Special Session: Water/Vapor Electrolysis

Session Description:

Water or vapor electrolysis using membranes or other mediums has a good application prospect in hydrogen production, water treatment, and even air dehumidification. This technology is promising as it is also suitable for using renewable energy. Transport phenomena (heat, mass, momentum, and energy transport) at different scales from molecular to macros determine the electrolysis performance and energy efficiency. This session aims to address the research related to the modeling and performance improvement of water/vapor electrolysis. The topics include, but are not limited to, multi-scale modeling of transport phenomena, numerical simulation, system thermodynamics, transport enhancement, system optimization, energy utilization improvement, and renewable energy applications (solar, wind, etc.).

Session Organizers:



Ronghui Qi (South China University of Technology)



Chuanshuai Dong (South China University of Technology)

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Topic 1: Multi-scale modelling and material manipulations on PEM-based electrolyte dehumidifier:

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Abstract

As an independent and ultra-compact method, PEM-based dehumidifiers are promising. This system operates through a low DC electric field, without any cooling/regeneration equipment. The dehumidifier can operate efficiently under extreme conditions, such as sub-zero dew point, high temperature (>60°C) and low humidity conditions (<45%). However, the accurate modelling of heat and mass transport with electrochemical reactions is still challenging. The presentation will introduce the multi-scale theoretical model developed for PEM-based dehumidifier, which is combined with the mesco-scale modelling of anode-side catalyst layer (CL) with reconstructed microstructures by the lattice Boltzmann method and the macro-scale modelling of air channel and diffusion layer (DL) by finite different method and the software COMSOL. Results showed that the CL microstructure (especially the particle shape) significantly affects the air outlet parameters of PEM dehumidifiers, especially in the beginning state. The randomly arranged catalyst particles makes CL the hottest (2~3°C higher) and driest (half the DL concentration) part of PEM element, which severely limits the whole performance. By applying the linear fillings of CL, the dehumidification rate was almost doubled. Based on this study, several material manipulations of catalyst were conducted.

Short bio:

Professor Ronghui Qi received her Ph. D degree in 2013, and was appointed as postdoctoral in 2013-2016 from the Hong Kong Polytechnic University. She joined the South China University of Technology in 2016 and was promoted to the professor on Sep, 2019. Prof. Qi's main research interests are advanced air dehumidification technologies, such as electrolytic and desiccant absorption/adsorption ones, and heat&mass transfer enhancement mechanism. As the first or corresponding author, she have published more than 50 international peer-reviewed papers, including 35 SCI papers. She has received the Distinguished Young Scholar from Natural



Science Foundation of Guangdong Province. She has in the editorial board for SCI journal *<International Journal of Green Energy>*, used to be a guest editor of SCI journal *<Heat Transfer Engineering>*.

Topic 2: Modulating molecular and microscopic structures of polymeric carbon nitride for boosting photocatalytic hydrogen and oxygen evolution

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Abstract

Photocatalytic water splitting to produce hydrogen provides an ideal solution to address the issues concerning energy shortage and environmental contamination. Developing semiconducting photocatalysts is critical to realize this hydrogen production technology. Although large quantities of semiconductor-based photocatalysts have been widely explored in recent years, none of them can meet the requirements for the practical application of this technology. It is still necessary to develop high-performance, low cost and robust photocatalysts. Amongst the reported photocatalysts, polymeric carbon nitride (GCN), a metal-free polymeric semiconductor, is a promising one, owing to its advantages of low cost, favorable energy band positions, and good stability. However, only a moderate photocatalytic activity has been achieved by PCN up to now. Consequently, it is of significance to explore effective strategies to increase the photocatalytic activity of PCN. In this talk, two kinds of highly active PCN photocatalysts, developed by our group, will be presented. The first one is a doped PCN prepared via the copolymerization between urea and theobromine, which exhibits improved performance for oxygen evolution; the second one is highly porous PCN microtubes, obtained from a one-dimension supramolecular precursor synthesized from a liquid-liquid interfacial self-assembly strategy, which showed remarkably enhanced activity for hydrogen evolution.

Short Bio

Professor Xiaoming Fang received her bachelor's degree in organic chemical engineering from Chengdu University of Science and Technology (now Sichuan University), China, in 1990 and her Ph.D. in chemical engineering from South China University of Technology in 2002, and did postdoctoral research at Kyushu Center, AIST, Japan, in 2003. She is now a full professor at South China University of Technology. Her research interests include photocatalytic materials, photo-thermal conversion materials, and composite phase change materials for thermal energy storage. She has contributed to more than 150 peer reviewed papers with over 7000 citations, along with an H-index of more than 40.



Topic 3: Hot carriers in metal-semiconductor photoelectrode for solar water splitting

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Abstract

Hot carrier is the basic energy transfer medium between photon energy, electric energy and chemical energy. More and more researches have paid increasing attention to the solar energy conversion theory based on hot carrier, which is of great significance to develop the eco-friendly "solar-to-hydrogen" technology. Above all, how to fabricate the metal-semiconductor composite with the optimized structure which is beneficial for the formation and transfer of the hot electrons. Another important problem is how to develop the hot carrier device in photoelectrochemical hydrogen production system. This talk aims to give some answers and reveal the energy transfer mechanism of hot carrier excited by the solar energy in micro/nano scale and the specific interface. **Keywords**: Hot carrier, solar-to-hydrogen, water splitting, photoelectrode

Short Bio

Professor Lixia Sang received her Ph.D. in 2004 in Industrial Catalysis from Tianjin University with Professor Shunhe Zhong, studying photo-stimulated surface catalysis. Since then, she has been a faculty member at Beijing University of Technology and Full Professor since 2013. She pursued his research as a Visiting Scholar at Case Western Reserve University from 2012 to 2013, where she was exposed to the advanced nanomaterials and the femtosecond laser technique under the directorship of professor Clemens Burda. She also became a member of 2019 International Clean Energy Talent Program of CSC and completed the three-month study and exchange mission in Sweden. Currently, her research is focused on solar energy conversion materials with specific interest in charge-transfer mechanism for solar fuels.



Topic 4: A new liquid desiccant regeneration method for air dehumidification coupled with hydrogen production

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Abstract

In recent years, the energy shortage caused by refrigeration and air-conditioning equipment in buildings has increased seriously, especially in high-temperature and high-humidity areas. When the dehumidification load of air is large, traditional refrigeration dehumidification method needs to cool the air below its dew point temperature to meet the dehumidification requirement. Then, the air requires to be heated to meet the temperature requirement, which causes a great waste of energy. Liquid desiccant air-conditioning method can solve this problem perfectly. In order to increase the regeneration performance of liquid desiccant under severe climate, this topic proposed a liquid desiccant regeneration system which can also produce hydrogen. The system can assist the solar thermal regeneration method for liquid desiccant under high temperature and humidity climate, meanwhile, this system effectively uses the polarization reaction in the electrode chamber of the electrodialysis regenerator to produce hydrogen, which is especially suitable for enterprise buildings carrying out hydrogen production. Moreover, this system can use low-cost electricity at night to store energy, alleviating the peak-to-valley difference in power load and achieving the goal of improving system economy.

Keywords: Dehumidification; Liquid desiccant regeneration; Electrodialysis; Hydrogen production

Short Bio

Dr. Qing Cheng has rich research experience in air dehumidification, building energy-saving and solar energy use, solar heat pump and heat pump drying and reverse Brayton air circulation. He has authored more than 30 technical papers published on and not limited to Renewable and Sustainable Energy Reviews, Energy, International Journal of Refrigeration, Building and Environment, Energy and Building.



Topic 5: Study of solid-state hydrogen storage based on metal hydride and its application in fuel cell power system

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Abstract

Hydrogen storage technology is one of the bottlenecks in the hydrogen energy industrial chain, especially when used in the portable and mobile occasions. Compared with traditional compressed hydrogen storage technology, the solid-state hydrogen technology based on metal hydride (MH) has the advantages of high energy density, low cost and intrinsic safety. During the hydrogen absorption process, the reaction between MH and hydrogen gas releases a large amount of heat; while the reaction needs external heating during desorption process. Therefore, efficient heat management is necessary for metal hydride reactor (MHR). In this study, we designed a kind of high-capacity metal hydride by co-doping transition metal and nonmetal for hydrogen storage, which has the hydrogen capacity of 9.7 wt.% at the dehydrogenation temperature of 85 °C. Besides, we proposed phase change material (PCM) as MHR heat management to recycle the heat released during hydrogen absorption process for hydrogen desorption process. The results showed that the hydrogen storage efficiency can achieve approximately 60% with no degradation of more than 10 cycles. As a result, the hydrogen storage process can be more energy-saving. In addition, the fuel cell power (FCP) system with this kind of MHR is independent from heat/cold sources, which makes the system simpler and more compact. It helps to facilitate the application of FCP system in the field of portable devices.

Keywords: Hydrogen storage, Metal hydride, Reactor design, Fuel cell

Short Bio

Dr. Zhen Wu, Ph.D, Associate Professor. He is the associate editor of *International Journal of Science and Technology: Material & Chemical*, the editorial board member of *Rare Metal* and *Science Journal of Chemistry* and the topic editor of *Energies*. He is also the reviews of the leading international journals of 'Applied Energy', 'Nanoscale', 'International Journal of Hydrogen Energy', 'Fuel' and 'Energy'. In 2017, he was selected as Hong Kong scholar fellowship in the Hong Kong Polytechnic University. His research interests include hydrogen storage materials and systems based on metal hydride, energy system modeling and optimization, DFT design and analysis, and so on. So far, he has published more than 100 scientific



and conference papers in the research field of hydrogen energy system. In 2015, his paper published in *Applied Energy* was awarded as the 'Best Paper Award of Excellence' jointly by *Elsevier* Publishing Co. Ltd. and the prestigious international journal of *Applied Energy*.

Topic 6: Experimental Study of Two-phase Flow in PEM Electrolytic Cells

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Abstract

A proton exchange membrane (PEM) electrolytic cell can be utilized at the areas of civil diving equipment, aerospace, etc. A PEM electrolytic cell can serve as a hydrogen reactant generator, which is combinedly utilized with PEM fuel cell to generate the electricity, on the other hand, oxygen is also produced to be supplied for breathing when it is used at the areas like submarines. In previous studies of our group, the gas and liquid two-phase flow characteristics in PEM electrolytic cells and the cell performance under various operation conditions are experimentally studied. A PEM electrolytic cell with a transparent window is fabricated to observe the two-phase flow behaviors during the cell operating. Experimental results show that the gas and liquid two-phase flow behaviors and cell performance are affected under various operation conditions, such as the flow field structure types, inclination angle, cell temperature and different gravity environments. Higher current densities and cell temperatures increase the generated bubble sizes, and higher current densities facilitates expelling the generated gases. In micro-gravity environment, bubble moving is slowed down. The cell performance is increased under higher cell temperature, and paralleled channel structure provided higher performance; in addition, the liquid water flow rate exhibits obscure effect on performance.

Keywords: PEM electrolytic cell; two-phase flow; mass transfer; microgravity

Short Bio

Hao CHEN received the Ph.D. degree at Beijing University of Technology in 2019. He is a post doctor at Beijing University of Technology. He researched the thermal fluid issues of proton exchange membrane fuel cells for 10 years, and the research interests include the numerical model improvement, two-phase mass transfer in proton exchange membrane fuel cell, and designing of flow channel structures. He has published 10 journal papers cited by SCI as the first author, including the top journals like Journal of Power Sources, Energy Conversion and Management. He received 1



excellence award and 3 special awards of science and technology innovation awards of Beijing University of Technology. He was invited to give the invited lecture at the 2nd International Conference on Electrochemical Energy Systems at May 2021, and serve as the session chair of 7TH International Conference on Renewable Energy Research and Application at October 2018. E-mail: <u>yefang@bjut.edu.cn</u>

Chuanshuai Dong (Session Organizer)

South China University of Technology



Biography

Dr. Dong received his Ph. D. in 2018 from Department of Building Services Engineering, the Hong Kong Polytechnic University, Hong Kong, China. He is currently an Assistant Professor/ Postdoc in South China University of Technology. Dr. Dong's research focuses on energy-related two-phase flow and heat/mass transfer, such as falling film liquid desiccant dehumidification, two-phase slug flow in pipes, etc. He has developed several constitutive equations for two-phase flow analysis. Dr. Dong has also authored 30 SCI journal papers in well-known journals, such as Physics of Fluids, Energy, and International Journal of Multiphase Flow, etc. As PI, Dr. Dong has presided over several research projects supported by National Natural Science Foundation, National Natural Science Foundation of Guangdong, and China Postdoctoral Science Foundation, etc.