The HKUST Energy Institute 香港科大能源研究院

中國科學院長春應用化學研究所—香港科技大學 氫能聯合實驗室 CIAC—HKUST JOINT LABORATORY FOR HYDROGEN ENERGY

Joint Seminar

Theory Guided Design of Ternary Alloy Pt_5(Ce)Co Multi-Layered Intermetallic Nanoparticles as Highly Active Catalysts for the Oxygen Reduction Reaction in PEMFCs

Prof. Jian XIE

School of Mechanical Engineering
School of Materials Engineering
Purdue University, West Lafayette, USA

Date 7 November 2025 (Friday)
Time 10:30 – 11:30 am
Venue **Room** 4503 (Lift 25/26) HKUST, (Location)

Abstract

The sluggish kinetics of the oxygen reduction reaction (ORR) presents a crucial barrier for proton exchange membrane fuel cells (PEMFCs). Alloying platinum (Pt) with transition metals such as cobalt (Co) can enhance catalytic activity by introducing strain and electronic effects, but controlling the extent of these effects at the atomic level remains a huge challenge. In this study, we demonstrate a novel approach of theory-guided synthesis that uses the rare-earth element cerium (Ce) to develop a Pt_5(Ce)Co/C catalyst with a finely engineered local structure. By creating a multi-layered catalyst architecture with Pt_5Co-like intermediate layers that controls the strain of a Pt-rich outer shell, we significantly enhance ORR kinetics and overall PEMFC performance. The design is guided by density functional theory (DFT) calculations, where among the Pt–Co alloys studied, the Pt_5Co sublayers is predicted to induce a unique mild compressive strain (1.24%) to the Pt(111) shell and an optimal *OH binding energy shift ($\Delta E \approx 0.11$ eV). This shift positions the alloy catalyst near the apex of the oxygen reduction reaction (ORR) activity volcano. The theoretical prediction is validated experimentally, showing the Pt_5(Ce)Co/C catalyst demonstrates a remarkable mass activity of 2.8 $A \cdot mgPt^{-1}$, far surpassing that of Pt_3Co/C and PtCo/C. After 30,000 accelerated stress test (AST) cycles in a rotating disk electrode (RDE), the catalyst retains a mass activity of 1.4 $A \cdot mgPt^{-1}$. In membrane electrode assembly (MEA) tests, Pt_5(Ce)-Co/C achieves an initial mass activity of 724 $mA \cdot mgPt^{-1}$ and delivers a current density of 1876 $mA \cdot cm^{-2}$ at 0.7 V under heavy-duty vehicle (HDV) conditions, maintaining 1450 $mA \cdot cm^{-2}$ at 0.7 V after 30,000 AST cycles. This work demonstrates a rational design strategy that DFT-guided strain engineering integrates with rare-earth templating to advance Pt-based catalysts for fuel cell applications.

About the Speaker

Dr. Xie is a professor of the School of Mechanical Engineering and School of Materials Engineering, Purdue University. He has published more than 80 journal papers and 2 book chapters, has 27 patents (14 issued). His research focuses on catalysis/electrocatalysis, energy conversion (i.e. fuel cells), energy storage (i.e. advanced batteries), nanomaterials, clear energy (i.e. electrolyzers etc.). He serves as a panelist for US National Science Foundation, Advanced Research Project Agency-Energy (ARPAE), Fuel Cell Technology Office, US Department of Energy Office of Technology Transfer, and the Canadian National Science Foundation. Before joining the university, he conducted research at Battelle Memorial Institute (fuel cell R&D, Li-ion batteries, and artificial lungs), Cabot Corp (catalysts for fuel cells), Los Alamos National Laboratory (membrane electrolytes, catalysts, membrane electrode assembly, and durability of fuel cells). He developed electric propulsion systems for Electric Vehicles (EVs) and Hybrid EVs at General Motors Advanced Technology Vehicle Center. Dr. Xie received his PhD in chemistry from Miami University and a BS in chemical engineering (emphasis on electrochemical engineering) from Tianjin University, China.

All are Welcome