Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-921~926 (invited)
June 30 - July 4, 2024, Ningbo, China

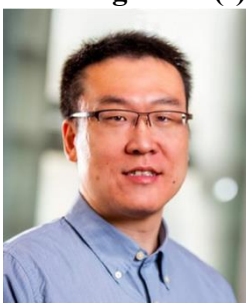
Special Session: Sustainable Energy Materials

Session Description:

Energy materials play a key role in determining the performance of electrochemical energy conversion and storage technologies, including batteries, supercapacitors, fuel cells, water electrolyzers, *et al*. Rational design and development of advanced energy materials with special consideration of sustainability ensures achieving the long-term goal of making a sustainable economy and society.

This special session provides a unique platform for researchers to present and discuss design principles, development strategies, their electrochemical/electrocatalytic behaviors and working mechanisms, as well as potential practical applications of various energy materials in the fields of electrochemical energy storage and conversion systems. Contributions from theoretical modeling, calculation, simulation, and prediction of energy materials are also welcomed.

Session Organizer(s):



Xiaolei Wang
University of Alberta

Ge Li
University of Alberta

Session Contents:

Topic **1**: Metal-based catalytic materials and their applications in electrochemical hydrogen conversion
Topic **2**: Design and synthesis of electrocatalytic materials with nanobionic structures
Topic **3**: Green fabrication of biomass carbon for high-performance supercapacitors
Topic **4**: Regulating Anode Behaviors in Lithium Metal Batteries
Topic **5**: Electrocatalysts Design for Two-Electron Oxygen Reduction Reaction
Topic **6**: Structural Regulation and Advanced Transmission Electron Microscopy Characterization of the Oxygen Reduction Reaction Electrocatalysts.

Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-921 (invited)
June 30 - July 4, 2024, Ningbo, China

Metal-based catalytic materials and their applications in electrochemical hydrogen conversion

Yujing Li*
School of Materials Science and Engineering, Beijing Institute of Technology
Email: yjli@bit.edu.cn

Abstract: Proton exchange membrane fuel cells (PEMFCs) have attracted significant interest as a promising alternative technology to the combustion engine to power next-generation vehicles with zero emission. Among the various technological targets, system cost and durability are currently identified as the main obstacles toward large-scale implementation of PEMFCs. Platinum-group-metal-based (PGM-based) catalysts are the most efficient catalyst for the rate-limiting cathodic oxygen reduction reaction in PEMFCs and take the highest share in the cost breakdown. Therefore, the stability of PGM-based electrocatalysts plays a significant role in the development of PEMFCs. In this presentation, the recent progress made in our group on the understanding of both the fundamental chemical and structural stability of PGM-based catalysts, and their durability in operational PEMFC devices will be discussed. It covers systematic studies on the chemical, structural, and operational durability of the PGM-based catalyst and the catalyst design with both superior activity and durability for cost-effective and high-performance PEMFCs.

Keywords: proton exchange membrane fuel cell, electrocatalysis, active site, stability

Prof. Yujing Li obtained his Ph.D. degree from University of California Los Angeles. He is now working at the School of Materials Science and Engineering in Beijing Institute of Technology (BIT). He is interested in the design of highly stable nanoscale structures and hybrid materials for the electrocatalytic and photocatalytic applications. His research is focused on the development of high-performance low-PGM catalysts for energy conversion devices including the proton exchange membrane fuel cells and water electrolyzers, and pursuing fundamental understanding on the degradation mechanism of electrocatalysts.

Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-922 (invited)
June 30 - July 4, 2024, Ningbo, China

Design and synthesis of electrocatalytic materials with nanobionic structures

Zhengyu Bai*, Yangdi Niu, Yang Yuan
School of Chemistry and Chemical Engineering, Henan Normal University
Email: baizhengyu@htu.edu.cn

Abstract: It has important research significance and application value to realize the height adjustment of the catalytic material active site in the application scenario of microbial fuel cells (MFCs). Therefore, on account of the material hybridization theory and biomimetic material synthesis technology, we developed a strategy of highly efficient coupling of multi-active site nanostructure units and living cells, and achieved important research progress. According to the biological properties of microbial cells with self-replication, continuous synthesis of redox proteins and degradation of organic matter, we designed for the first time to combine genetic engineering and nanoengineering technology to modify *Escherichia coli* (*E. coli*) with weak organic matter degradation ability and electrocatalytic performance and prepared a novel microbial catalyst enabling quick glucose degradation and efficient oxygen reduction reaction (ORR) catalyzation. The results showed that the engineered *E. coli* was applied to MFCs as a sustainable air cathode catalyst, demonstrating the rapid consumption rate of glucose and excellent battery output power, which made MFCs to rapidly treat sewage and generate electricity simultaniously, reaching the international first-class level in the field. This work not only opens up a new way for the rational design of bioelectrocatalysts, but also provides the feasibility for utilizing MFCs to solve environmental problems. Besides, this research provides a scientific basis for the construction and development of micro-cooperative regulation methods of nano-assembled biomimetic materials and the expansion and breakthrough of the concept of active site regulation of traditional catalytic materials for biofuel cells.

Keywords: Microbial fuel cells, Nanobionic structure, Oxygen reduction electrocatalysts, Design and synthesis

Zhengyu Bai is a professor at the College of Chemistry and Chemical Engineering of Henan Normal University, a recipient of the National Excellent Young Scientists Fund, and a leader of the scientific and technological innovation team of universities in Henan Province. Her main research interests are new green energy nanostructured materials, new energy or matter conversion electrocatalysts, including fuel cells, metal-air batteries, carbon dioxide and nitrogen reduction electrocatalytic materials such as green bionic synthesis and performance research. She has published over 130 articles in international journals, including those in *Nat. Commun.*, *Angew.Chem. Int. Ed.*, *Adv. Mater.*, *Adv. Energy Mat.*, *Adv. Funct. Mat.* etc.

Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-923 (invited)
June 30 - July 4, 2024, Ningbo, China

Green fabrication of biomass carbon for high-performance supercapacitors

Yao Li*, Yanyu Li, Di Zhang
State Key Lab of Metal Matrix Composites, Shanghai Jiao Tong University, China
Email: liyaosjtu@sjtu.edu.cn

Abstract: Electric Double-Layer capacitors (EDLCs) have the advantages of high-power density and long cycle life, while the energy density needs to be improved. It is crucial to develop porous carbon electrodes with high specific surface area and satisfactory pore structure to improve the energy density for EDLCs. Biomass are important precursors of porous carbon since their diverse structures and natural transmission channels. However, a large amount of strong alkali is consumed during traditional preparation of biomass-derived porous carbon, resulting in serious pollution and high carbon emissions. The concept of Fenton chemistry was adopted to pretreat the biomass precursor by oxidation, which can cut off the macromolecular chain segment, and initially construct the pore structure. This pretreatment increases the reaction site for activation, thereby improving the alkali activation efficiency and reducing the consumption of alkali. The optimized porous carbon has a specific surface area of 3440 m^2 g^{-1} and a mesoporous ratio of about 34%. The transportation of electrolyte ions in the pore structure was simulated by molecular dynamics to prove high transport efficiency of materials. In the electrochemical test, the maximum specific capacitance of the material reaches 425.2 F g^{-1}, and the capacitance remains 286.1 F g^{-1} at the ultra-high current density of 100 A g^{-1}. In addition, the porous carbon electrode materials have excellent cycle stability, the capacitance retention is greater than 98% after 20,000 cycles. This pretreatment method provides a new activation idea which constructs the porous structure through green and efficient means, with a wide application prospect.

Keywords: Electric Double-Layer Capacitor, biomass-derived porous carbon, activation efficiency, micro/meso-pores regulation

Short Bios of invited speaker: Yao Li, associate researcher, received Ph. D from Shanghai Jiaotong University, school of Materials Science and Engineers in 2015. Have published 40 papers as the first and corresponding author. He hosted the NSF, the Pujiang program, the research project of Shanghai Science and Technology Commission and many commercial projects. He is working on research of bio-inspired materials, as well as their application in environment treatment and energy storage.

Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-924 (invited)
June 30 - July 4, 2024, Ningbo, China

Regulating Anode Behaviors in Lithium Metal Batteries

Ge Li
Department of Mechanical Engineering, University of Alberta
Email: ge.li@ualberta.ca

Abstract: Lithium metal batteries (LMBs) are considered the most promising energy storage devices for applications such as electrical vehicles. Lithium metal is believed the most favourable anode for future LMBs owing to its extremely high theoretical specific capacity, low density, and lowest electrochemical potential among potential candidates. However, large-scale deployment of lithium metal anode in practical batteries still requires a scientific breakthrough in solving major challenges of dendrite growth and low plating/stripping efficiency of metallic lithium. To address the issues related to lithium anodes in LMBs, several effective strategies have been developed to stabilize Li anodes, including liquid electrolytes, surface coating, solid-state electrolytes, and porous current collectors. In this presentation, we will present our recent work on the materials design and development for next-generation LMBs by focusing on the in-depth understanding of interphase engineering. More specifically, we will discuss (1) the systematic electrolyte design and (2) the anode construction.
Keywords: Lithium Metal Batteries, Electrolyte Engineering, Anode Construction

Dr. Ge Li is an Associate Professor in the Department of Mechanical Engineering at the University of Alberta. Her research interests are in complex material design and synthesis, electrochemical investigation, and device construction for energy conversion and storage. She has so far published over 50 papers with a total citation over 3000 and h-index of 25.

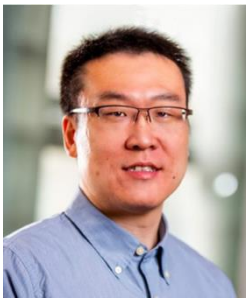
Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-925 (invited)
June 30 - July 4, 2024, Ningbo, China

Electrocatalysts Design for 2e^- Oxygen Reduction Reaction

Xiaolei Wang
Department of Chemical and Materials Engineering, University of Alberta
Email: xiaolei.wang@ualberta.ca

Abstract: Electrochemical production of hydrogen peroxide (H_2O_2) *via* 2-electron oxygen reduction reaction (ORR) offers a promising approach for sustainable decentralized production of H_2O_2. However, ORR goes through either 4-electron pathway to water or 2-electron pathway to H_2O_2. The need for controllable modulation of ORR pathways, as well as the kinetic challenges, calls for the discovery and optimization of efficient catalysts. Herein, we focus on various design strategies of electrocatalyst towards 2-electron ORR, including (i) developing advanced electrocatalysts with high activity and selectivity for both alkaline and acidic application media; (ii) elaborating *ex-situ* and *in-situ* characterization of electrocatalyst structure and electrochemical investigation; (iii) revealing the underlying factors that contribute to the high performance and providing guidance for future design; (iv) building up the gap between lab screening and practical application to facilitate its commercial utilization. Electrocatalysts were designed for alkaline electrolyte. A promising carbon-based catalyst, consisting of oxygen rich hollow mesoporous carbon spheres (HMCS) was developed, exhibiting high onset potential (0.82 V) and halfwave potential (0.76 V) as well as excellent H_2O_2 selectivity (above 95%). A series of HMCS were further developed for the investigation of porosity engineering on the performance. Electrocatalysts were designed for acidic media. A series of Au@Pd core@shell structures were developed to investigate the influence of Pd *4d* orbital overlapping degree on 2e^- ORR performance. Au@Pd NWs with Pd_4 with oxygen coverage causes electron redistribution and weakened *OOH binding strength on active sites, leading to enhanced activity of Pd_4 with only 0.06 V overpotential in acidic media. The influence of local coordination environment (LCE) manipulation was also studied. We underscore the influence of LCE on directing the 2e^- ORR, utilizing Pd cluster as a model catalyst.

Keywords: Electrocatalysts, Oxygen Reduction Reaction, 2-Electron Reaction, Hydrogen Peroxide



Prof. Xiaolei Wang is currently an associate professor in the Department of Chemical and Materials Engineering at the University of Alberta, and also titled Canada Research Chair in Batteries for Sustainability. He runs his *Nano For Advanced Clean Energy* (NanoFACE) laboratory and mainly focuses on the rational design, development, and application of novel nanostructured materials for energy-related technologies, including lithium (and other alkaline)-ion batteries, lithium-metal batteries, rechargeable aqueous batteries, metal-air batteries, supercapacitors, and electrocatalytic system for water splitting, CO_2 reduction and fuel cells.

Proceedings of the joint 16th International Green Energy Conference (IGEC-XVI)
& 5th International Conference on Energy and AI (ICEAI-V)
& Symposium on Chemical Engineering and AI
IGEC2024-926 (invited)
June 30 - July 4, 2024, Ningbo, China

Structural Regulation and Advanced Transmission Electron Microscopy Characterization of the Oxygen Reduction Reaction Electrocatalysts

Mingxing Gong
School of Materials Science and Chemistry, China University of Geosciences
E-mail: gongmingxing@cug.edu.cn

Abstract: Fuel cells (FCs) are regarded as the most promising green energy conversion technology in the 21st century because of their advantages. However, the industrialization process of FCs is restricted by several key problems, one of which is the cathode catalyst. The Oxygen Reduction Reaction (ORR) of FCs is a complex process involving 4 electrons, which has sluggish kinetics and high over-potential. Therefore, it is usually necessary to use a large number of precious metal platinum (Pt) catalysts to improve the reaction efficiency, but the characteristics of small reserves of Pt, high price, and easy to be poisoned and deactivated increase the operating cost of the whole system. It is imperative to develop substitutes for non-Pt-based ORR catalysts and reveal their structure-activity relationship with advanced characterization techniques.

There are two ways to solve this problem: one is to improve the utilization rate of platinum-based catalyst, the other is to develop non-platinum-based catalysts. In terms of improving the utilization rate of Pt, our research group mainly constructed new Pt-based ordered intermetallic compound catalytic materials, and improved the surface structure, alloying degree and electronic structure of Pt-based catalysts by changing the atomic types, proportions and post-treatment temperatures of Pt and transition metals, so as to regulate their electrocatalytic properties. On the other hand, the morphology control of ordered intermetallic compounds has always been a major challenge in this field, and we have made a preliminary attempt in the morphology control. At the same time, with the help of modern characterization techniques, it is of great significance to study the changes of structure and components during the service of Pd-based catalysts, and to understand their failure behavior and performance attenuation mechanism for the subsequent optimization and commercialization of Pd-based catalysts. Among them, visualization technology based on transmission electron microscopy (TEM) has become a research hotspot because it can directly observe the failure process of catalysts in service.

Keywords: Fuel cells; Electrocatalysts; Oxygen reduction reaction (ORR); Three-dimensional reconstruction; Decay mechanism

Author CV

Mingxing Gong received his Ph.D. from Huazhong University of Science and Technology in 2020. And then he joined in School of Materials Science and Chemistry, China University of Geosciences (Wuhan) as a full time researcher. Her research interests mainly focused on nanomaterials for energy conversion and storage, advanced visualization characterization technology based on transmission electron microscopy (TEM). Homepage: https://grzy.cug.edu.cn/gongmingxing/zh_CN/index/71516/list/index.htm and https://scholar.google.com/citations?user=vKRThXgAAAAJ&hl=zh-CN.