

*Promoting global cooperation in clean energy research and education*



PENN STATE AND DALIAN UNIVERSITY OF TECHNOLOGY

Joint Center for Energy Research



宾州-大连联合能源研究中心

# THE 4<sup>th</sup> PSU-DUT JOINT ENERGY WORKSHOP

## Technical Program

**November 9-10, 2016**  
**Dalian University of Technology**  
**Dalian, China**

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**Joint Center for Energy Research**



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## **Agenda for the 4<sup>th</sup> Joint Energy Workshop**

**Dalian University of Technology (DUT)  
November 9-10, 2016, Dalian, China**

## Wednesday, 9 November, 2016 – AM & PM

### Bochuan Library -Lecture Hall, DUT Campus, Dalian, China

8:15 Pick up of PSU Delegation members from the lobby of Bayshore Hotel

8:50 Arrival of PSU Delegation members in the Bochuan Library -Lecture Hall, DUT Campus

### Opening Session Chair: Dr. Chunshan Song, PSU-DUT JCER

09:00 to 9:05

Opening Remarks and Introduction by **Dr. Chunshan Song** (Co-Director, PSU-DUT JCER)

09:05 to 09:10

Welcome Speech by DUT Leader, **President Dongming Guo** (President and Professor of Mechanical Engineering at DUT, Member of Chinese National Academy of Engineering)

09:10 to 09:20

**Group photo of DUT and PSU leaders, faculty and student participants**

### Session #2 Chair: Dr. Xinwen Guo, DUT

09:20 to 09:35

**Dr. Chunshan Song** (*Co-Director of the PSU-DUT Joint Center for Energy Research, Director of PSU Energy Institute and Distinguished Professor of Fuel Science & Chemical Engineering*)

**Introduction to the Joint Center for Energy Research (JCER) between PSU and DUT,**

09:35 to 09:50

**Dr. Bruce E. Logan** (*Director of Engineering Environmental Institute, Evan Pugh Professor of Environmental Engineering at PSU*)

**Opportunities for Microbial Electrochemical Technologies and Thermal Regenerative Batteries to Provide Sustainable Solutions for the Water-Energy Nexus**

09:55 to 10:10

**Dr. Liping Huang** (*Professor of Environmental Engineering at DUT*)

**Heavy metal recovery and separation with simultaneous hydrogen production from microbial electrochemical systems**

10:15 to 10:35

**Coffee break**

**Session #3 Chair: Dr. Bruce Logan, PSU**

10:35 to 10:50

**Dr. Xinyong Li** (*Professor of Chemical and Environmental Engineering, Deputy Director of Group for Environmental Catalysis and Sustainable Energy at DUT*)

***In Situ* Spectroscopy Investigation of the Surface-interface Charge-Transfer Process over Tailored Nano-structured Based PEC Fuel Cells**

10:55 to 11:10

**Dr. Phillip E. Savage** (*Head and Professor of Department of Chemical Engineering at PSU*)

**Under Pressure and in Hot Water – Hydrothermal Reactions of Biomass and Biomolecules**

11:15 to 11:30

**Dr. Jieshan Qiu** (*Deputy Director of DUT Energy Research Center and Professor of Chemical Engineering at DUT*)

**Carbon Materials Synthesis and Characterization**

**Lunch Session Chair: Representative of Faculty of Chem, Env. Bio. Sci. Technol., DUT**

11:40 to 12:50

**Lunch Session Onsite**

**Remarks by Dr. Yang Li, Dean, Faculty of Chemical, Environmental and Biological Science and Technology, and Professor of Polymer Science and Engineering**

**Special Presentation:**

**Dr. Fengshou Xiao** (*Professor of Chemistry, Director of Catalytic Materials Group at Institute of Catalysis, Zhejiang University, Hangzhou, China*)

**Industrial Requirements of Porous Catalytic Materials and Design Synthesis**

**12:50 to 13:00 Break**

**Session #5 Chair: Dr. Phillip Savage, PSU**

13:00 to 13:15

**Dr. Xinwen Guo** (*Deputy Dean of Faculty of Chemical, Environmental and Biological Science and Technology, Professor of Chemical Engineering at DUT*)

**Design and Synthesis of Hollow Zeolites and Their Applications**

13:20 to 13:35

**Dr. Michael J. Janik** (*Professor of Chemical Engineering at PSU*)

**Computational Chemistry Studies of Heterogeneous Catalysis: the Impact of Self-assembled Monolayers on Selectivity**

13:40 to 13:55

**Dr. Anjie Wang** (*Professor of Catalysis at DUT*)

**Sulfur Removal from Engine fuels: Hydrodesulfurization and Oxidative Desulfurization**

14:00 to 14:15

**Dr. Robert M. Rioux** (*Associate Professor of Chemical Engineering and Chemistry at PSU*)

**Understanding Site Isolation of Pd and Ni in Zn-based Bulk Intermetallics during the Selective Hydrogenation of Alkynes**

14:20 to 14:35

**Dr. Yao Wang** (*Professor of Chemical Engineering at DUT*)

**Intensification of Chemical Reaction by Synergy of Non-Thermal Plasma and Catalysis**

14:40 to 14:55

**Dr. Sarma V. Pisupati** (*Professor and Chair of the Energy Engineering Program, Director of Online Education in the John and Willie Leone Family Department of Energy and Mineral Engineering at PSU*)

**Tar Formation and Characterization during Pyrolysis of Coal and Biomass at High Temperatures and Pressures**

15:00 to 15:15

**Dr. Haoquan Hu** (*Professor of Chemical Engineering at DUT*)

**Overview on Coal Direct Conversion into Liquid Products and Other Coal-related Works in Our Group**

15:20 to 15:40

**Coffee break**

**Session #6 Chair: Dr. Jieshan Qiu, DUT**

15:40 to 15:55

**Dr. Donghai Wang** (*Associate Professor of Mechanical Engineering and Chemical Engineering at PSU*)

**Development of Functional Composite Materials for Energy Storage Applications**

16:00 to 16:15

**Dr. Yujiang Song** (*Professor of Chemical Engineering at DUT*)

**Low- and Non-platinum Electrocatalysts of Polyelectrolyte Membrane Fuel Cells (PEMFCs) & Low-temperature Direct Biomass Fuel Cells (L-T DBFCs)**

16:20 to 16:35

**Dr. Xiaoxing Wang** (*Senior Research Associate of EMS Energy Institute at PSU*)

**Recent Progress of Developing Molecular Basket Sorbents for CO<sub>2</sub> and H<sub>2</sub>S adsorption separation**

16:40 to 16:55

**Dr. Chuan Shi** (*Professor of Department of Chemistry at DUT*)

**Environmental Catalysis: Catalytic Elimination of Environmental Air Pollutants and Green Process to Convert the Waste into the Useful Materials**

17:00 to 17:15

**Dr. Moses D.F. Ling** (*Associate Professor of Architectural Engineering at PSU*)

**Integrated Building Solutions – a Sustainable Design Strategy**

17:20 to 17:35

**Dr. Tianyi Zhao** (*Associate Professor of Civil Engineering at DUT*)

**Improving Building Energy Efficiency by Internet of Building Energy System (iBES)**

17:40 to 17:55

**Dr. Zhixian Ma** (*Lecturer of HVAC Engineering at DUT*)

**Heat Transfer Enhancement in Shell and Tube Condenser: Basic Research on Enhanced Tubes and Its Application**

17:55 to 18:00 Closing Remarks

**Dr. Chunshan Song** (*PSU-DUT JCER*)

18:10 to 18:50 Transportation for PSU and DUT Faculty Members to a separate place for joint dinner

19:00 to 21:30 Dinner

## **Thursday 10 November, 2016 AM & PM**

### **Session #7: Individual PSU-DUT Meetings**

08:30 to 10:15

**Individual DUT faculty members pick up of PSU faculty members from Bayshore Hotel**

**Individual DUT-PSU faculty group discussion and laboratory tour**

**Action items and plans for potential collaborations**

- (1) Bio-energy and water treatment (Liping Huang, to pick up Bruce Logan, for separate meeting/group discussion/lab visit)
- (2) Building energy (Tianyi Zhao, to pick up Moses Ling, for separate meeting/group discussion/lab visit)
- (3) Catalysis/chemical energy conversion (Xinwen Guo, Anjie Wang, Yao Wang, Chuan Shi and to pick up Phillip Savage, Mike Janik, Rob Rioux, and Chunshan Song; this group may be divided, for separate meeting/group discussion/lab visit )
- (4) Coal conversion (Haoquan Hu, to pick up Sarma Pisupati for separate meeting/group discussion/lab visit)

- (5) Electro-chemical energy (Yujiang Song to pick up Donghai Wang for separate meeting/group discussion/lab visit)
- (6) Separation of CO<sub>2</sub> and H<sub>2</sub>S (Shaoyun Chen to pick up Xiaoxing Wang, for separate meeting/group discussion/lab visit)

DUT faculty members accompany PSU faculty members to the Meeting Room of the State Key Laboratory of Fine Chemicals by **10:25** am

**Session #8: PSU-DUT Panel Discussion Facilitated by Dr. Chunshan Song**

10:30 to 11:30

**Panel discussions by DUT and PSU faculty members**

**Meeting Room of the State Key Laboratory of Fine Chemicals, DUT**

How to further advance the DUT-PSU collaboration?

Exchange of PSU and DUT students and faculty for collaboration

Joint efforts for potential international grants applications

11:40 to 13:00

**Lunch** (PSU-DUT faculty groups)

**Visiting Dalian Institute of Chemical Physics Facilitated by Dr. Chunshan Song**

13:00 to 13:20

**PSU Delegation Moving to Dalian Institute of Chemical Physics (DICP)**

13:30 to 17:00

**Visiting Dalian Institute of Chemical Physics, CAS**

Host: **Professor Tao Zhang, Director of DICP**

PSU faculty members meet with researchers at Dalian Institute of Chemical Physics (DICP)

**17:50- Dinner to be arranged by DICP**



# **Abstract and Biosketch**

## Overview of the PSU-DUT Joint Center for Energy Research

### Chunshan Song

*EMS Energy Institute, Departments of Energy & Mineral Engineering, and of Chemical Engineering  
The Pennsylvania State University ( [csong@psu.edu](mailto:csong@psu.edu) )*

*PSU-DUT Joint Center for Energy Research, School of Chemical Engineering, Dalian University of  
Technology*

This presentation gives an overview of the PSU-DUT Joint Center for Energy Research which was officially established between Penn State and DUT in April 2011. Significant progress has been made in collaborative research and education between Penn State and DUT through the efforts of faculty and graduate students in a number of research areas. Presidents of both universities have made mutual visits to the partner institutions. Three PSU-DUT Joint Energy Workshops have been organized, both in DUT and PSU with participation from both universities. Collaborative research between faculty members of the two universities have already resulted in ~60 peer reviewed journal articles. More collaborative research and education efforts are expected to result from the present Joint Energy Workshop, the 4<sup>th</sup> in the series since 2010.



Dr. Chunshan Song is the Director of the EMS Energy Institute, and a Distinguished Professor of Fuel Science and Professor of Chemical Engineering. He also serves as the Associate Director of the Penn State Institutes for Energy and the Environment and the Co-Director of PSU-DUT Joint Center for Energy Research at PSU and QianRen Chair Professor (Type B) at Dalian University of Technology. He is internationally known for his contributions to clean fuels, catalysis, and CO<sub>2</sub> capture and utilization research. He has over 280 refereed publications in leading journals, 8 patents, 6 books and 28 book chapters. He has delivered 50 plenary or keynote lectures at international conferences and 260 invited lectures worldwide. He has received many awards such as Henry Storch Award in Fuel Science and Fellow of ACS from American Chemical

Society, and QianRen Award (Type B) from Chinese government for which he holds the QianRen Professorship at School of Chemical Engineering at Dalian University of Technology. He has held numerous leadership positions with professional societies and international conferences. Dr. Song's current research interests include catalysis and adsorption for fuel processing, desulfurization of fuels and bio-gas, reforming of hydrocarbons and bio-fuels for hydrogen production and fuel cells, CO<sub>2</sub> capture, CO<sub>2</sub> conversion and utilization, shape-selective catalysis for chemicals, synthetic clean fuels from coal, heavy oil and biomass.

## Opportunities for Microbial Electrochemical Technologies and Thermal Regenerative Batteries to Provide Sustainable Solutions for the Water-Energy Nexus

**Bruce E. Logan**

*Department of Civil & Environmental Engineering, Penn State University, USA ([blogan@psu.edu](mailto:blogan@psu.edu))*

Continued population growth and urbanization is increasing the demand for food, energy and water. At the same time, the use of fossil fuels must be reduced to address climate change. Different microbial electrochemical technologies offer the promise for recycling food wastes, biomass, and organic matter in wastewaters directly into electricity and biofuels. Certain microorganisms can transfer electrons outside the cell during respiration, and therefore they can be used to develop new methods of renewable energy or chemical production based on: microbial fuel cells (MFCs) that can be used to produce electrical power; microbial electrolysis cells (MECs) for transforming biologically generated electrical current into transportable fuels such as hydrogen and methane gases; and other devices that can desalinate water, capture phosphorus, or produce acids and bases to fix carbon dioxide. In this presentation I highlight recent advances in materials and architectures that can transform MFCs into commercially viable technologies. Cathodes are the key component for power generation in an MFC, and activated carbon has been shown to be as effective a catalyst as Pt in MFCs, and activate carbon has greater durability and stability when MFCs are used to treat wastewater. Chemical modifications of the activated carbon can increase performance, with power densities in saline solutions as high as 4.7 W/m<sup>2</sup> using acetate. With domestic wastewater, power was about double that of a Pt catalyst, reaching 0.8 W/m<sup>2</sup>. Waste heat is an under-utilized source of energy for producing electricity. At Penn State, we are developing a new type of flow battery that can be charged using waste heat, as opposed to electrical power, so that energy in waste heat can be converted to electricity. So far energy conversion has reached ~7% of the Carnot efficiency, which is among the best efficiencies for these waste heat to electricity technologies. The use renewable biomass and waste heat or natural heat sources can be useful approaches for obtaining an energy sustainable water infrastructure.



Professor Bruce E Logan is an Evan Pugh Professor, the Stan & Flora Kappe Professor of Environmental Engineering, and Director of the Engineering Energy & Environmental Institute at Penn State University. His current research efforts are in bioenergy production and the development of an energy sustainable water infrastructure. Dr. Logan has mentored over 110 graduate students and post docs, and is the author or co-author of over 450 refereed publications (h-index=113, Google Scholar) and several books. He is the founding Editor of the new ACS journal Environmental Science & Technology Letters, and a member of the US National Academy of Engineering (NAE), and a fellow of AAAS, the International Water Association (IWA), the Water Environment Federation (WEF), and the Association of Environmental

Engineering & Science Professors (AEESP). Dr. Logan is a visiting professor at several universities including Newcastle University (England), Dalian University of Technology, Tsinghua University and Harbin Institute of Technology (China), with ties to several other universities in Saudi Arabia, Belgium and China. He received his Ph.D. in 1986 from the University of California, Berkeley. Prior to joining the faculty at Penn State in 1997, he was on the faculty at the University of Arizona.

## Heavy Metal Recovery and Separation with Simultaneous Hydrogen Production from Microbial Electrochemical Systems

**Liping Huang**

*School of Environmental Science & Technology at Dalian University of Technology*

Bioelectrochemical systems (BESs) including microbial fuel cells (MFCs) and microbial electrolysis cells (MECs) have been showing to be promising for producing chemicals and energy (H<sub>2</sub>, electricity, minor organic acids, etc) from wastes and wastewaters. Single metals such as aqueous Cr(VI) and Co(II), and even particles Co(III) have been shown in our laboratory to be successfully reduced/leached on the cathodes of BESs with various architectures/electrode materials (abiotic MFCs, abiotic MECs, biocathode MFCs and biocathode MECs), providing their potential as both environmental remediation technology and value-added metal recovery process from wastes/low grade ores in hydrometallurgical processes. In view of practical application, this metallurgical BESs also shows more efficient for recovering and separating mixed metals each other with simultaneous hydrogen production. Stacked BESs such as MFCs-MECs, serially stacked MFCs and MECs, and MFCs and MECs shift each other have been tested in our laboratory for recovery and/or separation of typical mixed metals including Cr(VI), Cu(II) and Cd(II), Co(II), Cu(II) and Li(I), Cr(VI) and Cd(II), and W(VI) and Mo(VI). Critical influence factors including reactor architecture, electrode material, bacterial community composition, stacked form of BESs and solution chemistry were highlighted and are being developed to potentially direct mixed metals recovery and separation from each other with simultaneous hydrogen production using this metallurgical BESs.



Dr. Huang is a Professor of Environmental Engineering at Dalian University of Technology. She began her appointment at Dalian University of Technology in July, 1994. Her research interests cover microbial/bioelectrochemical technologies for chemicals and energy (electricity, H<sub>2</sub>, minor organic acids, etc) generation from wastes and wastewaters. Current activities address bioelectrochemical technologies for multiple metals recovery and separation each other with simultaneous hydrogen production. She has co-authored about 80 papers and owned 6 authorized patents.

## ***In Situ* Spectroscopy Investigation of the Surface-interface Charge-Transfer Process over Tailored Nano-structured Based PEC Fuel Cells**

**Xinyong Li**

*School of Environmental Sciences and Technology, Dalian University of Technology*

The world has changed from the past decades and we are facing critical problems of global warming, energy crisis and environmental pollutions. Facing up to the problems, environmental catalysis has currently received enormous scientific attention and been extensively studied for environmental elimination and energy conversions process. Whereas, the environmental and energetic catalytic efficiency is still low in terms of practical requirements and long-term economic benefits. And to some extent, it is relatively difficult to get a whole and better understanding for environmental and catalytic process and mechanism as investigated and studied through traditional off-line techniques. Thus, how to further enhance the efficiencies of environmental and energetic catalysis and deeply understanding the environmental micro-interface processes have become a hot and cutting-edge research topic in modern environmental and energy science as well as corresponding interdisciplinary areas. This presentation will highlight some of our recent studies devoted to the design and fabrication of tailed active nano-structured materials for energy-efficient and environmentally friendly catalytic chemical transformations and sustainable energy conversions. Specific information on bunch of ferrite based PEC fuel cells will also be presented. It has been well recognized that development of powerful *in situ* spectroscopy techniques would allow us to study surface-interface charge transfers over the PEC fuel cells with high spatial and temporal resolutions and at relevant instant conditions. Follow up this point, several newly developed *In Situ* technique including EPR, FT-IR ESEM and EI-SPS with self-assembled accessories, adapted from the energetic catalysis and nanotechnology fields, to probe the intrinsic molecular adsorption and desorption, molecular oxygen uptake and ROS (reactive oxygen species) formation, surface-interface charge transfer, intermediates species interactions and stepwise transformations will be briefly discussed.



Dr. Xinyong Li is currently a Professor of Chemical and Environmental Engineering, the Deputy Director of the Centre for Environmental Catalysis & Sustainable Energy at Dalian University of Technology, and an Adjunct Professor in the Department of Chemical Engineering, Curtin University, Australia. He has established his exceptional research career having worked in a number of world-leading institutions such as CAS, University of Calgary, University of Georgia, HKUST, and Curtin University, with an international reputation in the field of Advanced Nanomaterials for Catalysis and Sustainable Energy, which was recently recognised through the award of the prestigious 2011 Second Prize of National Natural Science Awards (Engineering and Technology category) for outstanding scientific contributions. Dr. Li has an outstanding publication track record with SCI H-index 33 and Google i10-Index 55 (over 180 peer-reviewed journal papers, review articles, patents and book chapters, and over 90 technical presentations and reports), predominantly and consistently publishing in top tier A\* ranked Journals such as *Angew. Chem. Int. Ed.*, *Adv. Func. Mater.*, *Journals of Catalysis*, *J. Mater. Chem.*, *Nanoscale*, *ES&T* etc). Dr. Li has trained 2 Postdoctoral fellows, 11 PhD, 21 M.Sc and 27 Undergraduate students (UG Investigation Project) during his academic career, and now supervising 2 postdoctoral fellow, 11 PhD, 12 M.Sc postgraduate and 12 Undergraduate students. Many awards were credited to his research achievements including the prestigious Second Prize of National Natural Science Awards (Engineering and Technology category), the Distinguished Supervisor for Nominated National Excellent Doctoral Dissertation, the Distinguished Supervisor Provincial Award for Excellent PhD and M.S Theses, the First Prize of Natural Science Academic Achievement Awards of MOE, the Tin Ka Ping Scholar Prestigious Awards of HKUST, Elsevier Outstanding Reviewer Awards 2014 and 2015 Elsevier most cited Chinese researchers on environmental science. Dr. Li also makes active professional service as Regional Editor and/or Editorial Board including *Current Catalysis*. Dr. Li has also served on many national panels on Nanotechnology, Environmental Sciences and Energy Conversion processes and review committees for the National Academy of Sciences. He has been invited to serve as section chairs or advisory and organizing committee members for many international academic conferences.

## Under Pressure and in Hot Water – Hydrothermal Reactions of Biomass and Biomolecules

**Phillip E. Savage**

*Pennsylvania State University, Chemical Engineering Department, University Park, PA 16802*

There is much interest in using renewable biomass resources to meet demand for fuels and chemicals. Algal biomass is an attractive renewable feedstock because it requires less land area and has a higher photosynthetic efficiency than terrestrial biomass and it does not involve a food/feed vs. fuel competition as does corn ethanol or soy biodiesel. Being aquatic plants, harvested microalgae carry with them tremendous amount of water. Conventional algal bioenergy processes (e.g., lipid extraction for biodiesel production) first remove the water and then process the dried biomass. This drying step is costly and energy intensive. Thus, there is a need for wet biomass conversion processes that operate in the aqueous phase. We are helping to develop the chemical kinetics and reaction engineering foundations for hydrothermal processes that can convert wet biomass into biofuel intermediates directly (no drying) and thereby reduce process energy demands for biofuel production. This talk will outline recent progress made in understanding and optimizing the use of hydrothermal liquefaction for converting wet biomass into liquid fuels. Advancements in molecular characterization of the reaction products, understanding the hydrothermal reaction pathways and kinetics for biomass and model biomolecules, and reaction modeling will be highlighted.



Phillip E. Savage is the Head of the Chemical Engineering Department at Penn State and the Walter L. Robb Family Chair. He is also Arthur F. Thurnau Professor Emeritus at the University of Michigan. He earned a B.S. from Penn State and M.Ch.E. and Ph.D. degrees from the University of Delaware. All of his degrees are in chemical engineering.

Phil is Editor-in-Chief of *Industrial & Engineering Chemistry Research*. He is on the editorial boards for *J. Supercritical Fluids*, *Energy & Fuels*, and *Environmental Progress & Sustainable Energy*. He is past-chair of the Industrial & Engineering Chemistry Division of ACS and a past-chair of the AIChE Catalysis and Reaction Engineering Division.

Phil has published over 200 research articles in archival journals and given nearly 100 invited lectures at other universities and international symposia. He holds three U.S. patents, two of which have been licensed and put into practice commercially. Phil's research deals with reaction kinetics, pathways, and mechanisms in aqueous systems at elevated temperature and pressure. His recent work focuses on hydrothermal conversion of biomass to fuels. Phil has mentored 43 PhD students, nine of whom have been NSF and/or EPA STAR graduate fellows. Phil is a Fellow of both the AIChE and ACS. He received the inaugural (2015) *Energy & Fuels* Excellence in Publication Award from ACS, the 2014 Research Excellence Award from the AIChE Sustainable Engineering Forum, the Inaugural (2009) Michigan Governor's Award for Green Chemistry, and the 2001 National Catalyst Award from the American Chemistry Council in recognition of his outstanding teaching and contributions to chemical education.

## Carbon Materials Synthesis and Characterization

### Jieshan Qiu

*State Key Laboratory of Fine Chemicals, PSU-DUT Joint Center for Energy Research, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China.*



Dr. Jieshan Qiu is the executive director of the Institute of Energy Science and Technology and professor of chemical engineering and materials science. Dr. Qiu teaches in materials science and chemical engineering and his research interests focus on carbon materials and conversion of coal to advanced carbon materials. Dr. Qiu's current research includes preparation and application of high performance carbon adsorbents; adsorption separation technology and surface science; functional carbon materials for energy storage; preparation, characterization and application of carbon nano- and micro-materials; carbonbased novel catalysts and catalysis reactions; plasma chemistry and chemical engineering; novel nanomaterials from biomaterials.



## Design and Synthesis of Hollow Zeolites and their Applications

**Xinwen Guo**

*State Key Laboratory of Fine Chemicals, PSU-DUT Joint Center for Energy Research, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China.*

In recent years, hollow zeolites have attracted increasing attention for their versatile applications ranging from microreactors to metal supports. In our research work, hollow S-1 zeolite nanocubes could be easily controlled from about 150 to 600 nm by simply adjusting the size of parent silicalite-1. Using hollow S-1 nanocubes as host material, HPW@Hollow S-1, a novel solid catalyst which can be reused in the synthesis of ethyl acetate, was successfully prepared by the ship-in-bottle approach. Using “impregnation-dissolution-recrystallization” method, Ni-Pt binary metal nanoparticles with a small average size of 4 nm have been successfully encapsulated in hollow silicalite-1 single crystals. Compared with single metals (Ni or Pt) in the hollow crystals, Ni-Pt@Hol S-1 enhances the dispersion of nickel and platinum. Meanwhile, the encapsulation process enhances the interaction between nickel, platinum and support; making the catalyst sintering and coking resistant in dry (CO<sub>2</sub>) reforming of CH<sub>4</sub>. The synthesized hollow ZSM-5 exhibits desired acid catalysis with higher shape selectivity, as shown by higher 4-methyl biphenyl selectivity and similar activity in the biphenyl methylation with methanol as compared to solid ZSM-5. Furthermore, hollow ZSM-5 single crystals with double layer shells were successfully prepared with a layer-by-layer technique followed with dissolution-recrystallization strategy. Hollow ZSM-5 nano-sized crystals with encapsulated Fe<sub>2</sub>O<sub>3</sub>, carbon nanotubes (CNTs), and hollow ZSM-5 encapsulating bimetallic (oxide) nanoparticles such as CuO-Pd, and CuO-Pt as well as Fe<sub>2</sub>O<sub>3</sub>-Au have also been successfully synthesized. More interestingly, hollow pineapple-like nanovesicle assembly with hollow metal-encapsulated MFI type nanocrystals further improves the dispersion of encapsulated metal, which show superior activity and good reusability in the reaction of phenol oxidation.



Prof. Xinwen Guo is the Deputy Dean of Faculty of Chemical, Environmental and Biological Science and Technology and a Professor of Chemical Engineering at Dalian University of Technology (DUT). He is affiliated with PSU-DUT Joint Center for Energy Research. He received his Ph.D. in Industrial Catalysis at DUT in 1994. He began his faculty appointment at DUT in 1994. He has received a number of awards, including a Young Faculty Award, an expert of Dalian City, an expert of Liaoning Province, Award for Progress in Science and Technology of China. He has published approximately 200 papers in peer-

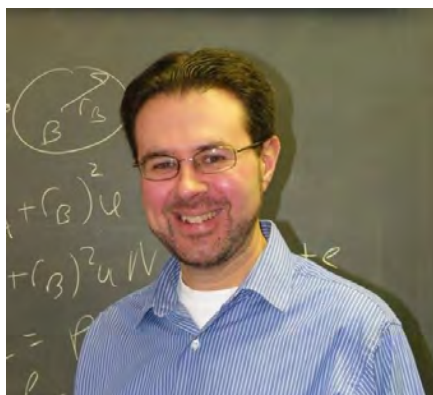
reviewed journals, and co-authored a book titled “Science and Engineering Fundamentals of Green Petrochemical Technology” (published by Petrochemical Press). He has been granted 30 patents in China. His group’s research currently focuses on the synthesis of novel zeolites and MOF materials and their applications such as shape-selective alkylation and selective oxidation, the conversion of carbon dioxide into fuels, and computational catalysis. His research has been financially supported by Natural Science Foundation (NSF) of China, the Education Ministry of China, the Science and Technology Ministry of China, and Industry.

## Computational Chemistry Studies of Heterogeneous Catalysis: the Impact of Self-assembled Monolayers on Selectivity

**Michael J. Janik**

*Department of Chemical Engineering at Pennsylvania State University*

Our group applies computational chemistry techniques to a range of catalyst and materials design challenges in energy technology. Quantum mechanics based computational techniques, such as density functional theory methods, are a useful tool in guiding catalyst design. Density functional theory (DFT) methods are widely used to evaluate surface catalytic reaction mechanisms and to predict the relative performance of various catalyst formulations or structures. Our group applies these methods to complex systems including metal and metal oxide catalysts and electrocatalysts. In each area, complexity is introduced to include features of the material or reaction environment that challenge straightforward application of DFT methods. Examples include the modeling of mixed oxide catalyst surfaces, inclusion of electrolyte impacts on electrochemical reactions, or the impact of self-assembled monolayers on catalyst selectivity. For this talk, I will overview the goals and approaches used to apply DFT methods to complex catalysts, and use the example of self-assembled monolayer effects on hydrogenation selectivity to illustrate these approaches.



Dr. Janik is a Professor of Chemical Engineering at Pennsylvania State University. He began his appointment at Penn State in August, 2006. His research interests are in the use of computational methods to understand and design materials for alternative energy conversion systems. Current activities address a wide-range of energy technologies including fuel cells and electrolysis, hydrogen generation, organic photovoltaics, and CO<sub>2</sub> capture and utilization. Research methods emphasize atomistic simulation using quantum chemical methods and kinetic modeling. Janik is affiliated with the Penn State Energy Institute, PSU-Dalian University of Technology Joint Center for Energy Research, the PSU Institutes of Energy and

the Environment, and the Battery and Energy Storage Technology Center. He also holds the title of HaiTian (Sea-Sky) Scholar from Dalian University of Technology. The Janik group currently includes 12 graduate students and 12 undergraduate students. Dr. Janik received his B. S. in Chemical Engineering from Yale University. He completed his doctoral studies at the University of Virginia under the advisement of Bob Davis and Matt Neurock. He has co-authored approximately 100 peer reviewed papers, and co-edited the book “Computational Catalysis” (with Aravind Asthagiri), published by the Royal Society of Chemistry in 2013.

## Sulfur Removal from Engine Fuels: Hydrodesulfurization and Oxidative Desulfurization

**Anjie Wang**

*School of Chemical Engineering at Dalian University of Technology*

Sulfur in gasoline and diesel is removed industrially by hydrodesulfurization (HDS), which is conventionally catalyzed by Mo- and W-based sulfides with Co and Ni as the promoters. However, sulfide catalysts are not effective in removing refractory sulfur compounds such as dibenzothiophenes (DBTs). Metal phosphides show great promise in the HDS of refractory sulfur compounds, in which the hydrogenation route predominates, because of their high hydrogenation activity. Unexpectedly, our group found that 4,6-dimethyl dibenzothiophene (4,6-DMDBT) is more reactive than DBT over supported MoP and WP. As a result, a combination of MoP bed and NiMoS bed led to enhanced HDS of a real diesel. Oxidative desulfurization takes place in mild conditions ( $< 100$  °C and atmospheric pressure), and is considerably efficient to turn the refractory sulfur molecules, which is less reactive in HDS, into their sulfones. The generated sulfones can be easily removed by extraction and/or adsorption. For this talk, I will outline the preparation of metal phosphides, the catalytic performance of metal phosphides in HDS, and the continuous oxidative desulfurization in a fixed-bed reactor.



Dr. Anjie Wang is a Professor of Catalysis at Dalian University of Technology. He began his appointment at Dalian University in July, 1988. His research interests include clean fuel catalysis, mesoporous and micro-mesoporous composite materials for catalysis, catalytic reaction engineering, and plasma catalysis. He is a member of Catalysis Society of China, and the Director of Liaoning Key Laboratory of Petrochemical Technology and Equipment. He is affiliated with the State Key Laboratory of Fine Chemicals and the PSU-DUT Joint Center for Energy Research. Dr. Wang received his Ph.D. degree in Coal Chemical Engineering from Dalian University of Technology in 1991. He has co-authored approximately 120 peer-reviewed papers, and co-authored two

books “Introduction to Heterogeneous Catalysis” (with Roel Prins and Xiang Li, published by Imperial College Press, 2016) and “Chemical Reaction Engineering” in Chinese (with Yuzhi Zhou and Bei Zhao, published by Chemical Industry Press, 2004).

## Understanding Site Isolation of Pd and Ni in Zn-based Bulk Intermetallics during the Selective Hydrogenation of Alkynes

**Robert M. Rioux**

*Department of Chemical Engineering and Department of Chemistry, The Pennsylvania State University, 165 Fenske Laboratory, University Park, PA 16802-4400*

The catalytic semi-hydrogenation of acetylene to produce ethylene is a common method for the removal of trace acetylene (~1%) in ethylene feed streams destined for ethylene polymerization. An effective catalyst for this reaction converts all of the acetylene to ethylene without further conversion of ethylene to ethane such that there is a net increase in the amount of ethylene. Pd-Ag alloys, and more recently, intermetallic Pd-Ga compounds, demonstrate high selectivity towards ethylene and long-term stability. Improved selectivity is a result of isolation of active Pd hydrogenation sites which reduces over-hydrogenation to form ethane, oligomerization products, and coke formation on the catalyst surface. Replacing Pd-based catalysts with base metal Ni-based catalysts would be highly beneficial in terms of cost and environmental impact. Bulk intermetallic catalysts contain little structural and compositional variance, a property that is not easily attainable with supported catalysts. We report on the catalytic selectivity of unsupported bulk intermetallic Ni-Zn and Pd-Zn catalysts for acetylene semi-hydrogenation. We demonstrate the addition of Ni to Zn improves selectivity to ethylene due to a reduction in acetylene oligomerization products rather than ethane over-hydrogenation. The most selective catalysts had the lowest Ni content with a  $\gamma$ -brass bulk structure. Structural investigation by neutron diffraction demonstrated the presence of well-defined Ni (or Pd) trimers in the  $\gamma$ -brass structure with the number of these trimers increasing with Ni (or Pd) content. The Ni alloys are active for H<sub>2</sub>-D<sub>2</sub> exchange, but all surfaces (i.e, different Ni content) are indistinguishable with respect to their catalytic behavior. In the case of Pd-Zn alloys with the  $\gamma$ -brass structure, there are apparent differences in the H<sub>2</sub>-D<sub>2</sub> rates and ethylene hydrogenation as the Pd content (and therefore number of Pd trimers) increases. While the Ni and Pd trimers are stable in the bulk structure, the differences in the surface stability of these trimers in the Zn matrix and the corresponding percentage of the trimer-containing surface present in a Wulff reconstruction explain the disparate catalytic results in the seemingly related systems. We demonstrate bulk intermetallics are useful systems to screen compositional and structural (from site-isolated to well-defined 2D clusters) variance on catalytic behavior. Transforming the bulk intermetallic structure into its nanoscale analog still remains a critical challenge for catalyst synthesis.



Robert (Rob) M Rioux is the Friedrich G. Helfferich Associate Professor of Chemical Engineering at the Pennsylvania State University. Prior to joining the Pennsylvania State University in 2008, he was a National Institutes of Health Postdoctoral Fellow at Harvard University in the Department of Chemistry and Chemical Biology working with Professor George Whitesides. He received his Ph.D. in physical chemistry from the University of California, Berkeley in 2006 working for Professor Gabor Somorjai. He holds a B.S. and M.S. degree in chemical engineering from Worcester Polytechnic Institute and the Pennsylvania State University, respectively. Since joining the Penn. State faculty, he has received a number of awards, including a DARPA Young Faculty Award, an Air Force Office of Scientific Research Young Investigator Program Award, a NSF

CAREER Award and a 3M Non-Tenured Faculty Award. Research in his laboratory is currently sponsored by NSF, DOE-BES, DARPA, AFOSR, AFRL, ACS-PRF and industry. His group's current research focus is on the development of spatially- and temporally-resolved spectroscopic techniques for imaging catalytic chemistry, single molecule methods to understand single molecule/particle catalytic kinetics and dynamics, elucidating reaction mechanisms in nanoscale systems, including catalyst synthesis, development of solution calorimetric techniques to understand catalytic processes at the solid-liquid interface and the development of base-metal catalysts for chemoselective chemical transformations.

## Intensification of Chemical Reaction by Synergy of Non-Thermal Plasma and Catalysis

**Yao Wang**

*School of Chemical Engineering at Dalian University of Technology*

Our group applies the combination of non-thermal plasma with catalysis techniques to the reactions which are unfavorable thermodynamically nor kinetically including high-purity hydrogen production from H<sub>2</sub>S splitting, CO<sub>2</sub> conversion into methane, and preparation of metal phosphides. Hydrogen sulfide (H<sub>2</sub>S) is a highly toxic and corrosive contaminant in large quantities. As a consequence, H<sub>2</sub>S must be detoxified, in general, by the Claus process, in which H<sub>2</sub>S is partially oxidized to produce elemental sulfur and water. On the other hand, H<sub>2</sub>S has often been considered a potential source of hydrogen for the future hydrogen energy economy. Recently, we found that the combination of semiconductor catalysis with non-thermal plasma in a dielectric barrier discharge (DBD) reactor was extremely efficient to decompose H<sub>2</sub>S for the production of hydrogen and sulfur at atmospheric pressure. In this presentation, decomposition of hydrogen sulfide in non-thermal plasma aided by supported Zn<sub>x</sub>Cd<sub>1-x</sub>S solid solutions will be presented. A series of Al<sub>2</sub>O<sub>3</sub> supported Zn<sub>x</sub>Cd<sub>1-x</sub>S solid solutions were prepared, and investigated in the plasma-induced H<sub>2</sub>S decomposition.



Dr. Yao Wang is a Professor of Chemical Engineering, School of Chemical Engineering at Dalian University of Technology (DUT), China. She specializes in heterogeneous catalysis, bio-oil upgrading, and process system engineering. Her current research interests address intensification of chemical reaction by synergy of non-thermal plasma and catalysis (high-purity hydrogen production from H<sub>2</sub>S splitting and CO<sub>2</sub> conversion), hydrodeoxygenation of bio-oil derived from cellulose-based biomass, and synthesis of transition metal phosphides via hydrogen plasma reduction and their applications in hydrotreating process.

Dr. Wang received her Ph.D. degree in Chemical Engineering from Dalian University of Technology, China in 2004. She has been a faculty of Dalian University of Technology since 1991. She is affiliated with PSU-DUT Joint Center for Energy Research. She has published over 50 quality papers in peer-reviewed journals, and co-authored two textbooks “Chemical Engineering Principles” (published by Chemical Industry Press) and “Chemical Engineering Design” (published by Chemical Industry Press). She is one of the recipients of the Third Prize of Natural Sciences of Liaoning Province. Her research has been financially supported by Natural Science Foundation of China, the Education Ministry of China, and Liaoning Province.

## **Tar Formation and Characterization during Pyrolysis of Coal and Biomass at High Temperatures and Pressures**

**Sarma V. Pisupati**

*Department of Energy and Mineral Engineering (EME) at Penn State University*

Tars are a group of compounds obtained during the rapid devolatilization of coal or biomass that can condense and merit a special investigation especially when biomass and coal are blended. Characterization of tars can provide meaningful information. It can help predict the amount and constituents of tars in processes where liquid products yield need to be maximized or minimized. Minimizing liquid product yield is for instance required in coal or biomass gasification, since tar in the product gas is undesirable. However, in combustion processes, tar becomes a valuable product as it carries a significant amount of the fuel's calorific value. In pyrolysis processes it is even highly valued as many species forming tar are the main constituents of bio-oil. Quantification and characterization of tar can also provide a good insight into the mechanism of thermal breakdown of solid fuels. There have been several studies investigating the formation and composition of tars in biomass and coal thermochemical processes. However, these studies have been conducted mostly in fluidized and fixed bed reactors offering a maximum temperature of approximately 1473 K. Therefore studies focusing on the formation and characterization of tar in high temperature systems such as entrained flow gasifiers are scarce.

The present study aims at bridging the gap that exists in the characterization of tars formed during high temperature pyrolysis of coal and biomass. Studies on tar species formation at high temperatures (1300-1500C) in a high pressure and high temperature entrained flow reactor have been conducted using Pittsburgh #8 Bituminous coal, White Pine sawdust and Swichgrass powder. Tar sampling was done using "European Tar Protocol". Identification and quantification of the compounds found in the tars was carried out by Gas Chromatography Mass Spectrometry (GC-MS). From the GC-MS results, the mass and the mole of the elements making up the tar species were calculated. The average molecular weight as well as the high heating value (HHV) of the each tar sample were also calculated. Variation of the H/C ratio of the tars indicated that this ratio decreased as the pyrolysis temperature is increased. Higher pyrolysis temperature resulted in an increase of the S/C ratio of the tar. The HHV, calculated by Dulong formula, decreased as the devolatilization temperature was increased.



Sarma V. Pisupati is Professor and Chair of the Energy Engineering Program, and Director of Online Education in the John and Willie Leone Family Department of Energy and Mineral Engineering at Penn State. He also codirects Coal Science and Technology Program of the EMS Energy Institute. He earned B.S. and M.S. degrees in Chemical Engineering and a Ph.D. degree in Fuel Science. He has been studying and teaching the issues related to the energy and environment for the past 35 years. He has worked in industry for five years before joining The Pennsylvania State University.

Prof. Pisupati's main areas of scientific research are combustion behavior of fossil fuels in fixed; fluidized and pulverized modes; computational fluid dynamic modeling of combustion systems for emission reduction; advanced power generation methods; oxy-fuel combustion; slagging and fouling in gasification; coal and biomass co gasification, energy conservation methods. He was Principal Investigator (PI) or co-PI on 60 externally funded scientific research projects and was involved in 15 other projects with specific responsibilities. He coauthored about 200 research publications and has one US patent.



## Overview on Coal Direct Conversion into Liquid Products and Other Coal-Related Works in Our Group

**Haoquan Hu**

*State Key Laboratory of Fine Chemicals, Institute of Coal Chemical Engineering, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, Liaoning, China*

Direct coal conversion into valuable liquid products, gas and char is an effective approach for clean utilization of coal. To improve the liquid product yield in coal pyrolysis, a novel process by coupling of traditional coal pyrolysis with catalytic reforming of low carbon hydrocarbon like CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> was developed in our group. By this way, above 50% tar yield than general pyrolysis can be obtained, which was resulted from the interaction of free radicals from coal with those from the hydrocarbon reforming confirmed by the isotope trace analysis. To clarify the coal pyrolysis process, some new apparatus like single-photon ionization time-of-flight mass spectrometry (SPI-TOF-MS) coupled with molecular beam sampling, *in-situ* coal pyrolysis- TOF-MS with EI and vacuum ultraviolet photoionization was applied to detect the free radicals or primary pyrolysis products. In the research on direct coal liquefaction (DCL), we focus on the catalyst effect and hydrogen transfer mechanism in DCL. We found that addition of small amount H<sub>2</sub>S to H<sub>2</sub> can obviously promote the conversion of preasphaltene and asphaltene into oil, and the interaction between hydrogen-donor and non-donor solvents affects the liquefaction performance. In addition, our group also conducts some studies on (i) synthesis and application of hierarchical materials (like activated carbon and zeolite) in hydrogen production by catalytic reforming of CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub> and catalytic decomposition of CH<sub>4</sub>, simultaneous capture and removal of hazardous pollutants during coal conversion, (ii) coal structure analysis and the theoretical calculation for the cleavage analysis of weak bonds in coal during thermal conversion, (iii) the mechanism and modeling of pore structure evolution in a coal particle during rapid pyrolysis by simulation based on CPD model. In this talk, I will overview the processes of direct coal conversion into liquid products and other coal-related studies in our group.



Dr. Hu is a Professor of Chemical Engineering at Dalian University of University (DUT). He began his appointment at DUT in July, 1985. His main research interests are in the coal and biomass conversion, preparation of porous materials and their application. Current activities address in fundamental research on coal structure and mechanism of coal thermal conversion, and developing new coal conversion technology including a process to integrate methane-rich gas activation with coal pyrolysis for high liquid product, coal direct liquefaction. He is the project leader of a National Key Research and Development Project on "Basic research on low rank coal conversion to high quality liquid fuels and chemicals". Hu is affiliated with School of Chemical Engineering of DUT, and is the director of Institute of Coal Chemical Engineering. He is also the Academic Committee Members of several state key laboratories including the State key laboratory on Coal Conversion in Shanxi institute of coal chemistry, Chinese academy of sciences; Editorial Board Member of several journals such as Fuel Processing Technology, J. of Fuel Chemistry, J. of DUT. The Hu group currently includes one associate professor, two lectures, 28 graduate students. Dr. Hu received his Bachelor degree in Chemical Engineering in 1982 from Zhejiang Institute of Technology, and his Master degree in 1985 and Ph.D. degree in 1990 from DUT. He has co-authored more than 100 peer reviewed papers and more than 10 granted or applied patents.

## Development of Functional Composite Materials for Energy Storage Applications

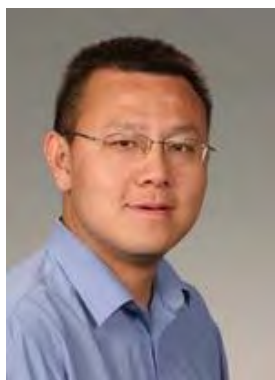
**Donghai Wang**

*Department of Mechanical and Nuclear Engineering*

*Department of Chemical Engineering*

*The Pennsylvania State University*

Electrical energy storage (EES) technologies are a key enabler to the future smart grid, particularly with the increasing penetration of renewable intermittent energy such as solar and wind energy. Similarly, EES technologies must be incorporated if transportation is to be partially or even totally electrified such as in plug-in hybrid and all electric vehicles. Li-ion batteries dominate portable electronic device and are the most likely EES system for transportation and small-scale stationary application; however, a large increase in the storage capability is needed, combined with lower cost and longer life. Today's intercalation based Li-ion batteries now are approaching their limits. My group is interested at development of new materials and technology for electrochemical energy storage application with emphasis on developing the functional composites and understanding the effect of controlled structure, interface and composition on its electrochemical performance. The presentation will cover development of cathode and electrolyte for Li-S battery and micro-sized Si-C composites for Li-ion anode and understand structure-property relationship for its excellent energy density and cycling stability of the batteries.



Dr. Donghai Wang is currently Associate Professor at Department of Mechanical Engineering and Department of Chemical Engineering at The Pennsylvania State University. Before joining Penn State in 2009, he was a postdoc and subsequently became a staff scientist at Pacific Northwest National Laboratories where he developed functional materials for catalysis and energy storage techniques. He received a B.S. and Ph.D. degree in Chemical Engineering from Tsinghua University and Tulane University in 1997 and 2006, respectively. Dr. Donghai Wang's research interests have been related to design and synthesis of materials for a variety of applications. His recent research is focused on material development for energy conversion and storage technologies such as batteries, fuel cells and solar fuels. Professor Wang has authored and co-authored over 80

peer reviewed publications and 4 book chapters.

## Low- and Non-platinum Electrocatalysts of Polyelectrolyte Membrane Fuel Cells (PEMFCs) & Low-temperature Direct Biomass Fuel Cells (L-T DBFCs)

**Yujiang Song**

*State Key Laboratory of Fine Chemicals, School of Chemical Engineering at Dalian University of Technology*

**Part I:** Platinum-based electrocatalysts are one of the key materials of PEMFCs and have been confronting the challenge of activity, cost, and durability, preventing this clean technology from widespread commercialization. We aim to create new types of low- and non-platinum electrocatalysts to tackle the problem, such as by developing controllable synthetic approaches and scaled-up preparative route for practical applications.

**Part II:** L-T DBFCs represents a new type of fuel cells directly converting biomass, especially solid water-soluble ones, to electricity. Unlike common hydrogen and alcohol fuel, biomass comes from photosynthesis, can be easily stored and transported, as well as has no fuel cross-over and is friendly to the polymer membrane. We focus on the selection of appropriate biomass molecules, advanced electrocatalysts for anodic fuel oxidation, and engineering issues.



Dr. Song received his M. S. in Inorganic Chemistry from Jilin University in 2000. He completed his doctoral studies at the University of New Mexico & Sandia National Laboratories (SNL) under the advisement of Dr. Prof. John A. Shelnutt in 2004. He was a Postdoctoral Researcher and later became a member of The Technical Staff at SNL from 2005-2009. He joined Dalian Institute of Chemical Physics of Chinese Academy of Science as a group leader in 2009. Dr. Song is a Professor of Chemical Engineering at Dalian University of University since 2015. His research interests include electrocatalysis, energy materials, PEMFC, L-T DBFCs, and CO<sub>2</sub> electrochemical reduction.

## Recent Progress of Developing Molecular Basket Sorbents for CO<sub>2</sub> and H<sub>2</sub>S adsorption separation

**Xiaoxing Wang**

*Senior Research Associate, EMS Energy Institute, the Pennsylvania State University*

Capture of CO<sub>2</sub> from various gas streams, especially from large sources of emissions such as coal fired power plants, is of critical importance in mitigating the greenhouse gas effect while meeting the increasing energy demand worldwide. Molecular basket sorbents (MBS) consisting of functional polymers immobilized in nano-porous materials have shown great potential as highly selective, high-capacity solid sorbent for CO<sub>2</sub> capture. Here, I will present our recent efforts in developing new generation of molecular basket sorbents (MBS), which includes using various commercially available supports such as fumed silica, silica gel, TUD-1 and carbon materials, and post-TEOS coating method to reduce the preparation cost, increase the capacity and enhance the sorption kinetics of MBS for CO<sub>2</sub> capture from flue gas. By using commercial supports, the MBS preparation cost and the associated cost for CO<sub>2</sub> capture are significantly lower compared to MCM-41 and SBA-15 (represents over 1000 times reduction in cost). Both the CO<sub>2</sub> sorption capacity and sorption kinetics were also improved. The addition of alkali carbonate promoted the CO<sub>2</sub> sorption capacity and stability of the MBS. The post-TEOS coating method was found to be effective in improving the thermal stability and regenerability of MBS. The current efforts make the new generation MBS more promising for practical applications. Additionally, through the collaboration with the engineering team at RTI International, the molecular basket sorbent has also been successfully scaled up from lab-scale powder to pilot-plant scale fluidizable particles with large quantities (>150 kg) and further evaluated in a fluidized-bed pilot plant with simulated flue gas which is engineered and operated by RTI International. The preliminary results collected from operating the pilot-plant system demonstrate that the sorbent is capable of rapid CO<sub>2</sub> removal and exhibits the ability to capture >90% of CO<sub>2</sub> in flue gas. At the end of this talk, the application of MBS for H<sub>2</sub>S adsorption will also be discussed.



Dr. Xiaoxing Wang is a Senior Research Associate of the EMS Energy Institute at the Pennsylvania State University. His research interests are in the areas of catalysis, renewable fuels and chemicals, and advanced materials for catalytic and adsorption processes. Dr. Wang has many years' research experience in developing advanced solid sorbents for CO<sub>2</sub> capture. His work has generated some important publications in prestigious journals including Journal of American Chemical Society, Journal of Physical chemistry C and Green Chemistry. So far Dr. Wang has about 57 publications and 2 issued patents. Dr. Wang received his PhD in Physical Chemistry (Catalysis) from Xiamen University with Prof. Ye Wang and has worked as postdoctoral researcher with Prof. Chunshan Song and late as Research Associate in the Pennsylvania State University.

## Environmental Catalysis: Catalytic Elimination of Environmental Air Pollutants and Green Process to Convert the Waste into the Useful

**Chuan Shi**

*Department of Chemistry at Dalian University of Technology*

Our research interests focus on **Nanocatalysis and Plasma assisted catalysis**. Nanomaterials have received much interest by virtue of their excellent properties suited for applications in various fields such as electronic, pharmaceutical, biomedical, cosmetic, energy, and catalysis. Physical, chemical, and biological properties of materials in nano-scale differ in fundamental from those of individual atoms and molecules or bulk materials. The extremely small size of the particles maximizes surface area exposed to the reactant, allowing more reactions to occur. We investigate the nanocatalysis on: (i) Supported nano-gold catalysts; (ii) Nano-sized transition metal nitrides/carbides/phosphides. We focus on the size dependent of nano-particles on catalysis, as well as the specific properties of nanomaterials for catalysis, i.e. noble like chemical properties. Meanwhile, hybrid plasma-catalyst systems have proven to be very efficient in VOC oxidation, automobile catalysis and water purification. However, no matter which kind of system is being used, the problem associated with the plasma-catalysis approach is the relatively high energy cost required to remove very low concentrations of pollutants. Therefore we propose a tandem “Non-thermal plasma-pulse” regeneration process which combines with the enrichment of low-concentration air pollutants on the catalysts at room temperature. Plasma is only applied for a very short time compared with the operating time for air pollutant enrichment, providing an energy-efficient method for the synergy of plasma and catalysis.



Dr. Chuan Shi is a Professor of Chemistry at Dalian University of Technology. She began his appointment at DUT in April, 2004. Her research interests are nanocatalysis and plasma assisted catalysis. Current activities address mainly on environmental catalysis, including automotive catalysis, VOC catalytic removal and small molecules of CH<sub>4</sub> and CO<sub>2</sub> activation and conversion. Her works have got the financial supports from National Science Foundation of China, and some research results have been published in Appl. Catal. B-Environmental, AICHE Journal, Green Chemistry and ACS Catalysis etc. Dr. Chuan Shi has been awarded as New Century Excellent Talents in University and Outstanding Young Teachers of Liaoning province.

## **Integrated Building Solutions – A Sustainable Design Strategy**

**Moses D.F. Ling**

*Architectural Engineering Institute at Pennsylvania State University*

Architectural Engineering Institute promotes “integrated building solutions” in its mission and vision statements. Ample opportunities to affect lower energy use and sustainability can be found in the practice of integrative design between architects and engineers. No longer should architecture and engineering be viewed as stand-alone disciplines. Buildings must be designed by collaborative efforts seeking synergic outcomes. Several projects of differing scale will be used to illustrate this approach to building design. Natural forces were used to achieve the goals of integrated building solutions.



Dr. Moses Ling is a professor and Undergraduate Program Officer in Architectural Engineering at Penn State. He is the past president and currently on the Board of Governors of Architectural Engineering Institute. As the Undergraduate Program Officer, Prof. Ling leads the Undergraduate Studies Committee in the design of educational objectives, pedagogical content, and learning outcomes, as well as the assessment process of an ABET accredited 5-year undergraduate program. For his research, an opportunity for investigation in architectural engineering is the practice of integrative design to affect energy efficient design. While most academic research focuses on the specifics of engineering disciplines, abundant opportunities exist at the intersection of architecture and engineering systems. Integrative design promotes passive design concepts. Passive Cooling Opportunities for Seasonal Energy Savings in Mass-produced Homes – Explore opportunities in current mass-produced homes for energy savings utilizing natural or low-tech ventilation techniques. Green Living – Survey of Hong Kong residents attempting to understand the life-style practices and expectations of residents of high-rise residential buildings.

## **Improving Building Energy Efficiency by Internet of Building Energy System (iBES)**

**Tianyi Zhao**

*Department of Civil Engineering at Dalian University of Technology*

Since building energy consumption has nearly 30% proportion of total energy consumption of entire society in China, building energy efficiency issue has become a major strategy for sustainable development in China. This presentation is about the progress of energy monitoring, efficiency evaluation and improvement based on Internet of Building Energy (iBES) technology during whole life cycle of buildings.



*A.P. Tianyi Zhao* received his Ph.D. degree in 2009 from HVAC department of Harbin Institute of Technology and then worked as a postdoctoral researcher in Civil Engineering Department of DUT. He was promoted to an associate researcher in 2014. His research focuses on internet of building energy system and intelligent control theory and optimization of HVAC system. Zhao was responsible for 2 National Natural Science Funds, 1 project of the ministry of housing and public building energy monitoring system construction and 1 China Postdoctoral science foundation. Zhao has undertaken nearly 30 projects including The National Natural Science Funds and National Key Technology Support Program with accumulative funding of 3 million RMB yuan. Also, he has undertaken nearly 280 projects of building energy monitoring and energy efficiency management covering 6.3 million square meters of large-scale public

buildings. He currently serves as consultancy expert for government energy saving agency in Liaoning province and Dalian City, China. He has published nearly 100 academic articles in international journal and conference.

## **Heat Transfer Enhancement in Shell and Tube Condenser: Basic Research on Enhanced Tubes and Its Application**

**Zhixian Ma**

*Institute of Building Energy, Faculty of Infrastructure Engineering, Dalian University of Technology*

Shell and tube condenser with vapor condense on a horizontal tube bundle are widely used in refrigeration and air conditioning field, petrochemical industry, energy power field, desalination field, etc. To meet the high efficient shell and tube condenser requirements of these energy-intensive industries, enhanced tubes was developed and then widely be used in this type of condenser. Our research and development(R&D) work on this topic mainly focus on four aspects, including new enhanced tubes, new tube arrange methods in a bundle, operating mode, lifetime maintenance and control systems for a high efficient condenser. These work improved our ability to analytically model the complex two-phase processes that occur on the outside of enhanced tubes, as well as the single phase convection heat transfer inside the enhanced tubes with multi-start helical fins, and validate such models with accurate experimental measurements. Once the detailed knowledge of these phenomena be revealed by the mathematic model, the condenser, as well as the enhanced tubes, can be designed more efficiently.



Dr. Ma is a lecturer of HVAC Engineering at Dalian University of Technology(DUT). He began his appointment at DUT in November, 2012. His research interests are in the use of experimental methods to understand the mechanism of heat transfer enhancement and design high efficient heat exchangers for heat pump systems and HVAC systems. Current activities address a wide-range of experimental heat transfer issues including film condensation, boiling, evaporation, inner tube convection, fouling, and corresponding heat transfer enhancement technologies. Dr. Ma received his B. S. and M.S. in HVAC Engineering from Harbin Institute of Technology. He completed his doctoral studies at the Harbin Institute of Technology under the advisement of Jili Zhang and Dexing Sun.