THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY | ENERGY INSTITUTE

THE HKUST ENERGY INSTITUTE 香港科大能源研究院

HKUST Energy Institute
Young Investigator Symposium Series:
Carbon Dioxide Electrochemical Reduction

Date: 12 April 2023
Time: 2 – 5:20 pm
Venue: Room 2405 (Lifts 17-18), HKUST ***(Location)***

<u>Program</u>

Time	
1:30	Registration
2:00 – 2:30	**Efficient Upgrading of C_1 Molecules to Fuels** ***(Abstract)*** **Prof. Xue Wang** Assistant Professor School of Energy and Environment City University of Hong Kong
2:30 – 3:00	**Electrode Process for Electrochemical CO2 Reduction Reaction in Acid** ***(Abstract)*** **Prof. Ying Wang** Assistant Professor Department of Chemistry Chinese University of Hong Kong
3:00 – 3:30	**Cu-based Nanomaterials with Unconventional Crystal Phases for Electrocatalytic CO2 Reduction** ***(Abstract)*** **Dr. Qinbai Yun** Post-doctoral Fellow Department of Chemistry City University of Hong Kong
3:30-3:40	Break
3:40 – 4:10	**Controlled Synthesis of Novel Low-dimensional Metal Nanomaterials for Electrocatalytic Carbon Dioxide Conversion** ***(Abstract)*** **Prof. Zhanxi Fan** Assistant Professor Department of Chemistry Hong Kong Branch of National Precious Metals Material Engineering Research Center (NPMM) City University of Hong Kong
4:10 – 4:40	**Catalyst Design and Mechanistic Study of the Electrochemical Carbon Dioxide Reduction Reaction to Hydrocarbons and Alcohols** ***(Abstract)*** **Dr. Ernest Pahuyo Delmo** Post-doctoral Fellow Department of Chemical & Biological Engineering The Hong Kong University of Science and Technology
4:40 – 5:20	**Panel Discussion** **Moderator:** **Prof. Minhua Shao,** Director of Energy Institute, HKUST **Dr. Ernest Pahuyo Delmo**, HKUST **Prof. Zhanxi Fan**, City University of Hong Kong **Prof. Xue Wang**, City University of Hong Kong **Prof. Ying Wang**, Chinese University of Hong Kong **Dr. Qinbai Yun**, City University of Hong Kong
5:20	End of the Program

Dr. Ernest Pahuyo Delmo
Post-doctoral Fellow
Department of Chemical & Biological Engineering
The Hong Kong University of Science and Technology

Dr. Ernest Pahuyo Delmo received his bachelor's degree in chemical engineering at the University of the Philippines Diliman. In 2022, he completed his PhD in Chemical and Biomolecular Engineering at The Hong Kong University of Science and Technology. He is now a post-doctoral fellow in Prof. Minhua Shao's group. His research is focused on designing catalysts and probing the mechanism of the electrochemical reduction of CO_2 to advanced products, such as hydrocarbons and alcohols.

Catalyst Design and Mechanistic Study of the Electrochemical Carbon Dioxide Reduction Reaction to Hydrocarbons and Alcohols

Abstract

The continuous burning of fossil fuels has caused a rapid accumulation of carbon dioxide in the atmosphere since the industrial revolution. To prevent an unprecedented shift in the Earth's climate, sustainable technologies that can lessen the societal dependence on fossil fuels and diminish greenhouse gas accumulation must be promptly developed. In this respect, the electrochemical CO_2 reduction reaction (CO_2RR) to advanced products, such as hydrocarbons and alcohols, is a promising method that can help alleviate climate change. However, the industrialization of CO_2RR electrolyzers remains hindered by insufficient faradaic efficiencies (FE), energy efficiencies, and device instabilities. Furthermore, the CO_2RR mechanism consists of multiple possible proton and electron transfer steps that are still poorly understood.

Our research aims to design electrocatalysts and unravel the multistep CO_2RR mechanism towards the production of alcohols and hydrocarbons. In the first project, we embedded imidazolium-based ionic liquids within copper metal organic frameworks to significantly improve the local environment during CO_2RR and enhance the thermodynamics of the CO_2-to-CH_4 pathway. A maximum FE of 65.5% towards CH_4 is then achieved on the HKUST-1/[BMIM][PF_6] electrocatalyst. We then utilized in situ FTIR spectroscopy and the electroreduction of stable reaction intermediates to probe the C_2 pathway of CO_2RR. Using in situ FTIR spectroscopy coupled with DFT calculations, we study how copper anodization can affect the adsorption of various C_1 intermediates on the oxide-derived copper (OD-Cu) surface. For the first time, we identify a C_2 dimer intermediate (*COCHO) on anodized copper, shedding light on how C_2 product formation is promoted on OD-Cu. Finally, we investigated the glyoxal pathway of CO_2 reduction on polycrystalline copper. We show that glyoxal is not the main intermediate towards the ethanol pathway. However, through a combination of electrochemical and chemical steps, we show that the glyoxal pathway of CO_2RR can allow us to access novel products, such as ethylene glycol, glycolate, and C_4 sugars. These findings offer valuable strategies and insights on designing CO_2RR electrocatalysts for selectively producing hydrocarbons and alcohols.

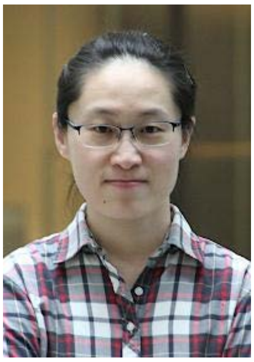
Prof. Zhanxi Fan
Assistant Professor
Department of Chemistry
Hong Kong Branch of National Precious Metals Material Engineering Research Center (NPMM)
City University of Hong Kong

Prof. Zhanxi Fan obtained his B.S. degree in Chemistry with guidance of Prof. Bai Yang and Prof. Hao Zhang from Jilin University (China) in 2010, and completed his Ph.D. under supervision of Prof. Hua Zhang at Nanyang Technological University (Singapore) in 2015. Then he worked as Research Fellow at Nanyang Technological University with Prof. Hua Zhang and Lawrence Berkeley National Laboratory (USA) with Prof. Haimei Zheng, respectively. Currently, he is an Assistant Professor at the Department of Chemistry in City University of Hong Kong. His research interests mainly focus on the controlled synthesis of novel low-dimensional metal-based nanomaterials and their potential applications in catalysis, clean energy, gas adsorption and separation, environmental remediation, *etc*. Until March 2023, he has published 99 SCI papers (79 with IF > 10) with a total citation of over 14,900 and H index of 53. Based on these works, he has been rated/honoured as a "Highly Cited Researcher" (Top 1%, World-wide) by Web of Science for consecutive 5 years from 2018 to 2022, a "Rising Star" by both *Advanced Materials* and *Small* in 2022, a "Top 2% of the World's Most Cited Scholar" by Stanford University for consecutive 3 years from 2020 to 2022, *etc*.

Controlled Synthesis of Novel Low-dimensional Metal Nanomaterials for Electrocatalytic Carbon Dioxide Conversion

Abstract

The excessive consumption of fossil fuels since industrialization has resulted in massive emissions and accumulation of carbon dioxide (CO_2) in the atmosphere. The global CO_2 concentration now is more than 50% higher than pre-industrial levels, reaching an ultrahigh level of above 420 ppm. As one of the dominant greenhouse gases, the increasing CO_2 concentration has led to a series of severe environmental problems, such as the global warming, glacier melting, sea-level rise and extreme weather, which pose serious threats to the living of human beings. Therefore, cutting CO_2 emissions has become a consensus to safeguard the future and destiny of mankind. In this presentation, I will talk about our recent progresses on the controlled synthesis of novel metal nanomaterials and their applications in electrocatalytic CO_2 conversion. Firstly, the synthesis and surface modification of unusual phase gold nanostructures for improved electrochemical CO_2 reduction reaction (CO_2RR) will be introduced. Then I will highlight the confined growth of well-defined silver-copper Janus nanostructures for the high-performance tandem electrocatalytic CO_2RR. Finally, the synthesis of unusual phase noble metal nanomaterials and their applications in aprotic lithium-CO_2 batteries will be systematically discussed as well.



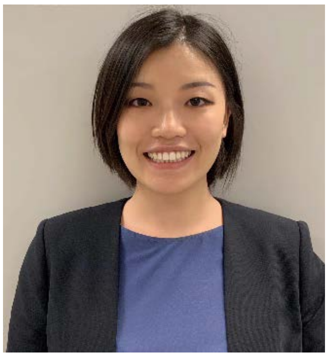
Prof. Xue Wang
Assistant Professor
School of Energy and Environment
City University of Hong Kong

Prof. Xue Wang received her Ph.D. degree in Chemistry from Xiamen University in 2015. During her graduate studies, she worked at the Georgia Institute of Technology as a visiting graduate student (2013-2015). After her Ph.D. graduation, she was appointed as associate professor at Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences (2016-2017). Then she worked as a postdoctoral fellow at University of Toronto, prior to joining the City University of Hong Kong as an assistant professor at City University of Hong Kong in 2023. Dr. Wang's research expertise covers nanomaterial design, electrocatalysis, and reaction engineering, with a particular emphasis on energy-related applications. To date, she has published over 60 peer-reviewed articles (including Nature Energy, Nature Commun., Nature Catalysis, JACS, Nano Letters, ACS Nano, Advanced Materials, Green Chem., etc. as the first/co-first/co-corresponding author).

Efficient Upgrading of C_1 Molecules to Fuels

Abstract

The CO_2 electroreduction reaction (CO_2RR) to feedstocks and valuable fuels, powered using renewable electricity, offers a sustainable approach to store intermittent renewable energy, and also to reduce CO_2 emission associated with chemicals. A wide range of different products from C_1 to C_3 is typically generated in CO_2RR; thus, to realize industrial application, improved selectivity, as well as high activity, stability, and energy efficiency, must be further pursued. In this talk, I will present our recent progress towards the more practical electrosynthesis of fuels from C_1 molecules, looking both at the catalyst and at the system. The mechanism of fuel electrosynthesis on the catalysts will also be discussed [1-3].



Prof. Ying Wang
Assistant Professor
Department of Chemistry
Chinese University of Hong Kong

Prof. Ying Wang received her D.Phil degree under the supervision of Prof. Richard G. Compton at Oxford University in 2015. During her D. Phil, Ying developed a joint computational and experimental approach to investigate the electrode process on nanoparticles for different electrochemical reactions. Before joining the Chinese University of Hong Kong in 2019, she was a postdoc research fellow with Prof. Thomas J Meyer at the University of North Carolina at Chapel Hill and Prof. Edward H Sargent at the University of Toronto. Ying is now an Assistant Professor working on fundamental electrochemistry and electrochemical CO_2 reduction reaction at the Chemistry Department at the Chinese University of Hong Kong. She has published more than 60 papers in prestigious journals, including Nature Catalysis, Nature Communications, Chem, Angewandte Chemie, Proceedings of the National Academy of Sciences of the United States of America and Chemical Science. She received the Excellent Young Scientists Fund (Hong Kong and Macau) 2022 and MIT Technology Review Innovator 35 Asia Pacific 2022

Electrode Process for Electrochemical CO_2 Reduction Reaction in Acid

Abstract

Developing high-efficiency carbon dioxide capture, storage, and conversion technologies has received extensive attention. Renewable electricity-powered CO_2 conversion offers an attractive means to produce low-carbon-footprint fuels and chemicals. In the past few decades, significant progress has been made in advancing CO_2RR technology under industrial-relevant current densities (> 100 mA/cm^2). One of the remaining critical challenges is to improve the carbon utilization efficiency of CO_2RR. Due to the hydroxide ion produced at the electrode interface during electrolysis, a significant amount of CO_2 will be converted to carbonate rather than reduced to targeted products. The maximum carbon conversion efficiency of CO_2-to-CO is only 50% for the current neutral/alkaline CO_2RR electrolyzer. This efficiency will further drop for multi-electron transfer products, such as ethylene (25%) and ethanol (25%). We are working on developing acidic CO_2RR electrolyzers for high carbon conversion efficiency to multicarbon products (C_{2+}). Converting CO_2 to C_{2+} in acid requires overcoming the competition from the hydrogen evolution reaction and the CO_2-to-C_1 pathways. Understanding the electrode process, including charge transfer and mass transport, is essential in developing efficient catalysts and electrolyzers for CO_2RR in acid.

Dr. Qinbai Yun
Post-doctoral Fellow
Department of Chemistry
City University of Hong Kong

Dr. Qinbai Yun obtained his B.E. degree in Mechanical Engineering in 2013 and M.S. degree in Materials Science and Engineering in 2016 from Tsinghua University, China. Then he completed his Ph.D. study in Materials Science and Engineering under the supervision of Prof. Hua Zhang at Nanyang Technological University, Singapore in 2020. Currently, he is a postdoc in Prof. Hua Zhang's group at City University of Hong Kong. His research interests focus on the preparation of micro-/nanostructured metallic materials with well-defined structure and their applications in catalysis and energy storage.

Cu-based Nanomaterials with Unconventional Crystal Phases for Electrocatalytic CO_2 Reduction

Abstract

Electrocatalytic CO_2 reduction reaction (CO_2RR) provides a promising strategy to convert CO_2 into valuable chemicals and fuels. Among the various CO_2RR catalysts, Cu is the only metal catalyst that can produce deep-hydrogenated multicarbon products with high values. However, the selectivity of Cu catalysts towards the production of specific product is still low. Therefore, tremendous efforts have been devoted to engineering the various structure parameters of Cu catalysts, including size, composition, shape, and defect, to enhance their selectivities. Recently, it has been revealed that tuning the crystal phase of CO_2RR catalysts can improve their electrocatalytic performance. Unfortunately, the preparation of Cu nanomaterials with unconventional crystal phases is still of great challenge. In this talk, our recent progress in developing Cu-based nanomaterials with unconventional crystal phases (*e.g.*, 2H, 4H, and 6H), including amorphous SnO_2-encapsulated crystalline Cu heterostructures and pure Cu nanomaterials, will be presented, and the influence of crystal phase on their CO_2RR performance will also be discussed.