Proceedings of the 15th International Green Energy Conference
IGEC2023-351~355 (invited)
July 10-13, 2023, Glasgow, UK

Special Session: Advances on Chemical Energy Storage: Hydrogen and Carbon Reduction

Session Description: Chemical energy storage is the process of converting and storing energy in the form of chemical bonds, which can later be released and utilized as needed. Hydrogen energy and carbon reduction are emerging as promising solutions within chemical energy storage for global energy challenges. This session will provide a comprehensive overview of recent advancements in these areas, bringing together esteemed researchers, engineers, and experts. It will cover the entire hydrogen value chain, from production to storage and utilization, including novel hydrogen production methods, storage technologies, and diverse applications in fuel cells for transportation, power generation, and industrial processes. The session will also highlight carbon reduction technologies, covering novel approaches for capturing, storing, and repurposing carbon dioxide, such as industrial processes, direct air capture, carbon utilization in value-added products, and geological and oceanic carbon storage techniques.

Session Organizers:

Prof. Kui Jiao received a PhD in mechanical engineering from the University of Waterloo, Canada in 2011. He is currently a professor in the State Key Laboratory of Engines at Tianjin University, China. His research interests include fuel cells, batteries, thermoelectric generators, and turbocharger compressors. He has published three books and over 100 papers in highly reputable international journals, including Nature. He has led more than 30 national and industrial projects in China and provided modeling and design services in the development of fuel cell engines for several major automotive fuel cell manufacturers. He serves as the founding editor of Energy and AI and associate editor of International Journal of Green Energy. He is also a Fellow of the Royal Society of Chemistry (FRSC) and a Fellow of the Institution of Engineering and Technology (FIET).

Dr. Bowen Wang received his PhD degree from Tianjin University in 2021. Now, he is an assistant professor in State Key Laboratory of Engines at Tianjin University, and the “Hong Kong Scholar” in the Hong Kong Polytechnic University. His research interest focuses on fuel cells, water electrolysis, hydrogen energy and machine learning modeling of energy conversion systems. He published more than 30 high-quality journal papers, including Nature, and three books, and had 10 Chinese invention patents and 3 software copyrights. He joined several national and industrial projects for automotive fuel cell modeling. He won the Best Reviewer Award of International Journal of Green Energy.

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Topic 1: Microenvironment design strategies for enhanced CO_2 electroreduction with a 60% full-cell energy efficiency

Qian Fu, Pengtao Yue, Jun Li, Liang Zhang, Xun Zhu, Qiang Liao
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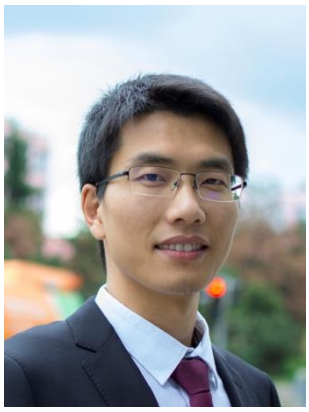
Abstract:

Electrochemical CO_2 reduction reaction (CO_2RR) integrated with renewable energy is an attractive approach for mitigating greenhouse gas emissions and converting CO_2 to value-added chemicals However, low current densities (production rates) and low energy efficiency (EE) caused by poor catalyst activities and limited CO_2 mass transfer in the catalyst layer (CL) prevent this technology from application. Herein, we report atomically dispersed Ni catalysts anchored on macroporous hollow nano-carbon sheets (A-Ni@CS) that simultaneously optimizes the coordination of Ni atoms and local CO_2 transport in the CL. The unique Ni–N_5–O/C structure of A-Ni@CS lowers the energy barrier of *COOH formation, and the layered nano-to-micro porous structure increases the effective diffusion coefficient of CO_2, enhancing the local CO_2 concentration in the CL. By employing a zero-gap flow cell, A-Ni@CS can mediate CO_2 to CO conversion with a 60% full-cell EE at 200 mA/cm^2. This work highlights the importance of tailoring the CL microenvironment as a means of improving the overall performance in the CO_2RR, and offers a unique insight to drive industrial applications of current systems.

Short bio:



Prof. Fu obtained his Ph. D degree from the Department of Systems Innovation, The University of Tokyo, Japan in 2013, and then worked as a Research Fellow at the Institute of Industrial Science, The University of Tokyo, Japan. He joined School of Energy and Power Engineering, Chongqing University as a scholar of "Hundred Talents Program" of Chongqing in 2015. He won the young scholar of “Chang Jiang Scholars Program” of Ministry of Education, China in 2019. Prof. Fu’s research interests include fuel cells and electrochemical CO_2 reduction. He has authored and co-authored more than 100 journal papers. He also acted as the guest editor of special issue of *Electronics*, academic editor of *DeCarbon*, and editorial board member of *Energy and AI.*

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Topic 2: Data-driven assisted functionally graded design of proton exchange membrane fuel cells

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Abstract:

Performance, durability, and cost are the trilemma for the commercialisation of proton exchange membrane (PEM) fuel cells. The use of Pt-based alloys as catalysts for the oxygen reduction reaction (ORR) and the nonuniform distribution of current density inside a membrane electrode assembly (MEA) result in high cost and low durability, which strongly hinders the wide adoption of PEM fuel cells in industrial and civil applications. For PEM fuel cells operated at various loads, the required activities and mass transport rates are different because the reactant and product are nonuniformly distributed inside the MEA. Thus, a rational design for a MEA, especially the porous electrode, with a spatial distribution of functional components is helpful for reducing the usage of precious components, improving cell performance, and achieving uniform distributions of current density and heat. To reduce the cost and improve the current homogeneity without sacrificing the cell performance, we studied the graded design of the functional components within the gas diffusion layer (GDL) and catalyst layer (CL), e.g., Pt loading, ionomer loading, electrode porosity, etc., along both the through-plane and in-plane directions and the spatial variation of operating parameters, i.e., temperature and pressure, as well as the interaction of multiple design variables. We developed the physics-based sophisticate model firstly, which is then used to generate the database for data-driven modelling after experimental validation. Therefore, physics-based simulation and machine-learning-based surrogate modelling are integrated to build a sophisticated M^5 model, in which **m**ulti-physics and **m**ulti-phase flow simulation, **m**achine-learning-based surrogate modelling, **m**ulti-variable and **m**ulti-objects optimisation are included. The novel approach is proved to be effective and efficient for the functionally graded design of PEM fuel cells.

Short bio:

Dr. Lei Xing received his PhD degree from Newcastle University (UK) in 2014, then worked as postdoctoral research associate in different word-leading universities, including Loughborough, Oxford, Purdue, and Birmingham, etc. He joined the School of Chemistry and Chemical Engineering at University of Surrey as a Lecturer in 2022. Dr. Xing's research interest lies in the sustainable growth of chemical and energy industries via industrial decarbonation and AI-based digitalisation within the context of circular economy, with focuses on the next-generation processes, devices and systems of carbon capture and utilisation, fuel cells and electrolysis. His current research focuses on the whole system thinking and optimisation of the industrial clusters consisting of advanced carbon capture and utilisation and intermittent renewable energy, in which AI-based adaptive optimisation, techno-economic analysis and life cycle assessment are performed to underpin the Net Zero target. He is a Chartered Member of IChemE, Editorial Board Member of *Energies*, *Frontiers in Energy Research* et al, and Guest Editor, Topic Editor and Review Editor of several journals. He has published **85+** (with **4 highly cited**) journal papers with *h*-index of **27** and **2500+** citation to date.

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Topic 3: Structure design to boost the power density of proton exchange membrane fuel cells

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Abstract:

Proton exchange membrane (PEM) fuel cell is an environmentally friendly electrochemical reaction device converting chemical energy into electricity, which is widely considered to play a vital role in future renewable energy system. However, its commercialization is currently largely hindered by the unsatisfactory power density, cost and durability. Increasing the power density not only requires high-performance membrane electrode assembly (MEA) materials, but also optimal cell structure for enhancing the 'gas-liquid-heat-electron-proton' transfer and reducing the cell/stack volume/weight simultaneously. Compared to the experimental test method, developing three-dimensional (3D) multi-physics model incorporating the full cell morphology, especially the bipolar plate (BP) and flow field, is a cost-effective and powerful tool in evaluating the influence of various cell structures on the multi-physics transfer and cell power density. Consequently, using a 3D fuel cell model that was comprehensively validated against experimental data regarding the polarization curves, electrochemical losses, spatial current density distributions, etc., we investigated the influence of several presentative BP and flow field structures on cell performance, including straight channel, wave-like channel, fine channel, channel inserting baffle, partially narrow channel, pin-type, 3D fine mesh and foam flow field. Additionally, we also compared the novel integrated BP-MEA and double-cell structure with conventional cell structure, and found significant power density improvement. This research indicates the importance of cell structure design and optimization in boosting the power density of PEM fuel cells.

Short bio:

Dr. Guobin Zhang received his Ph.D. in 2021 under the supervision of Prof. Kui Jiao at Tianjin University, China, and he studied in the University of California, Irvine as a visiting scholar during 2018-2019. He joined the Xi'an Jiaotong University in 2021 and now is an assistant professor. Dr. Zhang's main research interests are water and thermal management of fuel cells and electrolyzers, multiphase flow, heat and mass transfer in porous media, etc. As the first or corresponding author, he has published 19 international peer-review SCI journal papers in *Chemical Reviews*, *Small Methods*, *Applied Energy*, *International Journal of Heat and Mass Transfer*, etc.

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Topic 4: Experimental and numerical investigation of spatially resolved catalyst support degradation during start-up and shut-down of PEM fuel cells

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Abstract:

Degradation of PEM fuel cells during the start-up and shut-down is a major issue limiting its application in Automobiles. During the start-stop, the hydrogen and air coexist in the anode electrode, which could cause a sharp increase in the local cathode potential difference and lead to carbon corrosion. In this study, accelerated stress start-stop cycle tests are conducted on segmented PEM fuel cells where the local ECSA can be measured by cyclic voltammetry. The effects of operating temperature and flow rate are investigated. An interesting phenomenon is observed that the inlet segments which should suffer severe degradation don't loss much ECSA as expected. To investigate the underlying mechanisms, a transient quasi-2D model is developed with mass transport, electrochemical kinetics, and pseudo-capacitive effects all addressed. Through the literature, most works simply divide the anode into "power" and "load" regions through an artificially defined hydrogen/air front interface which doesn't exist in real operating conditions. In this model, for the first time, the effects of hydrogen/air mixed gas on degradation during start-up and shut-down are investigated and discussed. The local potential of each segment along the channel is calculated independently based on the local mixture gas concentration with no artificial front interface imposed. The model is developed on in-house code and implemented in Python. With the present model, a more detailed and realistic description of the start-up shut-down can be obtained. Results show that the membrane potential is very sensitive to the presence of hydrogen due to its fast chemical kinetic and the inlet segments can be protected by the remaining hydrogen in the pipeline during the short degradation time. The distribution of carbon loss obtained from the numerical model fits well with the ECSA loss observed in the experimental data. This work provides novel insights into the degradation mechanism during the start-stop.

Short bio:

Dr. Yuze Hou received his Ph.D. degree from Tianjin University in 2022, specializing in the field of PEM fuel cells. He then joined Fraunhofer ISE as a scientist, where he currently focuses on catalyst degradation, multi-scale modeling, MEA optimization, and the application of AI in MEA production.

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Topic 5: Time series health diagnosis system for polymer electrolyte membrane fuel cell based on convolutional neural networks

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Abstract:
Fault diagnosis is a critical process for the reliability and durability of polymer electrolyte membrane fuel cell (PEMFC) system. In this study, a comprehensive time-series health diagnosis system for PEMFC is proposed, coupling the fault mechanism model, sensor pre-screening method, and convolutional neural network. For a series of fault conditions, the multi-phase fault embedding model based on the physical transport processes is developed to simulate the performance evolution of the PEMFC under various health conditions. The physical model is validated by the experimental data and can be adjusted to accumulate data to address the problems of limited data samples and unbalanced data types. For the effect of various failure modes on system， the sensor pre-selection method based on adaptive network-based fuzzy inference system (ANFIS) as well as the analytical model is proposed to filter the insensitive data from the sensor set. The proposed sensor pre-screening method can improve not only diagnosis accuracy but also computational efficiency. Finally, the experimental data monitored by the optimal sensor set is utilized to build a high-precision fault diagnosis model based on the convolution neural network. It is verified that the final diagnosis accuracy rate 99.1 %, which is significantly better than the other popular methods of artificial neural network (ANN) and recurrent neural network (RNN) in this field.

Short bio:

Dr. Bowen Wang received his PhD degree from Tianjin University in 2021. Now, he is an assistant professor in State Key Laboratory of Engines at Tianjin University, and the “Hong Kong Scholar” in the Hong Kong Polytechnic University. His research interest focuses on fuel cells, water electrolysis, hydrogen energy and machine learning modeling of energy conversion systems. He published more than 30 high-quality journal papers, including Nature, and three books, and had 10 Chinese invention patents and 3 software copyrights. He joined several national and industrial projects for automotive fuel cell modeling. He won the Best Reviewer Award of International Journal of Green Energy.