bipy)_2]$. Cluster representation of the structure resulted in the interpenetrated net of the rare hextopological type.

Various substituted aryl and hetero arylboronic acids $RB(OH)_2$ [R = phenyl, 3-trifluoromethyl, 4-cyanophenyl etc.] underwent ipso-hydroxylation smoothly at room temperature to provide corresponding phenols in excellent yields. The main advantages of this protocol are the aqueous medium reaction, heterogeneous catalytic system, and short reaction time with excellent yields. All these and other results will be discussed.







Audience Take Away:

- From this presentation, the audience will learn how to develop new synthetic strategies for material design with an aim towards the real-world applications. They will be convinced that the work presented herein is important, valid and relevant to them. The audience also gets a chance to interact with the presenter and share ideas on an informal basis. This may lead them to new and fruitful directions.
- Through this presentation, the presenter will share his research findings and experiences with the audience. Interested research students and scientists of the relevant field can adopt the strategies discussed in the presentation for their own work.
- The work discussed in the presentation may be extended further for a fruitful outcome by the other researcher as well.

Biography

Dr. Sanchay Jyoti Bora is an Assistant Professor in Department of Chemistry, Pandu College, Guwahati, Assam, India. He completed his Ph. D in Gauhati University, Guwahati , Assam. He has done his M. Sc in Chemistry (Inorganic Chemistry) with Bioinorganic Chemistry and Analytical Chemistry as special papers, Gauhati University, Guwahati, Assam and B.Sc in Chemistry (Honours), Physics and Mathematics, Dibrugarh University, Assam. Other Qualification include GATE : Graduate Aptitude Test for Engineering (GATE), 2003, Percentile Score: 86.79. NET : CSIR-UGC National Eligibility Test (NET), LS (Lectureship) June, 2003. NET : CSIR-UGC National Eligibility Test (NET), JRF-CSIR (Junior Research Fellow-CSIR) December, 2003. Research Projects are FASTTRACK, SERB, DST.

Development of new Pd(0) catalysts immobilized on silica-gel : Study of reactivity according to stationary phases for Suzuki-Miyaura coupling reaction in water

Jaeyoung Ban*, Heejin Lee, Hakjune Rhee
Hanyang University, South Korea

Typically, diverse organic reactions using heterogeneous catalysts are less reactive than those using homogeneous catalysts. Several functionalized supporting bodies have been developed to solve this problem. In this study, we have synthesized new supporting bodies using 3-aminopropyl functionalized silica-gels which are reverse phase and normal phase. To the supporting bodies obtained, Pd(II) was loaded on the silica-gel supporting bodies and Pd(0) catalysts were obtained through $NaBH_4$ reduction. Therefore, new heterogeneous palladium catalysts were synthesized. In addition, reusability was proven by recycle tests. By using these catalysts, Suzuki-Miyaura coupling reactions have been carried out in the aqueous system.

As a result, the reverse phase silica-gel catalyst has shown better reactivity than the normal phase silica-gel one. It is expected that this reverse phase silica-gel palladium catalyst can be applied to diverse organic reactions in water such as hydrogenation and other coupling reactions.

Audience Take Away:

- They can learn the difference of reactivity according to stationary phase for Suzuki-Miyaura coupling reactions in water.
- They can understand the mechanism about Pd-catalyzed coupling reaction and synthetic procedure these catalysts.

Biography

I am a third year student pursuing Doctoral degree under supervision of prof., Hakjune Rhee at department of Bionanotechnology, Hanyang University in South Korea. I am majoring in Organic Chemistry and Organic Synthesis. I am interesting in the preparation of immobilized catalysts and the application for cross coupling reactions. In addition, I am studying synthesis of carbohydrate at the same time. As a result, I published one paper about total synthesis of L-ribose from D-ribose in this year.

Preparation and reduction behavior of carbon composite iron oxide pellets using woody biomass

Hirokazu Konishi*, Ph.D., Tateo Usui, Ph.D., Hideki Ono, Ph.D
Osaka University, Japan

Especially, biomass has a novel advantage, i.e., no CO_2 emissions, because of carbon neutral.Recently, charcoal composite iron oxide pellets were proposed to decrease CO_2 emissions for the iron-making. These pellets were promising to decrease the starting temperature for iron oxide reduction. From these backgrounds, we propose carbon composite iron oxide pellets using woody biomass in order to decrease CO_2 emissions. In this work, semi-charcoal composite iron oxide pellets have been prepared and the effect of residual V.M. and gasification rate of semi-charcoal on reduction of iron oxide were investigated. Furthermore, the effect of the semi-charcoal particle size was also investigated.

Audience Take Away:

- How to prepare and reduce carbon composite iron oxide pellets
- How to carbonize woody biomass
- Kinetics of gasification of carbon material
- Activation energy of carbon material

Biography

I received BD from Osaka City University, and MD and PhD (Doctor Energy Science) from Kyoto University. I worked as a research associate in National Institute of Advanced Industrial Science and Technology (AIST in Japan), in copper recycle process using electrolysis from ammonia solution. I has been working as an assistant professor in Osaka University. I earned ISIJ Young Researcher Award from ISIJ and Molten Salt Young Researcher Award from Molten Salt Committee of the Electrochemical Society of Japan. Now, titles of my works are reduction of iron oxide, sintering of oxide, recycle of rare- earth.

Copper(I)-catalyzed synthesis of 1,2,3-Triazoles from azidoformates, electron-deficient azides

Heejin Lee, Jaeyoung Ban*, Hakjune Rhee
Hanyang University, South Korea

Since the copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction was discovered, which is one of the classical click reactions, a various range of the 1,2,3-Triazole synthesis has been extensively developed. In case of formation of 1,2,3-triazole with electron-deficient azides such as N-sulfonyl , carbonyl, and cabamoyl, only a few system have been reported. We have first found the formation of regioselective 1,4-disubstituted 1,2,3-triazoles from terminal alkynes and azidoformates, which are electron-deficient azide groups, using commercialized $[(CH_3CN)_4Cu]PF_6$ copper catalyst with mild condition. This methodology can be applied to the synthesis of various bioactive triazole derivatives with other electron-deficient groups.

Audience Take Away:

- From this presentation, the audience can understand the [3+2] cycloaddition with azides using copper catalysts.
- They can learn the reaction tendency of CuAAC with electron-deficient azides such as N-sulfonyl , carbonyl, and cabamoyl azide.
- They can see the results having the different reactivity according to electron-donating or withdrawing groups.

Biography

I am a third year student pursuing Doctoral degree under supervision of prof., Hakjune Rhee at department of Bionanotechnology, Hanyang University in South Korea. I am majoring in Organic Chemistry and Organic Synthesis. I am interesting in the preparation of immobilized catalysts and the application for cross coupling reactions. In addition, I am studying synthesis of carbohydrate at the same time. As a result, I published one paper about total synthesis of L-ribose from D-ribose in this year.

Plasma assisted catalysis system for diesel PM combustion

Yoshiyasu Ehara*[1], Ph.D,Hirotaka Miyasita[1], Takashi Inui[2], Yukio Aoki[2]
[1]Tokyo City University, Japan
[2]Fuji Electric Co., japan

The particulate matters (PMs) emitted from marine diesel engine exhaust during the combustion process have low resistivity and extremely small in the range of 70-120nm.These particles cause a various human health and environment impacts. International standards limiting NO_x, SO_x, and PM emissions from ships are established through Annex VI of the international convention for the prevention of pollution from ships, otherwise known as MARPOL.

Authors have been developed non-thermal plasma (NTP) reactor for removal of PM emissions from a diesel engine. In the NTP reactor, the air is activated by discharge and produces ozone, oxygen radical and nitrogen radical, consequently the diesel particulates are oxidized under low temperature condition. Diesel PMs combusted by ozone produced in NTP. NO in the flue gas is oxidized to NO_2 by ozone and O radical, When the gas temperature is high, the oxidation of PMs by the resulting NO_2 using an applicable catalyst.

This research has been developed an after treatment system for removal of diesel PM from the ship exhaust. The PM was collected by electrostatic precipitator using corona discharge.The NTP reactor had a coaxial double tube structure. The pellets as a catalyst are packed between the inner and outer tubes. The catalysts surfaces depositing the PM were filled into the reactor. PM is taken from the diesel generator was operated with light oil. The catalyst used was NS-1A (Nikki-Universal., LTD.). It is spherical andthe diameter is about 4mm.NTP was generated by a high-frequency DBD. In the combustion experiment, plasma was generated in the heater which carried out temperature adjustment. The weight of PM before and after the experiment was measured and combustion efficiency was determined.

Audience Take Away:

- Facilitate the design of removalsystem of PM emissions from a diesel engine.
- The use of plasma assisted catalysis for air pollution matters.
- Instruct temperature characteristic to combustion efficiency of PM.

Biography

Yoshiyasu Ehara received the Ph.D. degree from Musashi Institute of Technology, Tokyo, Japan, in 1996. He is currently a Professor of electrical and electronics engineering with Tokyo City University, Tokyo. From 2002 to 2003, he was a Visiting Academic at the Ford Research Laboratory, Dearborn, MI, USA. His research interests include industrial application of nonthermal plasma and degradation diagnosis technology of the insulation materials in electric power apparatus. Prof. Ehara is a member of the Institute of Electrical Engineers of Japan.

Dopamine-mediated graphene/Ag NP hybrids for enhanced electrochemical activity

Wonoh Lee*, Ph.D
Chonnam National University, Republic of Korea

To facilitate the immobilization of the silver nanoparticles with high crystallinity and stability, the mussel-inspired dopamine is functionalized on the surface of the graphene. Considering the unique adhesive property of a catechol group in the dopamine toward metallic ions, a large amount of silver nanoparticles can be coated on the surface of the dopamine-functionalized graphene. To use the high surface area of graphene, large-sized graphene sheets are prepared using the microwave heat treatment of graphite powder followed by chemical oxidation and exfoliation. In addition, the large-area graphene sheets are selectively collected by a pH-assisted fractionation technique and are confirmed by the green-light filtered optical microscopic images. The dopamine-mediated graphene hybrid with silver nanoparticles shows superior electrochemical activity with enhanced electrical conductivity by promoting the decoration of stable silver nanoparticles on the surface of graphene. The resulting hybrid exhibits 7.6 times and 1.6 times higher electrochemical capacitance than that of the bare and graphene/silver hybrid-modified glassy carbon electrodes, respectively.

Audience Take Away:

- Various advantages of catecholamine chemistry such as high binding property toward metallic nanoparticles, easy functionalization with oxygen functional groups in graphene sheets, mechanically strong adhesive property, high carbon yield and nitrogen doping effect through high temperature annealing, and increase of hydrophilicity.
- Mussel-inspired dopamine functionalization on graphene surface.
- The catechol group in dopamine accelerated the surface immobilization of Ag NPs.
- The decorated Ag NPs had high stability and crystallinity.
- Dopamine-mediated graphene hybrid showed highly enhanced electrochemical activity.

Biography

Dr. Wonoh Lee is an associate professor at School of Mechanical Engineering of Chonnam National University, South Korea. He received a Ph.D in Department of Materials Science & Engineering at Seoul National University. His research interest are mechanics-based interdisciplinary researches for inelastic materials including metals, organic/polymeric structural materials, fiber-reinforced composites, advanced fiber/textile, and nano-carbon materials. Ongoing works focus on catecholamine-based graphene hybrids and their three-dimensional carbon nanostructures for electrochemical energy storage electrodes. He has over 60 peer-reviewed journal publications.

Design of a highly efficient natural gas fuel processor for residential PEM fuel cells

Wang Lai Yoon*, Un Ho Jung, Woohyun Kim and Kee Young Koo
Hydrogen Research Lab, New & Renewable Energy Research Division, Korea Institute of Energy Research(KIER), Republic of Korea

A scalable heat and system integrated coaxial cylinder type fuel processor is designed and fabricated. The unit process consists of desulfurizer, steam reforming with metallic structured catalyst, water gas shift(WGS), preferential oxidation and auxillary components(water pump, blower, heat exchanger and controller). The basic principle for scalability is explained to maintain the similarities in heat and mass flux. Since the strong endothermic steam reforming reaction of natural gas accompanies a very rapid surface reaction due to strong pore diffusion limitations with very low value of effectiveness factor decreasing from the reactor inlet below 0.1, as an alternative to conventional ceramic based pellet catalysts, a newly designed metallic structured catalyst with ruffled-fin type configuration using a FeCr alloy plate as a substrate to maximize geometric surface area per unit volume is applied. Subsequently, Ru, as an active reforming catalyst, is uniformly coated and highly dispersed onto the metallic substrate by deposition-precipitation method. The system reveals the fuel processing efficiency of ca. 80%(LHV) and the durability of up to 1,000 hrs with no decay in catalytic performance implying stable activity of the Ru on metallic structured surfaces is verified. The system volume including insulation is very compact with 12.5L/kW. In addition, Aspen+ commercial process simulation software is employed to optimize the heat exchange network of a fuel processor.

Quantification of ligand packing density on Cu nanoparticles and determination of nanoparticles surface area and sizes through quantitative ligand adsorption–chemisorption

Matumuene Joe Ndolomingo*, Ph.D., Reinout Meijboom, Ph.D
Meta-catalysis Research group, Department of Chemistry, University of Johannesburg, South Africa

The quantification of the ligand packing density of metal nanoparticles is of considerable importance for catalysis and for quality control in many applications. The effective catalytic properties of the metal nanoparticles are mostly based on their inherent high surface area to volume ratio. However, the determination of the true surface area of the metal nanoparticle in catalysis represents one of the greatest challenges due to the nanoparticle surface unevenness and morphological irregularity. In this contribution, we report on the ligand adsorption-based technique for quantification of ligand packing density on copper nanoparticles and determination of specific surface area of copper nanoparticles on gamma alumina supports. 2- mercaptobenzimidazole (2-MBI) was used as probe ligand. The adsorption of 2-MBI on the nanoparticle surface was evaluated by using different supported copper catalysts, and was followed by ultraviolet-visible spectrometry. The amount of ligand adsorbed was found to be proportional to the copper nanoparticles surface area. The ligand packing density was calculated based on the ratio of the mass fractions of 2-MBI and Cu as determined by UV-vis and AAS, respectively. With assumption that the self-assembly of thiol molecules onto the copper surface was completed, the amount of 2-MBI adsorbed per gram of copper nanoparticle was determined as the difference between the amount of 2-MBI added and the amount of unadsorbed 2-MBI. For 2-MBI with concentration of 40-65 µM, the calculated packing density of 2-MBI on copper nanoparticles is independent on the concentration, ranging from 2.88 to 3.26 nm^{-2}, and averaging 3.07 ± 0.13 nm^{-2} which would be equivalent to the saturation capacity of 0.510 ± 0.02 nmol cm^{-2}. On the basis of the packing density, the average surface area which each 2-MBI molecule occupies is 0.326 ± 0.01 nm^{2}. To validate this method, the quantification of 2- MBI packing density on gold nanoparticles was done under the same conditions. A good agreement was found between the saturation packing density obtained in this study, 0.586 ± 0.04 nmol cm^{-2} and those reported in the literature; 0.571 ± 0.005 nmol cm^{-2} and 0.574 ± 0.006 nmol cm^{-2}. A Langmuir–isotherm plot was used in order to determine the effective surface area per gram of the nanoparticles. Thus, the reciprocal of the slope of the Langmuir plot was multiplied by Avogadro's number and the cross section of the probe ligand. Although the specific surface area is the essential information acquired from the 2-MBI adsorption method, it is worth comparing the obtained particle sizes with those obtained by TEM. A fair agreement was found between copper particle sizes obtained from ligand adsorption and TEM methods; average sizes 3.0 ± 0.0 and 3.1 ± 0.2, respectively. To validate this method, 2-MBI and H_2 chemisorption methods were used for Pt/Al_2O_3 and Pd/Al_2O_3 catalysts. A good agreement was found between platinum and palladium specific surface area and particle sizes obtained from thiol adsorption and H_2 chemisorption. For palladium, both specific surface area and particle sizes deviate in the order of 5% and 7%, respectively.

Audience Take Away:

- Despite its significant merits and potential, catalysis by copper nanoparticles is relatively less explored compared to the noble and other base metals. Copper is environment-friendly, easily available and comparatively inexpensive. So, copper is of considerable importance as an alternative to these metals. For the first time, the 2-MBI packing density on copper nanoparticles was quantified using a simple and easy method.
- The physisorption method, BET is a reliable method for the surface area determination. The BET theory can be derived similar to the Langmuir theory; however, the BET does not allow the discrimination between a catalytic active species and the supporting material. Commonly, the specific surface area and the size of supported metal nanoparticle are investigated by chemisorption with H_2, CO, or O_2 as probe molecules. However, those methods are limited by the properties of the support and some metals, and could not be generally used. In addition, the method requires expensive instrumentation.

- True surface area and particle sizes determination are key aspects of the activity of metal nanoparticle catalysts. This study demonstrated that, a more easy, simple and precise determination of the specific surface area and particle sizes of metal nanoparticles is possible.

Biography:

Matumuene Joe Ndolomingo, studied chemistry at UJ (University of Johannesburg-RSA) and obtained his Ph.D. in 2016 under the guidance of Prof. R. Meijboom. Presently, he is a Post- Doctoral fellow at the same University in chemistry department at Prof. Meijboom's Research Center for Synthesis and Catalysis. His current research interests include the synthesis and development of mesoporous metal oxides supported metal nanoparticles for industrial oxidation and hydrogenation reactions, and development of a simple general approach for the easy determination of the true surface area and particles sizes of a wide range of metal nanoparticles using organothiols as probe ligand.

Effect of Transition metal promoter on Cobalt based Syngas to Olefin synthesis

Jayen Barochia*, Khalid Karim
SABIC R&T-Riyadh, Saudi Arabia

Introduction: Fischer-Tropsch to olefin synthesis has attracted much attention, especially to production of olefin feed stock mainly ethylene, propylene and butylene (C2=-C4=).

For selective formation of light olefin, iron based catalysts exhibits high selectivity and activity. However, iron based catalysts suffer from high selectivity to CO_2 and much faster deactivation due to carbide formation on catalyst, cobalt-manganese based catalyst has received much attention due to lower methane and CO_2 selectivity, especially using natural gas based feed stock.

In present study, prepared cobalt and manganese catalyst was promoted by various transition metals to enhance activity and selectivity to olefins and further reduction of CO_2 selectivity. Prepared catalysts were characterized by XRD, N2 adsorption, TPR and ICP and tested for catalytic activity.

Materials and Methods: Cobalt and Manganese catalyst was prepared using method published elsewhere using sodium carbonate as precipitating agent. Promoter in specified amount was impregnated with aqueous solution of promoter. Catalyst was dried and calcined. Catalyst are denoted as Co/MnOx-A (where A is Cr, Fe, Zn, Cu, and Ga).

Catalysts were shaped in 40-60 mesh size and tested in fixed bed high-throughput reactor at 513 K, 0.5 MPa, 2000 ml/g H2/CO=2. Prior to reaction, catalyst was reduced with 50% hydrogen in nitrogen at 623 K for 8 hours at atmospheric pressure.

Results and Discussion: XRD pattern shows presence of highly crystalline material with almost identical XRD of promoted and unprompted catalyst with presence of Co-Mn spinel phases (Co_2MnO_4 and $CoMn_2O_4$) with minor presence of $CoMnO_3$phase, no free oxide phase detected.

Surface area changes with promoter addition. Except Zn, all promoter decrease surface area of catalyst compare to control. Promoters has significant effects on pore volume. Fe and Zn tends to decrease pore volume, while Cu increases pore volume. Cr and Gahas almost no effect on pore volume.

TPR shows reducibility of catalyst changes with promoter.

Table 1. Characterization: N_2 adsorption and ICP

Catalyst	BET (m2/g)	Pore size (nm)	Pore volume (cc/g)	Promoter (% wt)
Co/MnOx	62	4.2	0.278	0
Co/MnOx-Cr	55	4.1	0.263	1.16
Co/MnOx-Fe	48	3.9	0.202	0.98
Co/MnOx-Zn	69	3.8	0.296	0.89
Co/MnOx-Cu	57	4.6	0.319	0.93
Co/MnOx-Ga	52	4.2	0.246	1.02

Catalytic performance at steady state (Table 2) shows Cu and Fe is decreasing catalyst activity, while Cr and Ga has almost no effect on its activity. Zn has positive effect on catalyst activity and olefin selectivity may be co-related to increased surface area and decreased pore size. Fe and Cu increase alcohol selectivity. Zn and Cu also decreases CO2 selectivity. Methane formation remains unaffected with promoter.

Table 2. Catalyst performance

Catalyst	Conversion	Olefin	C2+ Paraffin	Alcohol	CO2	Methane
Co/MnOx	65.7	40.6	28.1	9.1	15.7	6.4
Co/MnOx-Cr	64.6	39.7	29.7	9.0	14.8	6.7
Co/MnOx-Fe	45.3	41.7	22.2	11.0	18.1	7.1
Co/MnOx-Zn	67.7	44.3	29.2	8.6	11.6	6.4
Co/MnOx-Cu	37.2	46.2	21.9	12.1	11.3	8.6
Co/MnOx-Ga	66.1	42.1	26.7	9.2	15.5	6.4

Significance

Zn promoted Co/MnOx catalyst is prominent catalyst for direct production of olefin from syngas. It increases olefin selectivity with reduced CO_2 selectivity without affecting catalyst performance.

Audience Take Away:

- Researchers will familiarize with direct conversion of Syngas to lower olefin process.
- Transition metal promoters and link between characterization and performance will be discussed.
- The research work done is not for academic interest but for commercial technology development.

Biography

Jayen Barochia is Senior Scientist in SABIC Research and Technology Centre in Riyadh. Currently he is working on CO hydrogenation by modified Cobalt based FT catalysts, He is also working on Methane to Aromatics and Methane to Methanol catalyst development. His interest is practical usage of computational chemistry in catalyst design and development.

magnus
Group

DAY 3

Keynote Forum

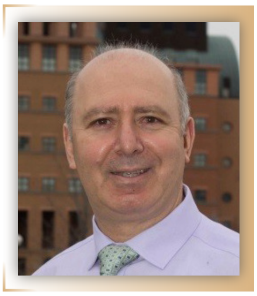
Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Base modified Bi_2WO_6: A facile route to improved photocatalytic activity under Visible light



Dionysios D. Dionysiou*
University of Cincinnati, USA

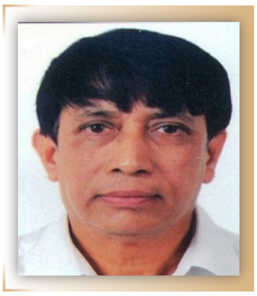
In this study, a facile approach was successfully employed to improve the photocatalytic activity of Bi_2WO_6. The pristine Bi_2WO_6 (p-Bi_2WO_6) nanoplates were prepared through a conventional hydrothermal method and then were subjected to sodium hydroxide aqueous solutions with concentrations ranging from 0.5 M to 10 M. Under visible light irradiation, the photocatalytic activities of base-modified Bi_2WO_6 (b-Bi_2WO_6) were significantly enhanced when compared to that of the p-Bi_2WO_6. However, as the concentration of base solution continues to increase, the performance of b-Bi_2WO_6 deteriorated. The b-Bi2WO6 nanoplates were characterized by various techniques including XRD, TEM, porosimetry analysis, UV–vis spectrometry, and XPS. The results indicated that the surface of b-Bi_2WO_6 was etched by alkaline solutions, which improved the surface area and produced active sites on the surface. The b-Bi_2WO_6 nanoplates were proved to be highly effective in photocatalytic degradation of emerging contaminants including ibuprofen (IBP) and microcystin-LR (MC-LR). The degradation byproducts and pathways of IBP were also investigated.

This study is beneficial to further understand the chemistry and properties of Bi_2WO_6 materials. The facile modification proposed here provides a novel strategy for improving the photocatalytic activity of Bi_2WO_6 materials, which could also be applied to other types of photocatalysts. In addition, the efficient degradation of IBP and MC-LR under visible light demonstrates the great potential of environmental remediation using sustainable solar energy.

Biography

Dr. Dionysios (Dion) D. Dionysiou is currently a Professor of Environmental Engineering and Science Program at the University of Cincinnati. He teaches courses and performs research in the areas of drinking water quality and treatment, advanced unit operations for water treatment, advanced oxidation technologies and nanotechnologies, and physical-chemical processes for water quality control. He has received funding from NSF, US EPA, NASA, NOAA/CICEET, USGS, USDA, Ohio Sea Grant, USAID, and DuPont. He is currently one of the editors of Chemical Engineering Journal, Editor-in-Chief of the Journal of Advanced Oxidation Technologies, and Editor-in-Chief of the Journal of Environmental Engineering (ASCE). He is a member of the Editorial Boards of several other journals. Dr. Dionysiou is the author or co- author of over 325 refereed journal publications, over 86 conference proceedings, 32 book chapter publications, 26 editorials, and more than 600 presentations. He has edited/co-edited 6 books on water quality, water reuse, ferrates, and photocatalysis. He is currently co-editing a book on harmful algal blooms. Dr. Dionysiou's work received over 15,000 citations with an H factor of 68.

Heterogeneous catalysts from waste biomass and their applications



Dibakar Chandra Deka*, Ph.D
Gauhati University, India

Use of ecofriendly and biodegradable heterogeneous catalysts is one of the key aspects one needs to consider while engaging in the development of newer generation of chemical processes. Such an effort would ensure, at least in part, the greener perspective of a process. In such an effort, we have come across a few interesting sources of biomass which have been converted to highly active heterogeneous catalysts with potential for use in industrial processes. Post-harvest banana plants (Musa balbiosiana Colla) are a huge waste of biomass which contributes little to the economic aspect of the farmers. We have converted this waste biomass to a useful heterogeneous catalyst which have been successfully tested in the transesterification process of vegetable oils to biodiesel and organic syntheses. Water hyacinth (Esichhornia crassipes) is an aquatic weed which grows in plenty in natural water bodies like ponds, lakes, and other natural water reservoirs. It has little economic value and is often considered a hazard for other economically important crops. A highly potent catalyst has been derived from this aquatic weed and successfully used in organic transformations. Red cotton (Bombax ceiba) is a huge permanent non-aquatic plant which produces tons of red flowers every year. The naturally fallen flowers find no economic value and simply a waste. We have discovered an application out of these waste flowers in converting them in to a heterogeneous catalyst which proves excellent in transesterification reactions and could find large scale applications in biodiesel industries.

Audience Take Away:

- Waste can be wealth if intelligently and innovatively used.
- Audience will learn to think how to use waste in their respective domains.
- The presentation will help in exploring more catalysts for chemical processes from easily available biomasses.
- The new catalysts may be of interest for Industrialists.

Biography

Prof. Dibakar Chandra Deka M.Sc., M.Tech., Ph.D., DTIT, D.Sc., FRSC is a senior professor in the Department of Chemistry, Gauhati University, Assam, India. Educated in Cotton College, Gauhati University and IIT Kharagpur, Prof. Deka was an UNESCO Research Fellow in Tokyo Institute of Technology, Tokyo, Japan from October/1989 to September/1990 and a Commonwealth Visiting Fellow in The University of Manchester, Manchester, UK from October 1997 to September 1998. In Tokyo, he worked in the research group of Prof. Takeshi Nakai and in Manchester he worked in the research group of Prof. Eric Jim Thomas. Currently, his research interests include organic synthesis, biofuels, natural products chemistry, applied catalysis, traditional alcoholic beverages, etc. He has successfully guided till now 23 research students to obtain Ph.D. degrees and a dozen more working in diverse areas.

magnus
Group

DAY 3
Speakers

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

GCR 2017

Sessions on: Catalytic systems and New catalysts | Photochemistry, photobiology and Electrochemistry | Advanced Synthesis and Catalysis

Session Chairs

Dionysios (Dion) Demetriou Dionysiou
University of Cincinnati, USA

Allen Apblett
Oklahoma State University, USA

Session Introduction

Title: **Single source precursor approach for the synthesis of bimetallic molybdate catalysts**
Allen Apblett, Oklahoma State University, USA

Title: **Synthesis of new water-soluble platinum(II) complexes by Phase Transfer Catalysis**
Ja'afar Kadhum Jawad, International University of Erbil, Iraq

Title: **Flexible CNT/metal-sulfide composite electrode for energy conversion and energy storage applications**
Chandu Venkata Veera Muralee Gopi, Pusan National University, Republic of Korea

Title: **Pycnoporus laccase production, properties and its novel application**
Jiayang Liu, Huanghuai University, China

Title: **CO_2 conversion from flue gas using a catalytic hybrid inorganic membranes**
Edidiong Okon, The Robert Gordon University, UK

Title: **Nanostructured metallic glasses and their powders as catalytic, chemical and biological materials**
Dmitri V. Louzguine, Tohoku University, Japan

Title: **Edible Lentinula edodes carbon with $NiCo_2O_4$ based hybrid super capacitive material for high capacitance**
Vivekanandan Raman, Pusan National University, Republic of Korea

Title: **Visible-light-induced degradation of polybrominated diphenyl ethers**
Chunyan Sun, Shaoxing University, China

Single source precursor approach for the synthesis of bimetallic molybdate catalysts

Allen Apblett*, Ph.D
Oklahoma State University, United States

Bimetallic molybdenum-containing oxides have a wide range of applications including numerous catalytic reactions. Previous work has shown that the preparation method has a marked influence on the physical and chemical properties of these kinds of metal oxides. Accordingly, a facile, low-temperature synthetic approach for the preparation of molybdenum-containing bimetallic oxide catalysts with controlled shape and chemical composition via the pyrolysis of water-based bimetallic single-source precursors will be reported. The precursors result from the reaction of aqueous solutions of alkaline earth metals or divalent first row transition metal salts of 2-hydroxycarboxylic acids (eg. lactic acid, 2-methyllactic acid, mandelic acid, and benzilic acid) with solid MoO_3. They crystalize with the exact ratio of divalent metal to molybdenum for formation of $MMoO_4$. TGA and XRD analysis has shown that the thermal decomposition of these single source bimetallic precursors produces the target materials. Several potential catalytic reactions will be discussed including oxidative dehydrogenation and production of petrochemicals via pyrolysis of biomass.

Audience Take Away:

- How single source precursors allow the synthesis of metastable more highly active catalysts
- How single source precursors permit the synthesis of metastable more highly active catalysts
- How single source precursors enable the search for novel catalysts
- Novel catalysts for biomass pyrolysis to produce fuels and commodity chemicals

Biography

Allen Apblett received a B.Sc.(Honours) degree from The University of New Brunswick in 1984 and a Ph.D. from The University of Calgary in 1989 under the supervision of Dr. Tristam Chivers. He was awarded a Natural Sciences and Engineering Research Council Postdoctoral Fellowship that he took up at Harvard University in Dr. Andrew Barron's research group. In 1991 he became an assistant professor at Tulane University and then moved to Oklahoma State University in 1997 where he is a full professor. He is a Fellow of the National Academy of Inventors, the American Chemical Society and the American Ceramic Society.

Synthesis of new water-soluble platinum(II) complexes by Phase Transfer Catalysis

Ja'afar K. Jawad*[1], Ph.D., Michael J. Morris[2], Ph.D., I.K.Ahmed, Ph.D
[1]International University of Erbil, Iraq
[2]University of Sheffield

The following issues will be discussed:

a)Synthesis of new Platinum(II) Complexes by Phase Transfer Catalysis.

Platinum(II) complexes have been synthesized by many different methods. In general, square-planar platinum(II) complexes contain stabilizing ligands (such as bipyridine, 1, 10-phenanthroline, 1, 5-cyclooctadiene, tri-alkyl or-aryl phosphines) and halides or organic groups. These complexes are not soluble in water at all. Therefore, Phase Transfer Catalysts (PTC) has become recognized as useful tools for performing reaction between anions (and certain neutral molecules and transition metal complexes) and organic substrates. PTC is needed because many anions (in the form of their salts) and neutral compounds are soluble in water and not in organic solvents, whereas the organic reactants are not usually soluble in water.

b)Synthesis of new water-soluble platinum(II) complexes by Phase Transfer Catalysis.

A great deal of attention has been paid to the search for water-soluble transition metal complexes and related catalysts since water has a variety of properties that set it apart from most organic solvents. Because most organometallic compounds have limited water solubility, the synthesis of novel water soluble transition metal complexes is central to the development of new complexes.

Platinum complexes are not soluble in water at all. The synthesis of novel water soluble transition metal complexes is central to the development of new complexes. The synthesis of water soluble platinum complexes, as most of the work in the literature, is to convert the stabilizing ligand into water soluble ligand having SO_3Na group for example. In this work we are modifying this method by replacing the halides by the water soluble ligand [8-hydroxy-7-(4-sulfo-naphthylazo)-5-quinoline sulfonic acid. disodium salt] (HSNQ).

c)Phase Transfer Catalysis.

As the chemical industry strives to increase efficiency, improve process safety, and reduce environmental impact, Phase Transfer Catalysts (PTC) has become recognized as useful tools for achieving these goals. Phase – Transfer Catalysis is useful primarily for performing reaction between anions and organic substrates. PTC is needed because many anions and neutral compounds are soluble in water and not in organic solvents, whereas the organic reactants are not usually soluble in water. The PTC acts as a shuttling agent by extracting the anion or neutral compound from the aqueous (or solid) phase into the organic reaction phase (or interfacial region) where the anion or neutral compound can freely react with the organic reactant already located in the organic phase. Reactivity is further enhanced, sometimes by orders of magnitude, because once the anion or neutral compound is in the organic phase, it has very little(if any) hydration or solvation associated with it, thereby greatly reducing the energy of activation. It has been shown that there are several advantages using PTC such as: An increased reaction rate, a lower reaction temperature, avoiding the need for expensive anhydrous or aprotic solvents, and the use of water together with an organic solvent as reaction medium.

Audience Take Away:

- The audience will be able to use this method whenever they face compounds or complexes which are not soluble in water. Moreover, there has been a steady development of interest in using Phase Transfer Catalysts (PTC) as useful tools for performing reaction between anions and organic substrates.
- Using this method is very easy. All we need is water and organic solvent plus one type of PTC catalysts. All types of PTC will be discussed in details.
- This method will help the researchers to find a practical solution when they face a problem of solubility, and this will expand their knowledge and give new information to assist in their research.

Biography

Dr. Ja'afar K. Jawad is an Associate Professor of Inorganic and Organometallic Chemistry. He completed his Ph.D in Liverpool University, Liverpool, England. Before that, he has done his M.Sc in Wales University, Aberystwyth, Wales U.K and B.Sc in Baghdad University, Baghdad, Iraq. A long time teaching, research, and administrative experience at the university level in addition to Industrial Work Experience. A chemical expert for the private & governmental factories in Iraq and Yemen.

- HOD, Department of Chemistry, College of Education, University of Salahaddin, Iraq.
- Assistant Dean for Scientific Affairs, College of Education, University of Salahaddin, Iraq.
- Acting Dean, College of Education, University of Salahaddin, Iraq.
- Academic Advisor, Inorganic Group Coordinator, General Chemistry,Head, Chemistry Department, College of Science, Sultan Qaboos University, Oman.
- Dean, College of Education, SABIS University, Erbil, Kurdistan, Iraq.
- President's Assistant for Administrative Affairs, International University of Erbil. Erbil, Kurdistan, Iraq.

Area of Research Interest:

- Application of New Platinum Complexes and Polymers as Models for Anticancer Agents.
- Application of New Transition Metal Complexes and Polymers for Polymerization, Catalysis and Biological Effects.

Flexible CNT/metal-sulfide composite electrode for energy conversion and energy storage applications

Chandu Venkata Veera Muralee Gopi*, Ph.D., Hee-Je Kim, Ph.D
Pusan National University, South Korea

Carbon nanotubes (CNT) and metal sulfides have attracted considerable attention owing to their outstanding properties and multiple application areas, such as electrochemical energy conversion and energy storage. Here we describes a cost-effective and facile solution approach to the preparation of metal sulfides (PbS, CuS, CoS, and NiS) grown directly on CNTs, such as CNT/PbS, CNT/CuS, CNT/CoS, and CNT/NiS flexible electrodes for quantum dot-sensitized solar cells (QDSSCs) and supercapacitors (SCs). X-ray photoelectron spectroscopy, X-ray diffraction, and transmission electron microscopy confirmed that the CNT network was covered with high-purity metal sulfide compounds. QDSSCs equipped with the CNT/NiS counter electrode (CE) showed an impressive energy conversion efficiency (η) of 6.41% and remarkable stability. Interestingly, the assembled symmetric CNT/NiS-based polysulfide SC device exhibited a maximal energy density of 35.39 W h kg^{-1} and superior cycling durability with 98.39% retention after 1,000 cycles compared to the other CNT/metal-sulfides. The elevated performance of the composites was attributed mainly to the good conductivity, high surface area with mesoporous structures and stability of the CNTs and the high electrocatalytic activity of the metal sulfides. Overall, the designed composite CNT/metal-sulfide electrodes offer an important guideline for the development of next level energy conversion and energy storage devices.

Audience Take Away:

- The energy crisis and global warming concerns have increasing the demand for progress into high performance energy conversion and energy storage devices. The development of new electrode materials for energy conversion and energy storage technologies, particularly quantum-dot-sensitized solar cells (QDSSCs) and supercapacitors (SCs) have attracted special attention.
- To date, there have been many reports on individual CNTs and metal chalcogenides used as electrode materials in both QDSSCs and SCs. None of these studies, however, examined composite CNT/metal sulfides as efficient electrode for high-performance QDSSCs and SCs. Therefore, the combination of CNTs with metal sulfides has been proposed to enhance the electrocatalytic activity and conductivity of CEs.
- Overall, these results indicate that the CNT/metal-sulfide composites provide a new path for the development of similar advanced electrochemical electrode materialsfor a range of applications. Fourth, the flexible property of the supercapacitor is highly desired for actual applications.

Biography

Chandu Venkata Veera Muralee Gopi is a Ph.D student of Department of Electrical Engineering at Pusan National University, Busan, South Korea. His current scientific interests focus on design, synthesis and application of nanomaterials for applications in energy conversion/storage. He has published over 43 papers and his works have been cited over 318 times.

Pycnoporus laccase production, properties, and its novel application

Jiayang Liu*, Ph.D
Huanghuai University

Many eco-friendly enzymes have been used in industries to promote cleaner production via enzymatic processes. Laccase (EC 1.10.3.2) is a very useful green catalyst for industrial, environmental, and medical applications due to its diverse capability in converting a wide range of substrates through catabolic or anabolic reactions As such, a rapid growth in the demand of laccase is expected worldwide, and the gap between production and demand will enlarge. It is thus of practical significance to seek microbes as potent cell factories to produce laccase with high yield at low cost.

We isolated a wild-type fungus from a rotten wood in subtropical area in China and characterized it as Pycnoporus sp. SYBC-L3. Laccase production was raised up to 45 U/mL from its original value of 0.8 U/mL by optimizing several parameters under submerged cultivation in flask. Productivity of laccase was further examined in bioreactors at different scales and showed scalability. In a 50 L stirred reactor, the highest activity of 110 U/mL was achieved. Cultivation in 65 L airlift bioreactor gave rise to 72 U/mL at day 6. A 5 ton bioreactor produced 80 U/mL laccase. The laccase was purified and characterized. Results showed that it was a thermostable one with strong stability at room temperature. Secondary structure β-sheet plays a critical role in maintaining laccase activity. Powdered laccase can be prepared using spray drying technique with >74% activity recovered. The production cost was calculated to be very low, in which the highest percentage was labor (50%) followed by electricity (36%). By roughly calculating the cost in 65 L airlift bioreactor, $1 for per liter fermentation crude was needed, equaling 72000 U in total.

The current novel application of laccase is to alleviate soil water repellency (SWR). SWR is the phenomenon that the soil is hydrophobic and does not spontaneously wet. SWR is caused by the formation of hydrophobic organic coatings on soil particle surfaces. These organic coatings include waxes, fatty acids, lignin, plant root exudates, fungal hyphae/exudates, etc. SWR can lead to serious loss in crop production and turfgrass quality. Laccase and other several enzymes were found to be effective in alleviating SWR, which is usually determined using water drop penetration times (WDPT) which involves placement of a droplet of water on an soil sample surface, with the WDPT classes being: <5 s penetration time means very hydrophilic soil. After enzyme treatment, all repellent soils were found to be hydrophilic with WDPT reduced to <60s from 7439s. One day treatment was proved effective. Laccase also showed stability in soil over treatment period. Other enzymes like chitinase, protease, and pectinase were also observed with high efficiency.

Audience Take Away:

- The audience will be able to get more information besides commercial laccases available.
- This might help the audience start and/or go further their work on laccase.
- This might also help enlarge applicable scope of laccase through interdisplinary communication.

Biography

Jiayang Liu received his PhD of fermentation engineering at Jiangnan University in 2013. In 2011-2012, he was invited as a visiting PhD student to the University of Georgia. He now is working as a faculty in Bioengineering Department at Huanghuai University, Zhumadian, China. From Feb, 2017 through Feb, 2018, he is working at the University of Georgia as a visiting scholar. His research interest focuses on production of enzymes from microbes and their application in environment. He has over 10 publications in English as first author and 5 publications as co-author.

CO_2 Conversion from flue gas using a Catalytic Hybrid Inorganic Membranes

Edward Gobina, Edidiong Okon*, Habiba Shehu, Ifeyinwa Orakwe
The Robert Gordon University Aberdeen, United Kingdom

Experiments have been carried out using a catalytic membrane reactor for the tri-reforming of power plant flue gas for CO_2 conversion. The experiments were performed at two different temperatures of 800 and 900 °C respectively. The gaseous stream was composed of O_2, CH_4, CO_2 and N_2. Two membrane sizes were used for the evaluation (10mm OD and 25 mm OD) with a length of 368 mm in each case. The reaction temperature was monitored by strategically located thermocouples with zonal control achieved using a power controller. At each operating temperature, tests were performed at atmospheric pressure and at four different volumetric flowrates (517, 994, 1,656 and 3,312 mL/min). Rhodium chloride ($RhCl_3$) solution was used as the catalyst precursor which was impregnated on the surface of an α-Al_2O_3 inorganic membrane having a commercial pore size of 600µm. For each membrane the 0.5 wt.% Rh/gamma-Al_2O_3 catalyst gave the higher conversions of CH_4 and CO_2 but the syngas ratio did not change significantly with increasing catalyst loading from 0.1 weight % to 0.5 weight %. The gaseous products were analysed using an Agilent Technologies Model 7890B equipped with an Agilent Technologies 5977A MS detector and a Varian CP – 3800 gas chromatograph equipped FID and TCD detectors respectively. The characterization of the membranes was carried out using scanning electron microscopy (SEM) coupled with energy dispersive x-ray (EDAX) and the Brunauer-Emmett and Teller (BET) gas adsorption method using liquid nitrogen. It was found that the calcined and reduced catalysts showed a lower surface area compared to γ-$Al2O_3$ support. The reduction in surface area was attributed to catalytic impregnation. It was observed that for each membrane, the 0.5 wt.% Rh/gamma-$Al2O_3$ catalyst gave the higher conversions of CH_4 and CO_2 but the syngas ratio did not change significantly with increasing catalyst loading from 0.1 weight % to 0.5 weight %. In conclusion, CO_2 reforming is more favourable at high temperatures, it was determined that by raising the temperature to the 900 °C range, a high CO_2 conversion was achieved.

Biography

Edidiong Okon is a Doctoral researcher/Research assistant at the School of Engineering, Robert Gordon University, Aberdeen, United Kingdom, having previously obtained her Bachelor and Master of Science degrees in Applied Chemistry and Instrumental Analytical Sciences respectively. She is currently working on ''Esterification of Lactic acid with Ethanol using cation-exchange resins impregnated metallic membrane reactor''. She has previously published and co-authored a number of academic papers in international journals. Her research interests are in the area of heterogeneous catalysis and metallic membrane reactor for ethyl lactate separation. She is a member of various Professional bodies including Royal Society of Chemistry and International Association of Engineers. She has also made several oral/poster conference presentations in the United State of America and United Kingdom.

Nanostructured metallic glasses and their powders as catalytic, chemical and biological materials

Dmitri V. Louzguine*, Ph.D
AIMR, Tohoku University, Japan

Here I am going to present the results of our long-term research activities on nanostructured metallic glasses and metallic glassy powders applicable as catalytic, chemical and biological materials. In particular, Au-based nanostructured metallic glasses produced by magnetron sputtering with a large surface area exhibited a high catalytic activity on the oxidation of the organosilane compounds with water. The catalyst was easily recoverable and was demonstrated to be used at least five times without loss of its activity. A nanograined $Pd_{78}Si_{22}$metallic glass was also produced which is also applicable for other reactions. In addition to the nanostructure-induced catalytic activity, these materials sustain good mechanical properties of a metallic glassy structure, showing a high hardness, good deformability and a low elastic modulus.

Ti- and Zr-based nanostructured metallic glasses exhibited excellent biocompatibility. A submicron-nanometer-sized hierarchical glassy structure of a $Ti_{34}Zr_{14}Cu_{22}Pd_{30}$ nanostructured metallic glass was used to tune the osteoblasts cell bioactivity. Our experimental results provide strong evidence that such a structure is extremely beneficial for cell attachment and proliferation. The $Zr_{62.5}Pd_{37.5}$ metallic glassy alloy exhibit a good thermal stability versus crystallization and good resistance to oxidation in dry air up to 573-673 K. The samples also show a very high corrosion resistance and spontaneous passivation in a simulated body fluid. The sample also exhibit catalytic activity in Suzuki-coupling reaction. The osteoblast cells cultivation on the nanoglass was also used to prove its good biocompatibility. The material has potential in biochemistry for biosensors and artificial tissue engineering.

Fe-based metallic glass powders were found to completely decompose the $C_{32}H_{20}N_6Na_4O_{14}S_4$ in aqueous solution in short time, about 200 times faster than the conventional Fe powders. MgZn-based metallic glassy powders also exhibited excellent ability in degrading azo dyes as typical organic water pollutants. Their azo dye degradation efficiency is about 1000 times higher than that of commercial crystalline Fe powders, and 20 times higher than their crystalline counterparts. The high Zn content in the amorphous Mg-based alloy enables a greater corrosion resistance in water and higher reaction efficiency with azo dye compared to crystalline Mg. Even under complex environmental conditions, in solutions with different pH, in a solution that contains several different azo dyes, at relatively low temperature and after exposure to air for a long time, the MgZn-based metallic glass powders retain their high reaction efficiency.

The above-described materials will be discussed in comparison with the metallic glassy samples for catalytic reactions produced by other research groups.

Audience Take Away:

- New functional metallic glassy materials will be presented in this talk. They exhibit excellent catalytic and biological properties as well as good chemical activity. These materials can be applied by the industry while their performance can be further improved by the researchers from academia.
- Explain how the audience will be able to use what they learn?
- How will this help the audience in their job? Is this research that other faculty could use to expand their research or teaching? Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient? Will it improve the accuracy of a design, or provide new information to assist in a design problem? List all other benefits.

Biography

2007-Present: Professor, Principal Investigator, WPI Advanced Institute for Materials Research, Tohoku University, Japan.
2005-2007: Associate Professor, Institute for Materials Research, Tohoku University, Japan.
1998-2005: Research Associate, Institute for Materials Research, Tohoku University, Japan.
1995-1998: Dr. Eng. Course Student, Tohoku University, Japan.
1991-1994: Researcher, Moscow State Institute of Steel and Alloys (Technological University), Moscow, Russia.

Edible Lentinula edodes carbon with $NiCo_2O_4$ based hybrid super capacitive material for high capacitance

Vivekanandan Raman*, Hee-Je Kim, Ph.D
Pusan National University, South Korea

A novel electrode of $NiCo_2O_4$ nanowire arrays (NWAs) on new carbon material which takes advantage of the high electrical conductivity to boost the pseudocapacitive performance. Graphene or carbon nanotubes based thin films have been used to fabricate flexible solid-state supercapacitors with high gravimetric specific capacitances (80–200 F/g), but usually with a rather low overall or areal specific capacitance (3–50 mF/cm^2) due to the ultra-small electrode thickness (typically a few micrometers) and ultralow mass loading, which is not desirable for practical applications. So we report that Edible Lentinula edodes will give more specific capacitance when compared to other carbon electrodes. $NiCo_2O_4$ mesoporous arrays together with the synergistic effect between $NiCo_2O_4$ and e-C will result in a high specific capacitance. Here we expect, with a e-C having high surface area combining with $NiCo_2O_4$ could enhance the specific capacitance, low leakage current, excellent cycling stability, and extraordinary mechanical flexibility.

Audience Take Away:

- In recent years, supercapacitors, the new devices between conventional physical capacitors and batteries, also known as electrochemical capacitors, have been extensively studied to serve as one of the most promising candidates for next-generation energy storage devices due to their intriguing properties, such as high power densities, long cycling lifespans and fast charge/discharge processes, which can be proven by the number of literature works.Recently the research has been focused intensively to develop supercapacitor devices with large areal capacitance to meet the demand of miniaturization of consumer electronics, hybrid electric vehicles and micro energy systems.
- By this topic they can know well about the carbon uses for the supercapacitor. We have been researching on natural carbon materials and its properties in the application of supercapacitor. It can make the peoples to do further researches in various other natural materials.
- This research is could expand the research in the area of natural materials and these materials provides good stability and more efficiencies due to its natural structures and high surface area. It can provide the practical solution because the materials used in this research is cost efficient and abundant in nature.

Biography

Vivekanandan Raman, doing Ph.D. student in Electrical Engineering at Pusan National University. Working in the field of synthesis of nano materials and its application, concentrating in the field of Super Capacitors and Solar Cells with two publications.

Visible-light-induced degradation of polybrominated diphenyl ethers

Chunyan Sun*, Ph.D
Shaoxing University, China

As typical persistent organic pollutants, polybrominated diphenyl ethers (PBDEs) have aroused highly environmental concerns because of their toxicity and recalcitrant degradation. Here, we will report the visible-light-induced degradation of PBDEs by several strategies. The reaction kinetics, influence factors and possible photoreductive mechanisms have been discussed. This research may provide the green and efficient methods to remove halogenated pollutants by using visible light.

Audience Take Away:

- Efficient degradation of polybrominated diphenyl ethers (PBDEs) under visible light irradiation.
- Mechanistic pathways of degradation of PBDEs were different under UV and visible light.
- It is a green and efficient method to remove halogenated pollutants by using visible light.

Biography

Chunyan Sun received her Ph.D. in Institute of Chemistry, Chinese Academy of Sciences (CAS) in 2010. She has been a Visiting Scholar in John C. Crittenden's group in School of Civil and Environmental Engineering of Georgia Institute of Technology, USA in 2017. She is an associate professor in the school of Chemistry at the Shaoixing University in China

Her research interestfocuses onthe photochemistry reactions in the environment and synthesis of novel photocatalytic materials for degradation of organic pollutants and the relevant mechanisms.

magnus
Group

e-Poster Presentations

Global Conference on

Catalysis and Reaction Engineering

October 19 - 21, 2017 | Las Vegas, USA

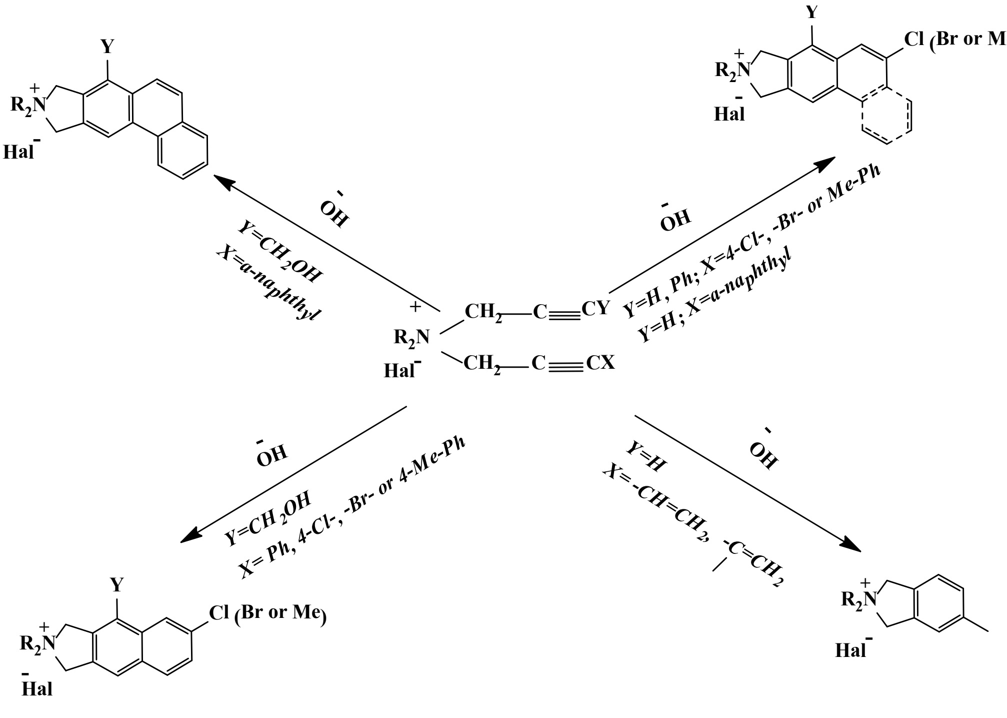
GCR 2017

Base catalized intramolecular cyclization of unsaturated ammonium salts and recylclization of derivatives of 4-hydroxymethyl isoindolinium chlorides

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

In 1969 by acad. Babayan A.T. and prof. Chukhajian E.O. with coworkers was discovered that ammonium salts, containing groups of allylic or propargylic type along with alkenylprop-2-ynylic, even in the presence of 0,2 mol of alkali per mol of initial salt at room temperature undergo with self-heating intramolecular cyclization; reaction ends within 5-10 min, forming potentially bioactive isoindolinium and 3a,4-dihydroisoindolinium bromides with quantitative yieds. Later it was shown that instead of expected last salts were obtained their isomeric forms – 2,6,7,7a-tetrahydro-1H-isoindolinium bromides.

In above mentioned conditions with self-heating undergo cyclization also ammonium salts containing propargylic type group alongside with 3-arylprop-2-ynylic fragment leading to formation of bioactive di-, three- and polycyclic isoindolinium and dihydroisoindolinium salts. As a result of cyclization of –(4-hydroxybut-2-ynyl)(3-alkenyl- or 3-arylprop-2-ynyl)ammonium chlorides–hydroxymethylisoindolinium salts and their condensed analogs are obtained.



In 2003 by us was discovered that mentioned salts in water-base cleavage conditions undergo intramolecular recyclization leading to derivatives of 1,3-dihydrobenzo[c]furans, formation of which includes the stages of nucleophylic attack of an alkoxy anion on partially charged carbon atom of isoindolinium cycle with the breaking of N-C and formation of C-O-C bond. It was established that voluminous substituents at nitrogen atom and in aromatic ring and also the increase of the number of aromatic cycles favorably act on recyclization. In contrast to intermolecular recyclization the process is not accompanied by any expansion or contraction of the cycle, and instead of isoindolinium cycle pharmacophore 1,3-dihydrofuranic ring is formed. Intramolecular recyclization is a domino process, has general character and besides of fundamental has also preparative significance. It was known that some of derivatives of 1,3-dihydrobenzo[c]furans are a part of molecules of diterpens and contained in sea sponges and algas and used in clinical practice as antidepressants and etc.

Base catalized intramolecular cyclization and recyclization are new directions in organic chemistry. Among cyclic products are representatives with high pharmacological activity.Activity is protected by numerous copyrights of Soviet Union and patents of Republic of Armenia.

The acquaintance with the results of base catalized intramolecular cyclization and recyclization enlarge the horizon of each organic chemist in this field.

Compounds which are result of these reactions can be objects of pharmacological investigations for creation of medicinal preparats and also representatives with new pharmacological activities.

New model for the description of sorptive and textural properties of CaO-based sorbents changing during repetitive sorption/regeneration cycles

Ya.B. Bazaikin[1,3], Ph.D., E.M. Malckovich[1,3], Ph.D., A.G. Okunev[3,2], Ph.D., A.I. Lysikov[3,2], Ph.D., V.S. Derevschikov*[3,2], Ph.D
[1]Sobolev Institute of Mathematics, Novosibirsk, Russia.
[2]Boreskov Institute of Catalysis, Novosibirsk, Russia.
[3]Novosibirsk State University, Novosibirsk, Russia

Carbon dioxide separation from gas mixtures is critical process in several emerging energy-related industries, including in hydrogen production by means of biomass utilization and exhaust gas clean up. Some studies on this topic suggest using calcium-based sorbents for effective CO_2 capture from gases at high temperatures because of potential advantages including: a wide range of operating temperatures; reduced energy penalties; avoidance of liquid wastes; the relatively inert nature of solid wastes.

However, the use of CaOas a regenerable CO_2 sorbent is limited by the rapid decay of the carbonation conversion with the number of carbonation/calcination cycles. The main reason for CaO capacity decay is sorbent sintering during sorption/retgeneration cycles.

The evolution of sorptive and textural properties of CaO-based sorbents during repetitive sorption/regeneration cycles has been mathematically simulated in this study. The proposed model takes into account the morphology of nascent CaO, sorbent sintering physics and CO_2 sorption kinetics. The results show that the model is in good agreement with the experimental data for real sorbents and predicts the dependence of the recarbonation extent on the number and duration of the sorption/regeneration cycles well. The model allows predicting the change of the textural properties of the sorbent (e.g. the values of specific surface area and mean pore size) during the sorption/regeneration cycles. The structure of the sorbent was modeled with the dense random packing of spheres using the Lubachevsky–Stillinger compression algorithm. The sintering was simulated under the following assumptions: the sintering proceeds via the lattice diffusion mechanism, and the sintering rate of $CaCO_3$ is higher than that of CaO. Note that, depending on the carbonation duration, our model predicts that the maximal thickness δ of the $CaCO_3$ layer constitutes 7% or 11% of the mean diameter of grains. Thus, taking into account that the radius of original CaO was near 300 nm, we can obtain that the effective thickness of the $CaCO_3$ layer is near 20–30 nm that is close to the experimental estimations. It should be noted that the calculated value 2.8 m^2 /g of the specific surface area of the parent sorbent is close to the experimental value of 4.2 m^2 /g for the sorbent produced by the $CaCO_3$ decomposition (Lu et al., 2006). To estimate the change in the sorbent pore size distribution during the cycling, we used the chord-length probability distribution (CLPD) method (Lu and Torquatoa, 1993). In this method, the mean chord length lC estimates a characteristic length of the porous space and can be interpreted as a first approximation of the mean pore half-size. Diminishing of the pore size from initial to final cycle also means the reducing of pore volume in the set of spheres i.e. its shrinkage. In this way sintering in the system drives to decrease the size and the volume of small pores inside the sets, but to increase of the pore volume which size comparable to the size of the sets in a multisets system. Similar pore size redistribution during cycling confirmed experimentally (Alvarez and Abanades, 2005). Indeed, some more advanced simulations approaches are needed to extract the exact morphological characteristics of porous systems (pore volume, geometry and size distribution) and it will be a task for our subsequent work. The work was performed under support of RFBR (Research project No. 16-33-00436 mol_a)

Audience Take Away:

- A method will be presented for modeling the change in the texture of porous bodies during the sintering process. The approach allows to monitor changes in the parameters of the porous medium during the sintering process: porosity, pore size distribution and sorption capacity.
- This approach can be used to describe the deactivation of catalysts and sorbents

Biography

Dr. Derevshchikov is a researcher at Boreskov Institute of Catalysis, Novosibirsk. Field of interests: Regularities in the formation of the texture of catalysts and sorbents.

Study of the migration of PVC plasticizers on ultrasonic metal welding

Sandra Matos*[1], Fernando Veloso[2], Carlos Santos[2], Leonardo Gonçalves[3], Emanuel Carvalho[4]
[1]University of Minho, Portugal
[2]PE, Delphi
[3]Setubal Polytechnic Institute
[4]Lisbon Superior Institute of Engineering

The ultrasonic metal welding process allows the joining of metals by the application of high frequency vibrations, under moderate pressure, in which the vibrations are applied parallel to the interface between the parts. The frequency between the parts, forms a solid-state weld through progressive shearing and plastic deformation over the surface asperities that disperses oxides and contaminants and brings an increasing area of pure metal contact between adjacent surfaces. The problems of metal oxides, high thermal conductivity, high electrical conductivity, intermetallic and brittle alloys are not significant in the ultrasonic welding since the ultrasonic equipment may be capable of monitoring energy and control the critical welding variables. However, on automotive industry, for applications that involve the ultrasonic welding of wires it has been seen that depending on the coating material of wires the metal bonding is not always stronger as it should be. Several studies were been done using different types of materials as insulators and as a results it was seen that PVC coated wires have worst results and even those are varying depending on the PVC formulation used. PVC is considered one of the most versatile polymers due to their ability to react with various additives before being processed into final products. By the choice within a wide range of chemicals, it is possible to obtain PVC compounds with the necessary features for each application but there are a large number of variables that affect the properties of PVC such as the degree of crystallinity, the glass transition temperature, molecular weight or morphology. The mechanical, thermal or chemical properties of the manufactured product may have specific characteristics, mainly due to two important factors: inclusion of appropriate additives in PVC formulations (plasticizers, pigments, lubricants, colorants, flame retardants, etc.) and a variety of manufacturing processes such as extrusion, injection, etc. As coating of wires, PVC is used in the flexible form, but due to PVC thermal instability, processing it is virtually impossible without the addition of additives. The additives are generally high molecular weight thermoplastic and are added in small quantities with three main functions, accelerate the fusion process, improve the rheological and mechanical properties. The biggest disadvantage of PVC is the easiness to degrade by the action of temperature or ultraviolet radiation. In order to identify the cause of negative effect on ultrasonic metal welding process of wires, a study was conducted using electrical wires coated with PVC with different formulations.

Audience Take Away:

- Understand the ultrasonic metal welding process used on electrical cables
- Understand the process limitations in regard the types of coating available in the market and be able to identify possible cause for bad results achieved during the process
- With the study already done it was seen that the type of plasticizers used on insulation material are directly related to results on ultrasonic metal welding of coated electrical wires
- The study can be followed on other universities since it seems to be possible the development of new methods to improve stability of materials.

Biography

Sandra Matos is a Ph.D student at Department of Polymer Engineering in University of Minho. She studied Chemistry Engineering at Lisbon Superior Institute of Engineering and had an M.Sc in Polymer Processing and Technology at University of Minho, she is been studying the behavior and the processing effects of materials used on coating of wires for Automotive Industry. She is mainly doing researches on chemical effect of materials used on coating of electrical automotive wires and its impact in processes used at that industry. She is also serving as a reviewer of several reputed journals.

INDEX

Notes

About GCR 2018

2nd Global Conference on

Catalysis and Reaction Engineering

September 20-22, 2018, Rome, Italy

www.catalysis-conferences.magnusgroup.org