



PRISM

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Venue

Mantra Bell City
215 Bell Street, Preston, VIC 3072
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Keynote Session

Catalysis for X-ray Nanochemistry

Ting Guo

University of California, USA

Abstract

Will be updated soon

Three Step Catalytic Synthesis of Furandicarboxylic Acid (FDCA) from Sugar Acids

Tuulamari Helaja

VTT Technical Research Centre, Finland

Abstract

Will be updated soon

Special Talks by the CatScience Board

Renewable Hydrogen Production at NanoStructured Interfaces

Ahmed F Halima

Hydrogen Group, RMIT University, Australia

Abstract

Will be updated soon

Engineering the Radical and Catalytic Properties of Graphene Oxide

Jingliang Li^{*} and Zahra Komeily Nia

Deakin University, Australia

Abstract

Graphene oxide (GO), as a precursor of graphene, has been widely studied. The surface functional groups, which contribute to its many applications, can be manipulated during the oxidizing exfoliation of graphite and by subsequent reduction treatments. Although an in-depth understanding of the surface chemistry of GO has been achieved, an important aspect has been overlooked. Compared to graphene, GO and reduced GO (rGO) have many structural defects, which are believed to contribute to the presence of radicals and the reactivity (e.g. catalytic activity) of these materials. However, a detailed understanding of how the content of radicals and thus the reactivity of GO can be optimized has not been achieved, which limits its applications. In the last few years, our group has focused on understanding the key structural features governing the free radical content of GO. The size and surface chemistry of GO were tuned by manipulating its degree of oxidization during its preparation and subsequent reduction treatments. It was observed that a maximal radical content of GO could only be achieved at a specific C/O ratio of c.a. 3.0 by a combination of oxidation and reduction treatments. We also observed that the catalytic reactivity of GO is linearly correlated to its radical content.

Our findings complement the current understanding of GO chemistry and are significant to many applications such as metal-free catalysis. In this talk, the progress in our fundamental understanding of the radicals and their applications will be presented.

Biography

Jingliang Li received his PhD in Chemical Engineering from the National University of Singapore. After a few years' postdoctoral research in the physics department of this university, he moved to Australia. He received a prestigious Future Fellowship from the Australian Research Council (ARC) and is an associate professor at the Institute for Frontier Materials of Deakin University, Australia. Dr. Li has expertise in a broad range of fields including nanomaterial, biomaterials and supramolecular materials.

An Approach to Sustainability: Agro-Waste as Catalyst for Value-Added Compounds

Pranjal Kalita

Central Institute of Technology, India

Abstract

With increasing population, the demands for production of agricultural, food, fuel and chemicals are increased along with huge amount of waste and pollution from the respective sectors per day globally. Thus, researchers are highly encouraged to develop sustainable technology and green novel routes for preparation of chemicals via several types of organic reactions. This is mainly for the protection of the environment, human health, atom efficiency, technological feasibility, and economically safer way. Solvents and organic reagents or homogeneous catalysts plays a key role for performing organic reactions. In addition, solvents are often essential for performing multi-step reactions, mixing between two substrates, workup procedures, separation of pure compounds, etc. After the reaction, dispose or storage of solvents and bi-products of the organic reagents are serious problems which create safety and environment issues as well as toxic effect to the water, soil and as a whole living being. With an aim to produce non-toxic, hazardous solvents / materials and low concentration of CO₂ in the environment, we are highly motivated for utilization of available biomass into its applicable. Thus, we have chosen commonly available waste biomass or agro-waste like waste banana peels & rhizomes, waste brassica Nigra plants and Sesamum indicum, etc. Due to basic in nature of all mentioned agro-waste, they are used as heterogeneous catalyst in the area of base-catalyzed organic chemistry. The high yields of 99 and 95% of catalytic activities were observed in transesterification for biodiesel synthesis and aldol reaction, respectively. The details of the work will be discussed in the presentation.

Biography

Presently, Dr. Pranjal Kalita is working as Associate Professor in the Department of Chemistry in Central Institute of Technology Kokrajhar (Deemed to be University, MHRD, Govt. of India), Kokrajhar, Assam. His broad research areas are heterogeneous catalysts, pyrolysis, alternative fuels and chemicals. With a PhD from National Chemical Laboratory, Pune (India) in 2008 and prior to joined in CITK & TERI, spent professional time in TERI, New Delhi and total 5 years of postdoctoral research including National Institute for Materials Science, Tsukuba, Japan; Iowa State University & Georgia Institute of Technology, USA. Presently, Currently, he is devoting his time utilization of biomass as heterogeneous catalyst and porous heterogeneous catalyst for synthesis of chemical intermediate and value-added products. Till now, he has credited 30 numbers of international publications including journals, book, book chapter, conference proceedings. In addition, delivered several numbers of talks as invited in international and national levels.

Adsorption and Decomposition of Lignin Fragments on a Platinum Catalyst

Javier B. Giorgi^{1*}, Cherif A. Ould Hamou¹, Mohammed Z. Asiri^{1,2}, Kusuma V. Adiningtyas¹, Romain Réocreux³, Carine Michel³ and Philippe Sautet^{3,4}

¹University of Ottawa, Canada

²Prince Sattam Bin Abdulaziz University, Saudi Arabia

³ENS de Lyon, France

⁴University of California, USA

Abstract

Catalysis plays an essential role in making biomass conversion viable for valorization by reducing activation energies for reaction and guiding product selectivity. Lignin, an important biomass component, can be simplistically described as a large molecule consisting of aromatic rings linked together by various forms of oxygen links. To valorize lignin as a renewable source of aromatics, it is necessary to develop selective heterogeneous catalysts for the hydrodeoxygenation reaction of aromatic oxygenates. Most of the metal-supported catalysts tested so far exhibit a high conversion but a low selectivity toward valuable aromatic hydrocarbons, yielding mainly phenolic compounds. To gain insights into catalytic activity, single-crystal investigations of aromatic oxygenates on transition metal surfaces have shown different preferences in C–H, C–O, and C–C bond cleavages. The decomposition pathways of aromatics seem to be strongly dependent on the coverage of adsorbed molecules on the surface and the interaction strength of the aromatic ring with the catalyst. Density functional theory (DFT) and surface studies (XPS, TPD and RAIRS) of increasingly complex small model molecules will be used to identify and explain reaction pathways for lignin decomposition with unexpected selectivity. As an example, whereas anisole leads to phenol under high pressures, in the absence of hydrogen pressure it leads to benzene. In contrast, veratrol leads to the formation of catechol, even in UHV conditions.

Biography

Javier Giorgi obtained his PhD from the University of Toronto (1999) and was a Humboldt fellow at the Fritz Haber Institute in Berlin. Since 2002, he has been a Professor in the Department of Chemistry at the University of Ottawa. Prof Giorgi has been the Chair of the Physical Chemistry Division of the Canadian Society for Chemistry and the Associate Director of the Centre for Catalysis Research and Innovation at uOttawa. He has been an active participant in national and international fuel cell and catalysis networks. Recent work has focused on the catalytic transformation of biomaterials into value added chemicals.

Esterification of Acetic Acid with Methanol using Sulfated Carbonaceous Catalyst: Parametric and Kinetic Study

Sarvjeet Kaur^{1,2*} and Rajiv Arora²

¹Shaheed Bhagat Singh State Technical Campus, India

²Government Polytechnic College Guru Tegh Bahadur Garh, India

Abstract

The esterification of acetic acid with methanol in the presence of sulfated carbon acid catalyst was studied in a batch glass reactor. In the present work, a strong solid acid catalyst, prepared by sulfonating carbonized wood, was proved to be an efficient and environmental friendly catalyst for the esterification of acetic acid and methanol. The influence of certain parameters such as stirring speed, catalyst loading, molar ratio and reaction temperature were carried out to optimize the conditions for maximum conversion of methyl acetate. A detailed kinetic study was carried out using second order pseudo-homogeneous kinetic model. The kinetics parameters and activation energy were determined from Arrhenius plot.

Keywords: Heterogeneous catalysis, kinetics, esterification, Acetic acid, Methanol, Sulfated carbon acid catalyst

Biography

Sarvjeet Kaur Kullar has completed her Master's degree in Chemical Engineering from a reputed institute: Shaheed Bhagat Singh State Technical Campus, Ferozepur, India. She is working as a lecturer in Government Polytechnic College G.T.B Garh Moga India since 2011. Her research work is around esterification and catalysis.

Manipulation of Internal Chemistry of Transition Metals Compounds for Enhanced Catalytic Processes

Nasir Mahmood

RMIT University, Australia

Abstract

Will be updated soon

Bifunctional CoMn-Oxide Catalysts for Catalytic Transfer Hydrogenation of Levulinic Acid to γ -Valerolactone

Jinyao Wang, Xiao Yu, Bin Yin, Chaohe Yang and Xin Jin*

China University of Petroleum, China

Abstract

The rapidly diminishing fossil fuel reserves and significant exhaust emission to environment have promoted the transition from fossil energy to renewable alternatives. Biomass, as one of the most abundant and renewable carbon resources on earth, can be transformed into transportation fuels and chemicals [1]. Levulinic acid (LA) is one of the most promising platform molecules produced from cellulose or C6 sugars with 5-hydroxymethylfurfural as an intermediate [2-4]. Hydrogenation of LA can produce γ -valerolactone (GVL), which is a sustainable chemical and has been used as green solvent, food additive or renewable bio-fuel [5]. Traditional hydrogenation processes are often conducted under harsh conditions, which unfavorably facilitate catalyst deactivation and significant formation of by-products. Catalytic transfer hydrogenation (CTH) in the absence of externally added H₂, however, display environmental and economic advantages.

Formic acid (FA) is an important co-product during the production of LA. Using FA as H-donor can make CTH process of LA more economical [6]. More importantly, most existing studies on CTH of LA were primarily focused on noble metals. The nature of non-noble metal catalysts on tandem H₂ generation and hydrogenation is still not clear. Therefore, in this work, we proposed unique hybridized CoMn oxide catalysts for CTH of LA to GVL using FA as H-donor in aqueous phase. The key finding is that, strong Co-Mn and Co-Con⁺ interaction induced structural reconstruction, leading to about 3 fold activity enhancement compared with monometallic CoO and MnO oxides. Catalyst characterization by XRD, XPS, BET, TEM and SEM techniques revealed the electronic coupling nature at CoO-MnO interface and significance of {Co, Mn}{Co, Mn}2O₄ phase for synergistic CTH of LA in the presence of FA. Conversion of LA and FA molecules were found to be follow high-temperature water (HTW) mechanism [7] where both substrates were adsorbed on active sites, thus H₂ transfer reaction from FA to LA occurred over CoMn oxide catalysts.

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Biography

Xin Jin obtained Ph.D from University of Kansas under the supervision of Professor Raghunath V. Chaudhari. Before joining China University of Petroleum, he worked as post-doctoral researcher at Center for Environmentally Beneficial Catalysis from 2014-2016. He received early promotion to Associate Professor in 2017. His research areas are focused on nanocatalysis, biomass conversion and multiphase kinetics. He is the recipient of Richard Kokes Award from North American Catalysis Society, ACS Catalysis Early Career Award, Frank Bowditch Excellent Research Award and Young Scientist Award from North American Symposium on Chemical Reaction Engineering.

Sulfated Tin(IV) Oxide Catalyst for the Partial Coupling Reaction of α -Pinene to Produce Less Viscous High-Density Fuel

Seong-MinCho*, Da-songLee, June-HoChoi and In-GyuChoi

Seoul National University, South Korea

Abstract

Brønsted acid-catalyzed reactions of α -pinene have been studied because of their ability to produce various types of fragrance molecules. Beyond this application, dimeric hydrocarbon products produced from coupling reactions of α -pinene have been suggested as renewable high-density fuel molecules. In this context, we present the application of a sulfated tin (IV) oxide catalyst for the partial coupling reaction of α -pinene from turpentine. Brønsted acid sites inherent in this solid superacid catalyst calcined at 550 °C successfully catalyzed the reaction, giving the largest yield of dimeric products (49.6%) at 120 °C over a reaction time of 4 h. Given that the low-temperature viscosity of the mentioned dimeric products is too high for their use as a fuel in transportation engines, lowering the viscosity is an important avenue of study. Therefore, our partial coupling reaction of α -pinene provides a possible solution as a considerable amount of the isomers of α -pinene still remained after the reaction, which reduces the low-temperature viscosity. On the basis of a comparison of the reaction products, a plausible mechanism for the reaction involving coinstantaneous isomerization and coupling reaction of α -pinene was elucidated.

Biography

Seong-Min Cho is a PhD candidate at the Department of Forest Sciences at Seoul National University, Seoul, Republic of Korea. He received a bachelor's degree in Environmental Materials Science in 2015 from Seoul National University, Seoul, Republic of Korea. His current research interests include the catalytic conversion of biomass to biofuels and biochemicals.

Long-Term Evaluation of Pre-Reforming Catalysts for Pressurized Liquid-Fuel Reforming

Joongmyeon Bae^{1*}, Jae Young Yoo¹, Jaemyung Lee¹, Aadesh Harale² and Sai Katikaneni²

¹Korea Advanced Institute of Science and Technology, South Korea

²Saudi Aramco, Saudi Arabia

Abstract

Due to its eco-friendliness and high energy density, hydrogen has recently gained wide attention as an important energy carrier for developing a future low-carbon society. Even with many advantages, hydrogen economy needs to reduce costs of production and delivery to be more attractive in the energy market. One possible approach is to install hydrogen filling stations, which produce hydrogen on-site from liquid fuel. We propose a novel and compact system that comprises a pre-reformer (PR) and a membrane reformer (MR) operating at high pressure. The PR produces a methane-rich gas by cracking liquid hydrocarbons. The product gas is then fed to the MR to reform the remaining methane and permeate high-purity hydrogen. One important consideration is to ensure long-term stability of the PR catalyst. In high-pressure liquid fuel reforming, however, multiple factors may degrade the catalyst. They include carbon coking, agglomeration, and evaporation of active metals. Several experiments were conducted to achieve continuous, stable catalyst performance. We tested engineering factors such as pressure, temperature, and steam-to-

carbon ratio. The lab-scale PR used our Ni-Ru/CGO catalyst. For its long-term stability, the steam-to-carbon ratio and temperature should be higher than 3.0 and 550°C, respectively. The catalyst successfully reformed heavy naphtha for 1,536 h. After wards, the PR produced ethylene, which indicated performance degradation. Catalyst analyses led to several results, which suggested that agglomeration may have been the leading cause of the degradation.

Biography

Prof. Joongmyeon Bae has been a professor in the Dept. of Mechanical Engineering at KAIST in South Korea since 2012. His research interests are SOFCs and reforming. He holds B.S. and M.S. degrees in Inorganic Materials from Seoul National University and a Ph.D. degree in Material Science from Imperial College, London. He was a researcher at the Electrotechnical Laboratory of NEDO in Japan from 1996 to 1999 and a senior researcher at Argonne National Laboratory in the U.S. from 1999 to 2002. He has published more than 100 papers. He founded H&Power, Inc. in 2009 and is currently its technical advisor.

Production of Phenolic Compounds from Bagasse Lignin via Catalytic Pyrolysis of $\text{CaZr}_x\text{Fe}_{1-x}\text{O}_3$

Yanguang Chen^{*}, Hua Song, Jun Wang and Mei Zhang

Northeast Petroleum University, China

Abstract

The greater demand for the fossil fuel associated with the lack of availability of some petrol fractions and an increased environment concerns warrant a replacement resource for energy and material. Large amounts of bagasse was produced in sugar industry. Chemical method is an important approach to convert bagasse lignin (BL) into chemical products, which favors in resource and high-value utilization of bagasse. A series of perovskite-type mixed ionic and electronic conductors $\text{CaZr}_{1-x}\text{Fe}_x\text{O}_3$ (CZFO-x) were prepared using the solid state reaction method. The crystal form, morphology, metal valence state of catalysts were characterized by XRD, SEM, XPS and the thermal stability of bagasse lignin were performed using TG-DTA, respectively. Productions of phenolic compounds from bagasse lignin via catalytic pyrolysis were evaluated in a fixed bed micro-reactor. The results show that the calcined CZFO-x pellets deposit randomly in the form of irregular grains or flake with compact structure. XRD spectra of the CZFO-x after calcination showed high intensity peaks characteristic in the presence of CZFO phase. Moreover, the pyrolysis temperature of lignin was significantly reduced under the action of CZFO-0.2. In the test of fixed bed micro-reactor, the yield of liquid product was about 23.71%. Under 500°C and atmospheric pressure, the phenolic products were mainly consisted with phenol, guaiacol, lilac phenol and catechol, whose selectivity was 35.19%, 6.18%, 10.68% and 14.21%, respectively. The rest of liquid products were benzene and methoxy aromatics. The CZFO-0.2 after regeneration exhibited the high structural stability and the better catalytic activity. A possible reaction pathway for the catalytic pyrolysis of bagasse lignin was proposed over CZFO-0.2 catalysts in a relatively mild condition under a nitrogen atmosphere.

Biography

Dr. Yanguang Chen, now is a professor of Chemical Engineering in Northeast Petroleum University, China. He got his B.S. at China University of Petroleum (Beijing) and Chemical Doctor's degree (Ph.D.) at Institute of Process Engineering, Chinese Academy of Sciences. Currently Dr. Yanguang Chen researches focus on Energy and Environmental Engineering, and Fossil and Biomass Energy Catalytic Conversion.

Green Polymers from Waste Glycerol: A Sustainable Catalytic Process

Shanthi Priya Samudrala^{1*}, Bhanuchander Ponnala² and Komandur V R Chary²

¹Monash University, Australia

²Indian Institute of Chemical Technology, India

Abstract

With the dwindling fossil-based energy reserve and increasing environmental awareness, the quest for sustainable energy production has become an urgent social issue. Apparently, alternative bio-based fuels are emerging as the long-term solution.

Glycerol, is a simple trihydroxy molecule with over 2000 known applications in various industries and is largely available as a by-product from the biodiesel production process. As the biodiesel industry is rapidly expanding, a glut of crude glycerol is being created, with an approximate global production of six million tons by 2025. The large volume of accumulated glycerol devalues the industrial biodiesel production process, dropping the market price of glycerol. Therefore, valorisation of glycerol for production of value-added fuels and chemicals is one manner of relieving the glycerol oversupply and to expand the scope of biobased fuels & chemicals. One of the most attractive routes of upgrading glycerol is the formation of 1,3-propanediol (1,3-PDO) by hydrogenolysis. 1,3-PDO is a valuable industrial chemical with wide applications from carpet and textile manufacturing to cosmetics, personal, and home care industry. It is mostly used as a building block in the synthesis of polytrimethylene terephthalate polymer. Vapor phase hydrogenolysis of glycerol performed over various loadings of tungstate platinum catalysts supported on titanium phosphate under reaction ambient conditions resulted in excellent selectivity to 1,3-PDO. The Bronsted acidity of the catalysts played a key role in enhancing the 1,3-PDO selectivity in a bifunctional dehydration-hydrogenation of mechanism of glycerol.

Biography

Shanthi Priya Samudrala is an early career researcher and received her PhD in 2016 from RMIT University. She is currently working at Monash University as a lecturer and researcher in the Department of Chemical Engineering. She holds research interests in the areas of heterogeneous catalysis, material development, biomass valorization processes, bio-based chemicals and fuel production. Her research primarily sits in the area of green chemistry and sustainability focusing on the development of novel and highly efficient catalytic materials for biomass valorization by using eco-friendly and economic viable synthetic routes that would increase the sustainability of biofuel and chemical industries.

Keynote Session

Dimethylether: A Plausible Clean Fuel for the Future? Yes, If Kegginheteropolyacid Catalysts are Properly Used to Convert Methanol: Mistakes to Avoid and Recipes to Follow!

Eric M. Gaigneaux* and Josefine Schnee

Université catholique de Louvain, Belgium

Abstract

Being a promising renewable fuel, the production of dimethylether (DME) via the gas phase condensation of methanol nowadays attracts growing interest. Because of their exceptionally high Brønstedsuper-acidity, heteropolyacids (HPAs) deserve to be explored in this context.

The Keggin H₃PW₁₂O₄₀ HPA indeed allows reaching high methanol conversions at much lower temperatures than conventional acid catalysts and leads to much better selectivity to DME. However, bulk H₃PW₁₂O₄₀ displays low surface area which might limit its overall performance.

A first option to cope with this is to exploit the capability of HPAs to catalyze reactions in the pseudo-liquid way, precisely to perform the condensation of methanol not only at the surface of HPA crystals but also within their bulk, so exploiting the protons located therein. This behavior has already been evoked in the past but yet not really exploited. Thanks to a Raman operando approach, we will show how to succeed this. Precisely, we will enlighten the pretreatment conditions allowing H₃PW₁₂O₄₀ to have its bulk simultaneously accessible for methanol and catalytically active [Catalysis Science & Technology, 2017, 7, 817-830].

A second option is to disperse HPAs on supports. TiO₂ is often claimed as an excellent choice... but it is actually not. We will demonstrate that, if indeed HPAs disperse well on it, their strong interaction with TiO₂ markedly lowers their acid strength, with correspondingly a lowered efficiency to convert methanol. In this context, we will point hexagonal boron nitride as a much better support. [ACS Catalysis, 2017, 7, 4011-4017].

Biography

Being bioengineer (UCL, 1993) EMG got his PhD (UCL, 1997, supervisor B. Delmon), and was fellow of the FNRS (1993-2004). After

stays in UK (ICI-Katalco, 1995), USA (University of Notre-Dame, supervisor E. Wolf, 1995), Germany (Fritz Haber Institute, supervisor R. Schlögl, 1998) and Japan (University of Tokyo, supervisor Y. Iwasawa, 1998-1999), he became professor (UCL, 2004). He is full professor since 2014, and guest professor at EPN (Quito, Ecuador, 2014-). EMG got the ExxonMobil Award (2003), and the Belgian Royal Chemical Society award (2013). He mainly works on heterogeneous catalysts preparation, in situ/oper and characterization, biofuel production, de-pollution, valorization of hydrocarbons/alcohols/biomass.

Special Talk

First-Principles Study of Catalytic CO₂/Water Decomposition on Layered Materials

Hong Seok Kang

Jeonju University, South Korea

Abstract

Based on a combination of various first-principles methods, we propose a layered material for photocatalytic CO₂ decomposition, which is tetragonal GeP₂ with optimal band offset with respect to two half-reactions (HRs) of the decomposition in wide pH range. Also will be described is a series of my recent collaboration with an experimental group for photocatalytic/electrocatalytic water splitting based on MoS₂/WS₂-guest hybrids. First, combined experimental and semiquantitative theoretical effort is described for efficient photoelectrochemical water splitting of p-GeAs/n-Si and p-GeP/n-Si heterojunctions based on the band edge positions obtained from the HSE06 hybrid band structure calculation, band offset, build-up of space charge in the junctions, and the band bending of the n-Si at the electrolyte interface. Second, our extensive DFT calculation complemented by analyses of sulfur vacancy formation, charge transfer, electronic structure, and the activation barrier of Volmer-Heyrovsky reactions give a panoramic insight into our experimental results, which have shown that the 1T'-phase guest-intercalated MoS₂/WS₂ nanosheetssynthesized by one-step hydrothermal reaction exhibit excellent stability as well as higher catalytic activity toward hydrogen evolution reaction. A variety of guest species is taken into account such as cobaltocene, porphyrin, phenylenediamine, and ammonium ion. Finally, we show that an extensive ab initio molecular dynamics simulations not only reproduce collaborative experimentalvoltage-charge capacity curves for WS₂@graphite and WS₂@nitrogen-doped graphitecomposites in lithium ion battery but also gives us a detailed picture on the structural evolution in the charge-discharge process, which is essential for its high performace.

Scientific Session-2

Materials | Chemical Kinetics

Development, Characterization and *in vitro* Assessment of pH Sensitive Gelatin-Sodium Dodecyl Sulfate/Sodium Alginate Blend Hydrogel Film for Controlled Drug Release

Lisa Sreejith* and P.K Muhammed Adnan

National Institute of Technology Calicut, India

Abstract

A cost effective and viable method to synthesis and characterize a drug carrier film for the controlled and safe oral drug delivery is reported. In the present study, alginate is blended with gelatin-SDS gel complex to achieve improved performance and attempted to synthesize and characterize a pH sensitive drug carrier film for controlled drug delivery. Calcium is used as the cross linking agent in the film preparation to replace toxic organic cross-linkers which may harmfully interact with the entrapped drug. As a physical hydrogel, the drug delivery matrix which is completely degradable and comes under swellable mucoadhesive drug carrier for controlled and targeted drug release in the stomach. Ciprofloxacin hydrochloride (Cip HCl) was used as the model drug and the drug-loaded films were prepared by casting/solvent evaporation method. It is further characterized by Scanning Electron

microscopy (SEM), Fourier Transform Infrared Spectroscopy (FT-IR), X ray diffraction (XRD), Transmission Electron Microscopy (TEM) and studied for its invitro release. The results showed the prepared film is stable, homogenous, and is pH sensitive in drug release.

Biography

Dr. Lisa Sreejith, Professor, Department of Chemistry, National Institute of Technology Calicut, India did her doctoral studies with Prof. Kabir-ud-Din of Aligarh Muslim University, Aligarh, UP in 1996 and continued in the department as research associate till she joined the then Regional Engineering College, Calicut in 1997. She had developed a Soft Materials Research laboratory where 6 students completed their Ph.D, 4 more research scholars are in different stages of their doctoral work. She has 48 international journal publications, 63 papers presented in various national/international conferences and 2 Indian patents to her credit. More than 80 M.Sc projects were completed under her guidance she is the reviewer for 4 International research journals and is the editorial member for International Journal of BioSciences and Technology.

Theoretical Study of Electronic Structure and Catalytic Activity in Metal Nanoparticles

Takayoshi Ishimoto

Yokohama-City University, Japan

Abstract

Metal nanoparticles are widely used in environmental applications and energy-related devices. It is reported the bimetallic core-shell and solid-solution nanoparticles show different properties, such as stability and catalytic reaction. To obtain the target function of nanoparticles, the control of the phase stability is one of the important approaches. For example, Pd/Pt solid solution system can absorb larger amount of hydrogen compared with pure Pd nanoparticles, although Pd and Pt are phase separation system in bulk. However, the mechanism of phase change between core/shell and solid solution of PdPt nanoparticle is still unclear. In this study, we calculated electronic structure and optimized geometry of PdPt nanoparticles by using density functional theory. We found that the PdPt solid solution phase was found to be a stable phase in the nanoparticles compared with Pd-Pt core-shell nanoparticles. Details of the results and related calculation results for other metal nanoparticles are also shown in the presentation.

Biography

Takayoshi Ishimoto received his Ph.D. at Rikkyo University in 2004. After Grid Research Center and Research Institute of Computer Science in National Institute of Advanced Industrial Science and Technology, he moved to Kyushu University as Assistant Professor of INAMORI Frontier Research Center in 2009. Since 2016, he has been an Associate Professor at Graduate School of Engineering, Hiroshima University. Now he is an Associate Professor at Graduate School of Nanobioscience, Yokohana City University. Recent his research interest is catalytic reactivity design based on electronic structure modification of metal nanoparticles.

Synthesis of Porous Hybrid 2D-3D CeO_{2-x} and Heterojunction Nanostructures for High-Performance Catalysis

Charles Christopher Sorrell^{1*}, Sajjad Mofarah¹, Esmaeil Adabifiroozjaei², Pramod Koshy¹, Constantine Tsounis¹, Jason Scott¹ and Yin Yao¹

¹UNSW Sydney, Australia

²Research Center for Functional Materials (RCFM), Japan

Abstract

Two-dimensional (2D) nanomaterials exhibit unique chemical and electronic properties that are absent in other-dimensional nanostructures. These properties arise from their high surface-to-volume ratios, with highly exposed sites, thereby making the nanostructures suitable for surface-dependent applications, i.e., catalysis. This newly emergent class of 2D materials consists of nanosheets containing nanovoids that maximise the number of unsaturated covalent bonds at the edge sites. Despite promising performances, their fabrication processes are challenged by complexity and the requirement of templates. Consequently, large-scale production of such unique architectures remains elusive.

The present work reports the development of a versatile and uncomplicated fabrication of a new type of cerium-based

coordination polymer (Ce-CP) with a stratified structure. Rapid exfoliation of this bulk-layered Ce-CP in liquid triethanolamine (TEA) at room temperature. Followed by heating at 450°C, resulted in the formation of a highly porous hybrid 2D-3D CeO_{2-x} structure consisting of clustered mesoporous nanosheets. This unique architecture of CeO_{2-x} yields a high specific surface area of 251 cm²g⁻¹ and associated high density of accessible active sites. These structures were used as catalysts for CO oxidation and exhibited outstanding performance with T90 value of ~148°C. MnO- and CuO-based heterojunctions also were synthesised and revealed further improvements in performance.

The present work discloses a high-yield, simplified (infrastructure and process), and template-free strategy to synthesise a hybrid 2D-3D CeO_{2-x} architecture for energy and environmental applications.

Biography

Prof. Charles Christopher Sorrell has degrees from the University of Missouri-Rolla (Ceramic Engineering 1977, Chemistry 1980), Pennsylvania State University (Ceramic Science 1980), and the University of New South Wales (Ceramic Engineering 1987). He has supervised ~20 postdoctoral fellows and ~100 postgraduates to completion. His research focus for more than 35 years has been the processing of ceramics, often informed by phase equilibria considerations. His research activities, documented in >500 publications and 4 patents, have been commensurately broad, including most areas of ceramics except fracture mechanics. This work has generated an H-index of 44 and over 11,000 citations.

Modeling of the Influence of the Mechanical Aspects (Static, Dynamic) on the Production of Electric Power of a Fuel Cell (PEMFC)

Raed KOUTA

Charles Delaunay Institute (ICD), France

Abstract

A fuel cell is a multi-physical system. Its electrical performance depends on chemical and fluid parameters in addition to mechanical ones. Many studies deal with the physical-chemical aspects. Our study contributes to the evaluation of the influence of mechanical aspects on the performance of a fuel cell. Only those who are characterized with low-temperature proton exchange membrane type (PEMFC) batteries can deliver the required power level. One of the main scientific and technical challenges is to know its behavior in its actual environment of use.

The study proposes to highlight the influence on the production of electric power:

-Mechanical design and fabrication parameters and their uncertainties (Young module, GDL porosity, permeability, etc.). The influence of the tooth geometry of the bipolar plates is also taken into consideration. An experimental design is proposed with two types of materials as well as three geometric shapes for three assembly pressures. Other experimental design is also proposed for the study of the influence of the mechanical parameters' uncertainties on the performance of the cell.

-Mechanical (static, dynamic) and thermal solicitations (tightening - compression, vibrations (road rolling and testing on vibro-climatic bench, etc.). This study is also carried out according to an experimental design on a fuel cell system for vibratory solicitations recorded on a vehicle test track with three temperatures and three expected performance levels.

The work will enhance the coupling between mechanical and physical-chemical phenomena.

Biography

Raed KOUTA, Research Director, Associate Professor at Charles Delaunay Institute and at Belfort Montbéliard University of Technology (France). My areas of expertise are in Dependability, Reliability, Risk Management, Statistics and Physical-Probabilistic Coupling. My research is in the area of coupling between physics and dependability of technological entities in their real conditions of using. I have already supervised eight PhD, and now, I currently lead four. Research topics are always about reliability, the influence of uncertainties on the performance of complex systems. Responsible at Belfort Montbéliard University of Technology for teaching robust engineering, reliability and statistical probabilities for the engineer.

Catalytic Biohybrid Polymer Materials for Biomedical Applications

Lewis Blackman

CSIRO, Australia

Abstract

Will be updated soon

Mn/Fe Mixed Oxide Catalysts with Enhanced Water Resistance Property for Low Temperature Selective Catalytic Reduction of NO_x

Zongli Xie*, Derrick Ng, Durga Acharya and Xingdong Wang

CSIRO Manufacturing, Australia

Abstract

Nitrogenous oxide (NO_x) exhaust from the burning of hydrocarbon-based fuels, has been identified as major atmospheric pollutant for its direct effects as well as role in the generation of ozone and impact on human health. Mitigation of NO_x, particularly NO, generation from flue gas is thus of great importance and selective catalyst reduction (SCR), which utilises NH₃ as the reducing agent and heterogeneous reaction of NO on a catalyst, is one of the most widely used technology. Vanadium based catalysts vanadium-based catalysts have been successfully employed in the temperature range 300-400°C but its efficiency is very limited at low temperature. In addition, the current catalysts activities are often inhibited by the flue gas water vapour due to the -OH competitive adsorption with NO_x as well as with -H. In our work, we have fabricated monolithic manganese and iron based mixed oxides catalysts, and then doped with hydrophobic agents; polytetrafluoroethylene (PTFE) and cellulose siloxane (CS), in an effort to increase catalysts water vapour resistance while attaining superior catalyst coating. Our analyses and test results show that doping PTFE (up to 10%) and CS (up to 5%) do not adversely affect catalyst overall morphology, surface and bulk activities. By adding an appropriate amount of doping agent, we can increase NO_x conversion at the water vapour content of 10% in simulated flue gas and at a temperature as low as 125°C. Biography Dr Zongli Xie is a senior research scientist and a team leader of Catalysis and Materials Discovery at CSIRO Manufacturing. Zongli has worked on more than 30 research and development projects with Australian and international companies in various aspects of advanced materials development, commercial scale production of materials for industrial emission control and wastewater treatment. She has over 80 journal publications and 3 invited book chapters. Her research area includes environmental catalysts for industrial emission control and wastewater treatment, nanocomposite mixed matrix membranes for desalination and industrial wastewater treatment. She is also a director of Membrane Society of Australasia (MSA).

Upgrading Ultra-heavy Oil with Iron-based Oxide Catalysts under Sub-/Supercritical Water Conditions

Takao Masuda*, Hisaki Kondoh, Tatsuya Kitaguchi, Yuta Nakasaka, Takuya Yoshikawa and Teruoki Tago

Hokkaido University, Japan

Abstract

Our studies on the application of iron-based oxide catalysts to upgrade ultra-heavy oils under sub-/supercritical water conditions are presented. At first, the influence of reaction parameters, such as temperature and pressure, on the product yields were investigated for upgrading oil sand bitumen over iron-based oxide catalysts. Reaction pressure was found to be affect markedly the product yield, revealing that the formation of carbonaceous solid materials, called coke, were decreased with increase in pressure, and the yield of lighter component (Gas Oil and VGO: vacuum gas oil) reached the highest under sub-critical water condition using both a batch and a flow type reactors. Furthermore, kinetics and reaction path for the decomposition of oil sand bitumen were analyzed. The decomposition reaction of VR (vacuum residual oil) in the bitumen was expressed as second order reaction rate equation, and the activation energy was obtained as 132 kJ/mol. Reaction kinetics was analyzed by using Lumping Model. The assigned reaction rate constant for each lump revealed that VR was sequentially converted in order of VGO, Gas Oil and Gas. And the coke formation was found to be suppressed under sub-critical water condition, as compared with the rates of the main reaction path. Accordingly,

the reaction process using iron-based oxide catalyst is expected to be applied for the on-site upgrading of ultra-heavy oil including the bitumen derived from SAGD (Steam Assisted Gravity Drainage) method, in which bitumen was mined accompanied with high temperature and pressured water.

Biography

Takao Masuda got Ph.D. in 1988 from Kyoto University, Japan. He was dean (2017-2018) of engineering faculty of Hokkaido University. He served directors of the chemical society of Japan (2009-2010) and of the catalysis society of Japan (2010-2011), president of the Japan association of zeolite (2014-2015), vice president of the Japan petroleum institute (2016-2017). He received the Catalysis Society of Japan Award in 2012, and the Japan petroleum institute Award in 2017. His major is chemical reaction engineering with solid catalysts. His research projects focus on biomass-refinery, upgrading extra-heavy oil and preparation of nano-sized zeolite crystals uses as catalysts and adsorbents.

The Formation of Dead Zones in Nonisothermal Porous Catalyst

Piotr Skrzypacz^{1*}, Vsevolod V. Andreev² and Boris Golman¹

¹Nazarbayev University, Kazakhstan

²Chuvash State University, Russia

Abstract

We consider the formation of dead zones in the porous catalyst pellets due to the chemical reaction and diffusion. We established and investigated the model with nonisothermal reaction of fractional order and activated temperature-dependent diffusivity. The effects of process parameters, catalyst shape, and reaction and diffusion parameters on the formation of the dead zone are studied numerically and characterized by the critical Thiele modulus. The lower bounds for the critical Thiele modulus are derived analytically in terms of process parameters for exothermic and endothermic reactions and verified numerically. The critical Thiele modulus increases with increasing Arrhenius number for diffusion and decreasing Arrhenius number for reaction in the case of exothermic reactions, whereas the opposite trends hold for the endothermic reactions. The critical Thiele modulus also increases with increasing fractional reaction order as well as with decreasing energy generation function, and increasing Biot numbers for heat and mass transfer. Moreover, the critical Thiele modulus is the highest for spherical pellets and the lowest for pellets with planar shape.

Improved Synthesis of Mesoporous SBA-15-CTA Using Citric Acid Under Mild Condition and Its Application in Catalysis

Yan Liu^{1*}, Luming Li^{1,2} and Wei Chu²

¹Institute of Chemical and Engineering Science, Singapore

²Sichuan University, China

Abstract

The dry reforming of methane (DRM) process has aroused particular interest, as it can convert two greenhouse gases (CH₄ and CO₂) into syngas (CO and H₂), as a suitable resource for the production of sulfur-free liquid fuels and oxygenated chemicals. In this contribution, novel mesoporous materials were developed under mild condition and used as supports for DRM catalysts. The synthesis parameters were carefully investigated, while the materials were well characterized. Through increasing nickel's dispersion and adjusting the metal and support interaction, high performance catalysts were formulated with stable activities.

Biography

Yan Liu is a Senior Scientist in Institute of Chemical and Engineering Sciences, A*STAR, in Singapore, a Team Leader in Material Synthesis Team. After receiving her PhD in Chemical Engineering in 1998 at Tianjin University and carrying out two-year postdoctoral studies at State Key Laboratory of Catalysis in Dalian with Prof Can Li, She has worked in ICES since 2001. She has published near 100 articles in the leading journals and proceedings, and more than 10 patents. Her research interests are mainly on the novel catalytic materials development and their applications in C1 Chemistry, Biomass conversion, and so on.

Design Catalysts for Catalytic Wet Air Oxidation of Ammonia

Bing Hui Chen*, Jile Fu, Songshou Ye, Lili Geng, Nuowei Zhang and Jinbao Zheng

Xiamen University, China

Abstract

Catalytic wet air oxidation (CWAO) has shown great potential for the treatment of industrial wastewater, owing to its high efficiency and simple operation. However, it will be much better if the catalysts can have higher activity especially better stability of the catalysts, in addition to the various demand for catalysts among treatment of different compounds.

For the CWAO of ammonia, the performance of metal-based catalysts was thought to be related to the oxygen affinity, which should be moderate (e.g. Pd, Ru) for high ammonia conversion and nitrogen selectivity. Thus, the RuCu bimetallic catalysts could be the excellent option. The strong interaction between Ru and Cu could adjust the overall oxygen affinity of the catalysts, thereby affecting the oxidation of ammonia. The optimized RuCu catalysts showed both satisfactory activity and selectivity as well as stability than that of either Ru or Cu catalysts. When investigating the reaction pathways and pH effect in the CWAO of ammonia using RuCu catalysts, the results confirmed the fact that ammonia oxidation was confined by the moderate oxygen affinity using all the reported metals. To break the limitation, we tried to introduce new oxygen source, the hydroxide on the surface of Au based catalysts. The results showed that the activity of AuPd catalysts is at least ten times higher than that of RuCu catalysts. Besides, the oxygen affinity of AuPd is low according to the CO-TPR and H₂-TPR, and the TPSR experiments clearly proved that the H₂O greatly enhanced the activity of AuPd catalysts.

Biography

Binghui Chen received his Ph.D. degree from University of Leeds in 1998, Master degree from Zhejiang University in 1990, and Bachelor degree from Huaqiao University in 1984. All are in chemical engineering. Currently, he is a full professor of College of Chemistry and Chemical Engineering at Xiamen University, as well as the dean of School of Energy and Chemical Engineering at Xiamen University Malaysia. He has won awards including the National Academic and Innovation Award in 1997 and the SinoPec Science and Technology Award (1996 and 1997). His research interest is mainly in catalysis in hydrogenation and oxidation.

Less Aggregated ZSM-22 Prepared by a Seed Silanization Strategy for N-Dodecane Hydroisomerization

Xiangyu Wang*, Xiangwen Zhang and Qingfa Wang

Tianjin University, China

Abstract

Less aggregated ZSM-22 zeolite was synthesized by a seed silanization strategy. An organosilane PHAPTMS (phenylaminopropyltrimethoxysilane) was applied as seed silanization agent. The textural structure and acidity of the as-synthesized ZSM-22 zeolite was characterized by XRD, SEM, TEM, ICP, N₂-adsorption, 27Al MAS NMR, NH₃-TPD and FTIR. Low pre-crystallization temperature (40°C) favored the nucleation and growth of pure ZSM-22. Seed silanization agent could effectively reduce the aggregation of ZSM-22 nanorods. Acidity of as-prepared ZSM-22 was also reduced as the amount of added PHAPTMS increased and the aggregation of ZSM-22 reduced. This zeolite supported with platinum (Pt/ZSM-22) showed high performance of n-dodecane hydroisomerization, because its less aggregated crystals and reduced acidity favored the formation of 2-methyl isomers through pore-mouth mode, and restrained cracking.

Biography

Xiangyu Wang is a PhD candidate in Key Laboratory for Green Chemical Technology of Ministry of Education in Tianjin University. His research work aims to improve the performance of ZSM-22 in the hydroisomerization of n-paraffins through top-down and bottom-up strategies.

Well-Defined Zinc Imine POSS as a Highly Active Catalyst for the Synthesis of Cyclic Carbonates from Epoxides and CO₂

Sławomir Szafert^{*}, Mateusz Janeta and Łukasz John

University of Wrocław, Poland

Abstract

Carbon dioxide is a greenhouse gas originating from the carbon footprint of human activities. It is - at least partially - responsible for a global warming effect, hence, there is an ongoing search for effective methods to mitigate its amount and - at the same time - its effect on the environment. One of the approach is to use gas CO₂ as a substrate in chemical transformations. A well-working example would be the synthesis of cyclic carbonates from epoxides and gaseous CO₂, which is catalyzed by for instance zinc complexes. Although, the reaction is quite effective, usually high pressure of CO₂ must be applied, what is always less favorable from an industry point of view (but of course feasible). We have envisioned an imine side-armed polyhedral oligomeric silsesquioxane (POSS) as convenient macromolecule to anchor zinc ions. Such constructed multi-centered complex (in one isomeric form) was obtained in a direct reaction of octa-substituted T8-type imine POSS with ZnEt₂. The compound was fully characterized by x-ray crystallography and numerous spectroscopic (NMR (1H, 13C, 29Si), UV-vis, DRIFT, CP-MAS NMR (13C, 29Si)) and thermal methods (TG-DTA) as well as MS spectrometry (ESI-MS). The four-centered complex was next tested as a catalyst for the above mentioned reaction. It showed spectacular activity in formation of cyclic carbonates from CO₂ and different epoxides with low working pressure.

Biography

Sławomir Szafert received his PhD at the University of Wrocław (Poland) in 1996. He was subsequently awarded a Fulbright Foundation fellowship to join prof. John A. Gladysz group at the University of Utah for postdoctoral research. In 1999 he returned to Poland to take a position at his Alma Mater. He was a visiting researcher/professor at Erlangen-Nürnberg Universität (Germany), Rennes Université (France), Tokyo Institute of Technology (Japan), Fudan University (China) and some others. His scientific interests are focused on the synthesis and reactivity of long chain polyynes as well as on materials chemistry.

Poster Presentations

Nanoporous Metal Oxide Catalysts by Hard-Template Method with Concurrent Improvement of Activity and Stability for Water Oxidation Reaction

Chanho Pak

Gwangju Institute of Science and Technology, South Korea

Abstract

Will be updated soon

Recovery of Phenols from Degraded Lignin Dissolved in Inert Solvent over Mixed Catalyst of TiO₂-FeOX and MFI-Type Zeolite

Takuya Yoshikawa^{1*}, Hiroya Ishimaru¹, Yuki Kawamata¹, Yoshihito Koyama^{1,2}, Yuta Nakasaka¹, Eri Fumoto³, Shinya Sato³, Teruoki Tago⁴ and Takao Masuda¹

¹Hokkaido University, Japan

²Idemitsu Kosan Co., Ltd., Japan

³National Institute of Advanced Industrial Science and Technology, Japan

⁴Tokyo Institute of Technology, Japan

Abstract

Lignin, which is a main component of lignocellulosic biomass composed of alkyl phenol units, has attracted attention as a renewable resource for phenolic compounds. Our previous study has suggested a lignin conversion process, in which lignin were depolymerized into lower molecular weight fractions using a solid acid catalyst in water/1-butanol mixture, then the obtained degraded lignin was further reacted over iron oxide based catalyst to produce phenols. At the beginning, in this study, the catalytic cracking of guaiacol as a lignin model compound over TiO_2 -FeOX catalyst using 1-butanol as a solvent, which was employed in the original treatment, was carried out. The result revealed that 1-butanol reacted, decreasing product selectivity, whereas benzene as a solvent did not react, exhibiting a reasonable material balance, but the degraded lignin did not dissolve. Therefore, an investigation was done to find a solvent that could dissolve lignin and yet was inert to the catalyst using Hansen solubility parameters and screening tests with a microreactor coupled to a GC/MS instrument. The results suggested lignin had good solubility in quinoline, which also was inert over TiO_2 -FeOX and MFI-type zeolite catalysts at the reaction temperature. A physically mixed catalyst of TiO_2 -FeOX and MFI-type zeolite was used for catalytic cracking of the degraded lignin dissolved in quinoline to obtain phenol selectively, with 10.0 mol% yield of monomeric phenols and 56.5% phenol selectivity.

Biography

Takuya Yoshikawa is currently Assist. Professor of Faculty of Engineering, Hokkaido University, Japan. He graduated from Hokkaido University, and received Ph.D. in 2013 from the same university. After he worked at Hokkaido Research Organization, Japan, he moved back as a current position in 2015. His major is chemical engineering, and his research topics are separation technique of inedible biomass via organosolv treatment, conversion of lignin into useful chemicals with solid catalysts, upgrading of heavy oil to lighter fuels or directly to bulk chemicals and so on.

Visible Light Active $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ Nanocomposites for Photocatalytic Applications

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¹Kuvempu University, India

²Sir M.V. Government Science College, India

Abstract

Water treatment technologies are in a need of depollution materials which can efficiently eliminate wide range of toxic and non biodegradable pollutants. This reason aims for the generation of new photocatalytic materials with enhanced efficiency and applicability. Herein, $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ nanocomposites were fabricated by microwave-assisted approach. These samples were characterized by numerous spectroscopic techniques to examine their crystalline structure, morphology and elemental composition. The result demonstrated that $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ nanocomposites exhibited cubic spinel structure with no impurity at 600 °C calcination. FTIR spectrum resulted in two main characteristic peaks of metal-oxygen bonds of $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ at tetrahedral (594 cm^{-1}) and octahedral (397 cm^{-1}) sites. As measured by diffused reflectance spectroscopy, the composite show strong absorption in the visible region with the optical energy band gap of 1.9 eV. The NiFe_2O_4 - CoFe_2O_4 nanocomposite exhibited maximum efficiency for the photodegradation of rose bengal (97%) and methylene blue (94%) under visible light in 150 mins due to the synergic effect between NiFe_2O_4 and CoFe_2O_4 , as confirmed by photoluminescence spectroscopy. Lower the PL emission intensity higher will be the photocatalytic activity of $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ nano-photocatalyst which profits a delay in the recombination rate. Main active species $\bullet\text{OH}$ radical were responsible for the degradation as confirmed by quenching/radical trapping experiment using Coumarin as a probe molecule. These nanocomposites demonstrated extraordinary chemical stability and reusability even after five repeated cycles. These results conclude that the prepared nanocomposite will be applicable as potential photoactive material for textile and wastewater treatment.

Keywords: $\text{NiFe}_2\text{O}_4/\text{CoFe}_2\text{O}_4$ Nanocomposites, Photoluminescence, Rose Bengal, Methylene blue

Biography

H.S. Bhojya Naik is a faculty in Department of PG Studies and Research in Industrial Chemistry, Kuvempu University, India since 1998 with present position of professor. His research interests are development of metal based materials for catalytic/biological applications. He has supervised 28 Ph.D and 02 PDF students with 205 research articles & 01 Indian patent. His scientific citations are 2075 with hindex 22 and i10-index 77 as of now. Attended and organized national/international conferences/seminars/symposia/

workshops. Visiting scientist for USA, UK, Europe and other countries and presented research outputs. Is life member of scientific/academic bodies. He completed major projects funded by DST, BRNS, UGC, NRB India and Wichita State University, USA and editor of more than 05 books.

Regioselective Synthesis of Ru(II)-Chiral Oxazoline Complexes Containing RuC(sp²) Bond and their Application for Catalytic Asymmetric Cyclopropanations

Hayato Inoue*, Thanh Nga Thi Phan, Ikuhide Fujisawa and Seiji Iwasa

Toyohashi University of Technology, Japan

Abstract

We designed and regioselectively synthesized a new variety of ruthenium complexes containing Ru(II)-C (sp²) bond as a chiral catalyst. (Scheme 1). Various Ru(II)-Pheox complexes cat.A and B were evaluated for catalytic asymmetric intramolecular cyclopropanation reactions of diazoesters with olefins. (Scheme 2). The reaction was proceeded smoothly to give the corresponding optically active cyclopropanes derivatives in high yields with high diastereoselectivities. We found that cat.A type gave relatively higher enantioselectivities (99% ee, trans) than cat.B.

Preparation and Characterization of Electrospun Nanofibrous Membranes for Adsorption of Heavy Metals

Jun Cong Ge¹, Dong Guk Ko¹, Jiaqing Li², Min Soo Kim¹ and Nag Jung Choi^{1*}

¹Chonbuk National University, South Korea

²University of Wollongong, Australia

Abstract

The rapid development of industry has led to a serious decline in water quality, especially the pollution of heavy metals in water has received increasing attention. Therefore, in order to remove heavy metal pollutants such as lead ions (Pb²⁺) and cobalt ions (Co²⁺) in waste water, we successfully synthesized fly ash, silver nitrate and polyacrylonitrile (PAN) into nanofibrous membranes by an electrospinning technology for adsorbing heavy metal ions in sewage. It also has antibacterial activity against Gram-negative *Escherichia coli* (*E. coli*) and Gram-positive *Staphylococcus aureus* (*S. aureus*) bacteria. The fly ash particles and silver particles were successfully combined on PAN nanofibers by scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD) analysis. The results show that the nanocomposite membrane has a good adsorption effect on Pb²⁺ than Co²⁺. This may be attributed to the electrostatic attraction between the phosphate anions contained in the fly ash and the Pb(II) cation, and the phosphate group precipitates lead in the form of lead hydroxide. In addition, the adsorption of metal ions by the nanocomposite membrane mainly depends on the type of metal ions, such as ion size, positive and negative charges on the surface of metal ions. On the other hand, the antibacterial activity of the electrospun nanofibrous membrane against *S. aureus* was obviously better than that against *E. coli*. It may be electrostatic adsorption caused by positively charged Ag nanoparticles and the negatively charged cell membrane of bacteria play a dominant role by creating structural alterations in the membrane, which result in more permeability to the bacterial cell membrane. As a result, the Ag nanoparticles combined with negatively charged functional groups on the cell walls of bacteria and interfere with cell permeability and respiratory functions, and led to the loss of bacterial activity.

Introduction: Electrospinning is one of the most convenient technologies for fabrication of durable fibrous membranes with unique properties such as a high surface area and multiple inter/intra porosity, and also with other advantages such as low cost, easy operation and controlling [1-3]. Therefore, the multifunctional nanofiber membranes fabricated by electrospinning have great application potential, such as heavy metals removal and bacterial activity. In this study, the electrospun multifunctional membranes with heavy metal adsorption and bacterial activity were investigated.

Methods: PAN precursor fibers (Mw=150,000) were purchased from SIGMA-ALDRICH, Co., USA. Fly ash powder as adsorbent was purchased from Won Engineering Company Ltd., Korea. Analytical grade N, N dimethylformamide (DMF) as received was purchased from Samchun Chemical Co., Ltd., Korea. AgNO₃ crystal powder was purchased from Sigma Aldrich and was used as an antibacterial agent against *E. coli* and *S. aureus* bacteria. Figure 1 shows the electrospinning system for fabrication of the

multifunctional membranes.

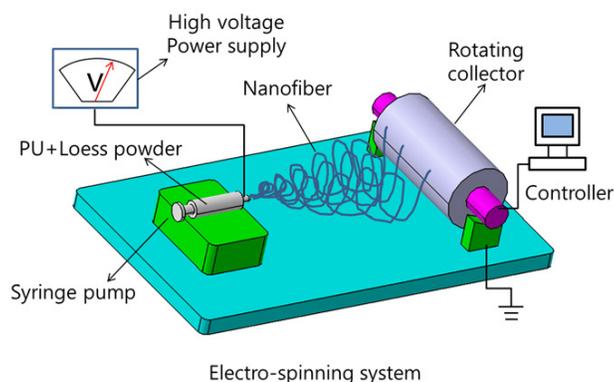


Figure 1: Schematic diagram of the electrospinning system.

Results and discussion: Figure 2 shows the SEM images for all samples. As shown in Figure 2, it can be seen that the Fly ash particles were well loaded on PAN fibers. This shows that the electrospinning technology can combine the fly ash and PAN fiber well. Figure 3 shows the adsorption of Co(II) and Pb(II) for fly ash powder and FA4. They all showed good adsorption capacity, in which the adsorption of Pb(II) is greater than that of Co(II).

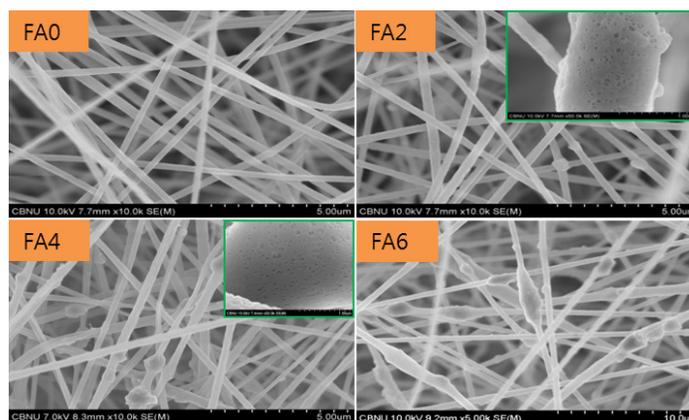


Figure 2: SEM images for all samples.

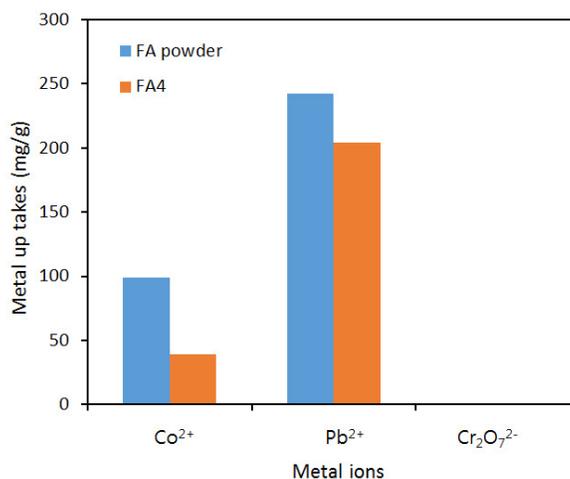


Figure 3. Electrospun membranes for adsorption of metal ions.

Conclusions: The multi-functional fibrous membranes meant to remove heavy metals were successfully fabricated via simple, economical, and one-step electrospinning technology. SEM images showed that all ratios of fly ash and Polyacrylonitrile can be spun into composite membranes.

Acknowledgement

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Effect of Different Solvents on the Properties of Copper Nanoparticles Produced via Pulsed Laser Ablation and its Enhanced Catalytic Activity

Talshyn Begildayeva*, Seung Jun Lee, Juhyeon Park, Tae Ho Kim and Myong Yong Choi

Gyeongsang National University, South Korea

Abstract

Comparative experiments were carried out to specify the effect of various solvents (deionized water, methanol, ethanol, 1-propanol, butanol, ethylene glycol, hexane and acetonitrile) on the final composition, morphology and catalytic activity of copper based nanomaterials. Copper nanoparticles with a range of different surface morphologies were synthesized by pulsed laser ablation method using a copper plate as target in liquid media. When laser ablation of a solid copper plate was carried out in acetonitrile, a core-shell nanostructure of copper@graphitic carbon (Cu@GC) and copper (I) cyanide particles were formed. While spherical and rod-like structured particles of copper (I) and (II) oxide was obtained in deionized water and methanol, respectively. The catalytic activities of the synthesized copper nanoparticles were evaluated for the reduction of 4-nitrophenol to 4-aminophenol, and nitrobenzene to aniline, as a model reaction. Based on the obtained results and pseudo-first order kinetics, the synthesized nanoparticles of copper (II) oxide and copper encapsulated in graphitic carbon layers demonstrated an enhanced catalytic performance towards the reduction of 4-nitrophenol and nitrobenzene. The enhanced catalytic activities of this catalysts might be due the unique surface morphologies and positive synergistic effect between copper nanostructures and graphitic carbon layer. The present investigation was revealed that the pulsed laser ablation of copper plate in various liquid medium is a facile method for producing of copper and copper-based nanoparticles with unique surface structure, compositions and act as an excellent catalytic material.

Novel Plasmonic ZnO/Au/g-C₃N₄ Nanocomposites for Solar Light Active Photocatalysts

Yiseul Yu*, Talshyn Begildayeva, Seung Jun Lee, Hyeon Jin Jung, Juhyeon Park, Tae Ho Kim and Myong Yong Choi

Gyeongsang National University, South Korea

Abstract

Novel ZnO/Au/graphitic carbon nitride (g-C₃N₄) nanocomposites were fabricated through a facile and eco-friendly three-step pulsed laser ablation method in liquid followed by calcination, without the use of a capping agent or surfactant. The as-prepared photocatalysts were examined by electron microscopic and spectroscopic techniques, and the results further confirmed the good dispersion of gold nanoparticles (NPs) on the surface of spherical ZnO particles and g-C₃N₄ nanosheets. The ZnO/Au/g-C₃N₄ nanocomposite exhibits substantially enhanced catalytic activity toward the degradation of methylene blue (MB) under simulated solar light irradiation. This improved photocatalytic activity of ZnO/Au/g-C₃N₄ is attributed to the surface plasmon resonance of Au NPs and the synergistic effect between ZnO and g-C₃N₄. The boundary between ZnO/Au and g-C₃N₄ enables the direct migration of photogenerated electrons from g-C₃N₄ to ZnO/Au, which can easily retard the recombination of electron-hole pairs and boost the carrier separation efficiency. A reasonable MB degradation mechanism over the ZnO/Au/g-C₃N₄ photocatalyst is proposed on the basis of the results.

Metals Recovery Method from Waste Solution Containing Metal Ions Using a Pulsed Laser

Seung Jun Lee*, Hyeon Jin Jung, Juhyeon Park, Tae Ho Kim and Myong Yong Choi

Gyeongsang National University, South Korea

Abstract

In this study, effective metals recovery are confirmed from the metal waste solution containing metal ions using Pulsed Laser Irradiation in Liquid (PLIL) technique. In PLIL technique, when a laser having strong power and energy is irradiated through a focusing lens into a waste solution containing metal ions, plasma plumes are generated by the temperature and the pressure. As a result, it was confirmed that metals can be recovered as metal particles by using only laser without any other additive or reducing agent, which is a more environmentally friendly method than the conventional recovery method.

Catalytic Au and Acid-Resistant Graphitic Carbon-Encapsulated Au(Au@GC) Nanoparticles Prepared by Pulsed Laser Ablation in Various Solvents

Myong Yong Choi

Gyeongsang National University, South Korea

Abstract

Will be updated soon

Development of Multicomponent Quantum Chemistry Methods for Accurate Prediction and Elucidation of Hydrogen-Functional Mechanism

Masanori Tachikawa* and Yusuke Kanematsu

Yokohama City University, Japan

Abstract

Recently, Mori et al. developed the κ -H3(Cat-EDT-TTF)2 (H-TTF) with a hydrogen-bonded π -electron system, which was found to reveal C2/c symmetry in 50-293 K, while its isotopologue, κ -D3(Cat-EDT-TTF)2 (D-TTF), showed the phase transition at 185 K from C2/c to P-1. To elucidate the origin of such difference, we have theoretically analyzed the difference between H-TTF and D-TTF using quantum chemistry approaches. First, we have performed multicomponent density functional theory (MC_DFT) calculations, taking account of the nuclear quantum effect with the 3-unit model that considering interaction by b1 (π - π stacking). In the H-TTF, the shape of the eff-PEC becomes single-well potential, since the energy barrier obtained with conventional DFT is removed by protonic quantum effect. This is in reasonable agreement with the corresponding experimental observation that the hydrogen is located at the center of H-bond in X-ray structures of H-TTF both at 50 and 293 K. On the other hand, in the D-TTF, the eff-PEC still holds double-well. This means that deuterium is localized at one side of oxygen rather than the center of H-bond in low temperature phase, due to the small thermal effect. Therefore, it is expected that the phase transition in D-TTF occurs due to the localization of the deuterium. We would like to mention that the phase transition temperature of D-TTF is determined by the π - π interaction and the nuclear quantum effect.

Biography

Masanori Tachikawa got Ph.D. in Waseda University in 1995, became a JSPS(PD) in Emory University, and a Special Postdoctoral Researcher (SPDR) in RIKEN in 2000. In 2003 he moved to Yokohama City University as an associate professor, became a professor in 2006, and now director of Department of Materials System Science, Graduate School of NanoBioScience. He is developing new quantum simulation methods, in which both electrons and hydrogen nuclei are treated quantum mechanically. He has applied these methods to the various systems from material science to biochemistry.

A Study on Spray Characteristics according to Nozzle Tip Diameter at Water Injection

Min Soo Kim*, Jun Cong Ge, Nag Jung Choi and Dong Guk Ko

Chonbuk National University, South Korea

Introduction: Siphon nozzles are used to transport the liquid in the stored state to other places using pressure and gravity differences. Those generally have a horizontal spray angle. Therefore, the droplet size is not uniform due to the influence of gravity and is difficult to apply to the nozzle for spraying pesticide of agricultural drone in the vertical direction. In this study, to apply siphon nozzles to the drone spray those, the droplet size according to the change of tip diameter was analyzed.

Experiment: Figure 1 shows the spraying schematic of water through the siphon nozzle tip. The spray pressure is 10bar. The diameters of nozzle tip are 0.5 mm, 0.7 mm and 1.0 mm and the spray measurement distances are 5 cm, 10 cm, 15 cm, 20 cm and 30 cm. The particle diameter of the droplet was measured using LDPA (Laser Diffraction Particle Analyzer).

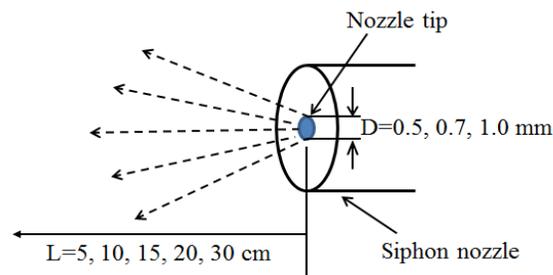


Figure 1: Spraying schematic of siphon nozzle.

Results and Discussion: Figure 2 SMD Values according to tip diameter of siphon nozzle.

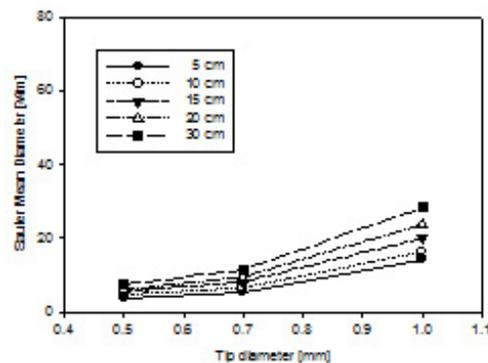


Figure 2 shows SMD (Sauter Mean Diameter) values according to the tip diameter and spray measurement distance. The SMD is a degree of atomization of the injected liquid through surface contact with the surrounding gas. The SMD value can be expressed as follows.

Where N and D is the number and diameter of droplets, respectively. I is any number of droplets. The average particle diameter of the SMD is affected by larger droplets than smaller those. As the diameter of tip and the measurement distance increased, the surface area of droplets became smaller due to the surface tension, and consequently the SMD value increased. The SMD value at the measurement distance of 30 cm increased by 1.98 times compared to the value at 5 cm when the tip diameter was 1.0 mm. Therefore, the atomization of liquid was more active.

Conclusion: In this study, we analyzed the droplet size according to the tip diameter when the water was spread through the nozzle.

- 1) The SMD value at the measurement distance of 30 cm increased by 1.98 times compared with the value at 5 cm when the tip diameter was 1.0 mm.
- 2) The atomization of water particles increased due to the surface tension and dispersion of droplets in the downstream direction of flow.

$$SMD = \frac{\sum_i N_i D_i^3}{\sum_i N_i D_i^2}$$

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Nanoporous Black Silicon for Hydrogen Photogeneration in Solar Water Splitting

Ahmed F Halima

RMIT University, Hydrogen Group Australia

Abstract

Will be updated soon

Keynote Session

3D Printed Catalytic Reactors for Continuous Flow Hydrogenation

Christian Hornung

CSIRO Manufacturing, Australia

Abstract

Will be updated soon

Scientific Session-3 Electrocatalysis | Photocatalysis

3D Printing and Electrocatalysis

Chong-Yong Lee

University of Wollongong, Australia

Abstract

Will be updated soon

Enhancing the Oxidation Efficiency of Hg0 by Using CuO/TiO₂ Photocatalysts

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¹National Sun Yat-Sen University, Taiwan

²Huaqiao University, PRC

Abstract

Synthesized CuO/TiO₂ photocatalysts prepared by sol-gel method were applied to enhance the oxidation of Hg⁰. The experiments were conducted at temperatures of 100-200°C with 300 ppm SO₂ and 300 ppm NO simulated flue gas under the irradiation of near UV. The surface properties of photocatalysts were characterized by XRD, SEM, TEM, EDX, PL, XPS, and BET. Experimental results indicated that the photocatalysts had larger specific surface areas than the commercial TiO₂, and were uniform nano-sized grains. CuO was well-dispersed on the surface of TiO₂ and Cu²⁺ was the dominant species contributing to Hg⁰ oxidation. TiO₂ doped with CuO can enhance the oxidation efficiency of Hg⁰ while compared with the commercial TiO₂. 5% CuO/TiO₂ was the optimal photocatalyst for Hg⁰ oxidation. The oxidation efficiency of Hg⁰ in the simulated flue gas containing SO₂ and NO rose up to 85% and 70% at 120°C, respectively. NO inhibited Hg⁰ oxidation since NO could consume surface oxygen and competed with Hg⁰ for active adsorption sites, while SO₂ could promote the oxidation of Hg⁰ due to the formation of HgSO₄. Simulated by Langmuir-Hinshelwood model and Arrhenius equation for Hg⁰ oxidation, the equilibrium constant (K), the reaction rate constant (k), and the activation energy (E_a) were determined for various CuO/TiO₂ photocatalysts. We also found that CuO presented excellent sulfur resistance to SO₂. The mechanism for Hg⁰ oxidation was further proposed for CuO/TiO₂ photocatalysts.

Keywords: CuO/TiO₂ photocatalysts, Oxidation efficiency of Hg⁰, Simulated flue gas, Operation parameters, Langmuir-Hinshelwood model

Biography

Chung-Shin Yuan is a Distinguished Professor in the Institute of Environmental Engineering at National Sun Yat-sen University in Taiwan. He served as the Associate Editor of JA&WMA and the Senior Editor of AAQR and ASE. His research field covers air quality monitoring, air pollution control technology, and catalytic science and technology. Recent studies focused on urban and marine PM_{2.5}, atmospheric speciated mercury, photocatalytic degradation of VOCs, photothermal oxidation of Hg⁰, and on-line monitoring of greenhouse gases. Prof. Yuan has published 155 SCI journal papers and 746 conference papers and owned 19 invention patents of Taiwan, USA, and China.

Developing TiO₂-based Nanocomposites for Selective Photocatalysis and Visible-Light-Induced Activity

Esfandiar Pakdel

Deakin University, Australia

Abstract

Will be updated soon

Instability-Directed Architectural Design of Multiscale Nanostructures

Sajjad Mofarah^{1*}, Esmaeil Adabifiroozjaei², Pramod Koshy¹, Hamidreza Arandiyani³, Constantine Tsounis¹, Jason Scot¹, Yin Yao¹ and Charles Christopher Sorrell¹

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Abstract

The widely reported disadvantageous weak bonding between the metal cation and the organic linker in some coordination polymers (CPs) is the source of their instability. This has led to studies aimed at stabilisation of these phases. In contrast, this instability can

be converted readily into an advantage since unstable CPs can be disassembled at room temperature in different solvents and, upon solvent removal, reassembled into nanostructures of unique architectures not previously observed. These architectures can be designed according to the type of polar solvent, its concentration, and the evaporation kinetics. The nanostructures are defect-rich and so they offer the potential for new levels of functionalities not obtainable otherwise. This approach to fabrication is of low complexity, reproducible, high-yield, rapid, and economical compared to conventional methods. The examples to be presented are a Ce-based CP used to generate highly defective CeO_{2-x} -based heterojunction structures and an unstable MOF-5 used to synthesize different ZnO nanostructures.

Structural and Morphological Effects on the Activity and Durability of the Electrocatalysts

Pei Kang Shen* and Xinyi Zhang

Guangxi University, China

Abstract

The development and manufacturing of cost-effective, environmentally friendly and high-performance catalysts have attracted tremendous interest due to their importance in the field of energy and sustainable chemistry. In this talk, we will describe the design and synthesis of novel electrocatalysts for energy storage and conversion applications including oxygen reduction reaction, alcohol oxidation, and water splitting. We will offer a summary of the development of unique Pt-based nanoframes or nanocages, stereotaxically constructed graphene-based heterostructure, particularly, noble metal free electrocatalysts. Through rational design, these catalysts exhibit excellent catalytic activity and high durability. Experimental evidence and theoretical calculation show such achievement can be attributed to the strong structural and morphological effects.

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Biography

Pei Kang Shen is a Professor and Director at the Collaborative Innovation Center of Sustainable Energy Materials in Guangxi University, China. Dr. Shen obtained his BSc degree in Electrochemistry at Xiamen University in 1982, and he continuously carried out his research and teaching at the same university for seven years before he became a visiting researcher in the United Kingdom. He received his Ph.D. in Chemistry at Essex University in 1992. From then on he has been working at different universities both in UK, Hong Kong and China. Since 2001, he has been the Professor at the Sun Yat-sen University (Guangzhou, China). He is the author of over 400 publications in qualified journals, including 35 ESI (Highly Cited Papers, 1%) papers and 3 Hot Papers (0.1%) or specialized books (9 in English and Chinese), of 80 patents, and of more than 150 meeting presentations. He has organized eight international conferences on Electrochemical Energy Storage and Conversion as a conference Chairman. He is now working in Guangxi University. His research interests include fuel cells and batteries, electrochemistry of nanomaterials and of nanocomposite functional materials, like graphene powders for different applications and electrochemical engineering.

2D Material-based Nanostructures for Electrocatalysis Applications

Wenping Sun

University of Wollongong, Australia

Abstract

Developing sustainable renewable energy sources along with efficient energy storage and conversion systems is vital to address the global environmental and energy challenges. Two-dimensional (2D) nanomaterials and other materials with sheet-like morphologies possess unique physicochemical properties compared with their bulk counterparts, such as confined atomic thickness, high specific

surface area and quantum confinement of electrons, which make 2D nanomaterials have great potential in electrochemical energy conversion and storage applications. Currently, many non-noble metal electrocatalysts for electrochemical water splitting are layered 2D materials, but their catalytic performance still cannot reach the level of noble metal electrocatalysts. Developing efficient strategies to further improve the electrochemical performance of 2D nanomaterials still remains a big challenge. Also, some electrochemically inactive 2D materials like RGO and g-C₃N₄ have great application potential in constructing hybrid electrocatalysts or battery electrodes. In this talk, I will be sharing some recent work on the design of efficient 2D material-based nanostructures by surface engineering and interface/heterostructure engineering strategies for electrocatalysis applications.

Biography

Wenping Sun received his B.S. in 2008 and PhD in Materials Science in 2013 from University of Science and Technology of China (USTC). From September 2013 to May 2015, he worked as a postdoc fellow at Nanyang Technological University, Singapore. In June 2015, he moved to Institute for Superconducting and Electronic Materials at the University of Wollongong. His research is mainly focused on the development and rational design of efficient materials and nanostructures, and the fundamental understanding of electrochemical processes for energy conversion and storage applications, including electrocatalysis, fuel cells, batteries, and supercapacitors.



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