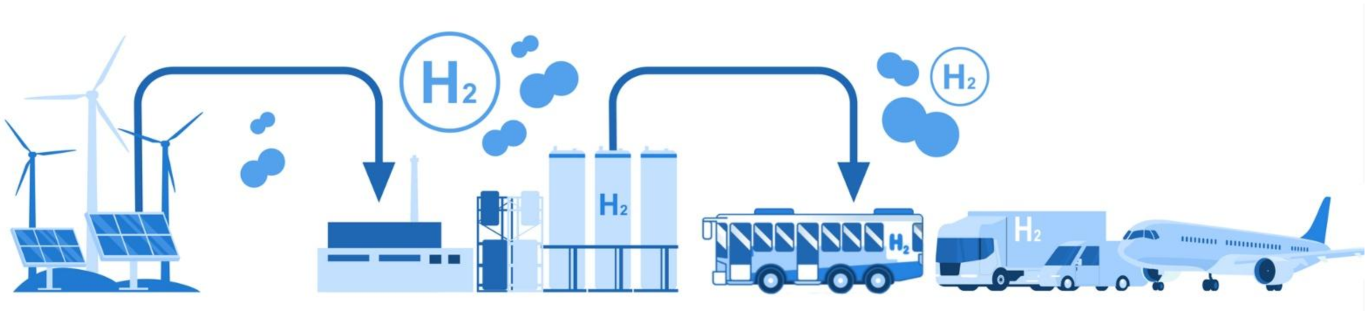
The International Workshop on Green Hydrogen and Hydrogen Energy (H_2⚡)

August 22-23, 2025

Purdue University



PURDUE UNIVERSITY

東北大学
TOHOKU UNIVERSITY

Institute for Basic Science
ibs
기초과학연구원
CENTER FOR NANOPARTICLE RESEARCH
나노입자 연구단

TOYOTA

UL Research Institutes

Organizing Committee:

Dr. Zhenhua Zeng, Assistant Research Professor, Purdue University

Dr. Naoto Todoroki, Associate Professor, Tohoku University

Dr. Taeghwan Hyeon, Distinguished Professor, Seoul National University

Dr. Luna Lu, Vice President of Industry Partnerships, Indiana ACPA Professor of Civil Engineering, Purdue University

Dr. Guang Lin, Associate Dean for Research and Innovation, College of Science, Professor of Mathematics and Mechanical Engineering, Purdue University

Dr. Jeff Greeley, Davidson Professor of Chemical Engineering, Purdue University

Dr. Brian Tackett, Assistant Professor, Purdue University

Dr. Christina Li, Associate Professor of Chemistry, Purdue University

Dr. Qi (Tony) Dong, Assistant Professor of Chemistry, Purdue University

Dr. Jian Xie, Professor of Mechanical Engineering, Purdue University

Sponsorships:

Purdue University, Office of Global Partnerships

Purdue University, Office of Industry Partnerships

Purdue University, College of Science

Tohoku University

Center for Nanoparticle Research, Institute for Basic Science

Toyota Research Institute of North America

UL Research Institute

Agenda for the International Workshop on Green Hydrogen and Hydrogen Energy

Venue: Purdue Chemistry and Chemical Engineering (Parking: Grant Street Garage)

Day 1 (August 22)			
Time	Name of speaker	Institute	Chair
8 am onward	Registration (Wetherill Hall 104)		
8:30-9:00 am	Opening Ceremony (Wetherill Hall 104)		
8:30-8:45 am	Dan Delaurentis	Purdue U	Zhenhua Zeng & Guang Lin
8:45-8:55 am	Luna Lu	Purdue U	
8:55-9:00 am	Li Qiao	Purdue U	
9:00-9:15 am	Workshop photo (In front of Wetherill Hall)		
9:15 am-12 pm	Scientific presentation (Wetherill Hall 104)		
9:15-9:45 am	Taghwan Hyeon	Seoul National U	Guang Lin (Purdue U)
9:45-10:15 am	Naoto Todoroki	Tohoku U	
10:15-10:30 am	Coffee break (Wetherill Hall 225)		
10:30-11:00 am	Liang Wang	Toyota Research Institute	
11:00-11:30 am	Jacob Spendelow	LANL	
11:30-12:00 pm	Jeff Greeley	Purdue U	
12:10-2:00 pm	Lunch and posters (Forney Hall atrium)		
2:00-5:30 pm	Scientific presentation (Wetherill Hall 104)		
2:00-2:30 pm	Kotaro Sasaki	BNL	Jeffrey Dick (Purdue U)
2:30-3:00 pm	Yue Wu	Iowa State	
3:00-3:30 pm	Kasun Gunasooriya	U Oklahoma	
3:30-4:00 pm	Coffee break (Wetherill Hall 225)		
4:00-:4:30 pm	James Wortman	GM	Xingchen Ye (Indiana U)
4:30-5:00 pm	Jian Xie	Purdue U	

Day 2 (August 23)			
Time	Name of speaker	Institute	Chair
8:30 am-12 pm	Scientific presentation (Wetherill Hall 104)		
8:30-9:00 am	Hong Yang	UIUC	Brian Tackett (Purdue U)
9:00-9:30 am	Kazuyuki Iwase	Tohoku U	
9:30-10:00 am	Venkata Yarlagadda	GM	
10:00-10:30 am	Coffee break (Wetherill Hall 225)		
10:30-11:00 am	Xiao-Dong Zhou	Uconn	Tony Dong (Purdue U)
11:00-11:30 am	Samira Siahrostami	Simon Fraser University	
11:30-12:00 pm	Yulia Pushkar	Purdue U	
12:00-2:00 pm	Lunch and posters (Forney Hall atrium)		
2:00-5:30 pm	Scientific presentation (Wetherill Hall 104)		
2:00-2:30 pm	Junhang Dong	U Cincinnati	Swami Kumaraguru (GM)
2:30-3:00 pm	Ahmed Farghaly	ANL	
3:00-3:30 pm	Jeff Wu	UL Research Institute	
3:30-4:00 pm	Coffee break (Wetherill Hall 225)		
4:00-:4:30 pm	Kensaku Kodama	Toyota Central Lab	Zhenhua Zeng (Purdue U)
4:30-5:00 pm	Christina Li	Purdue U	

Optional Day 3 (August 24): Turkey Run State Park personal meetings and hiking

Presentation Titles (in order of appearance):

Friday (Day 1) Morning

1. **Taeghwan Hyeon**, *Single atom catalysts and nanocatalysts for photo-& electro-catalytic hydrogen production* (pg. 7)
2. **Naoto Todoroki**, *Engineering Surface and Interface Structures for Efficient and Durable Water Electrolysis Electrodes* (pg. 8)
3. **Liang Wang**, *Accelerating PEMFC Technology toward Commercial Applications: ORR Catalysts for LT and HT PEMFCs* (pg. 9)
4. **Jacob Spendelow**, *Engineering Fuel Cell Catalysts, Supports, and Electrodes for Heavy Duty Trucking and Beyond* (pg. 10)
5. **Jeff Greeley**, *First principles treatments of oxygenate electrooxidation – structure sensitivity and influence of solvent on chemically diverse elementary reaction steps* (pg. 11)

Friday (Day 1) Afternoon

6. **Kotaro Sasaki**, *Designing Advanced Low-PGM Electrocatalysts using Nitride-based Cores/Supports for Fuel Cells and Electrolyzers* (pg. 12)
7. **Yue Wu**, *Sub-nanometer Cobalt on Tungsten Titanium Carbide MXene (W2TiC2Tx): An Electrocatalyst for Highly Efficient and Stable Alkaline Hydrogen Evolution at Industrial-Scale Current Density* (pg. 13)
8. **Kasun Gunasooriya**, *Theoretical Insights into Material Discovery and Design for Oxygen Electrocatalysis* (pg. 14)
9. **James Wortman**, *Improved durability of PEMFC cathode enabled by engineering ionomer-catalyst interactions and catalyst agglomeration* (pg. 15)
10. **Jian Xie**, *Super Stable and Highly Active Pt and Pt Alloy Catalysts over Nanostructured Single-Pt-Atomic-Site Support for PEMFCs* (pg. 16)

Saturday (Day 2) Morning

11. **Hong Yang**, *Defect Engineering in Complex Oxides as High-Performing Electrocatalysts for Oxygen Evolution Reaction* (pg. 17)
12. **Kazuyuki Iwase**, *Hydrothermally Synthesized Nano-Sized High-Entropy Spinel Oxide Particles as Oxygen Evolution Electrocatalysts* (pg. 18)
13. **Venkata Yarlagadda & Swami Kumaraguru**, *Overview of Catalyst and Electrode Development Efforts Targeting Improved Fuel Cell Performance and Durability* (pg. 19)

14. **Xiao-Dong Zhou**, *Electric Aviation: Triple-Breakthrough Fuel Cells for Lightness, Power, and Fuel Flexibility* (pg. 20)
15. **Samira Siahrostami**, *Emerging Electrochemical Routes for Green Hydrogen: Water and Hydrogen Sulfide Electrolysis* (pg. 21)
16. **Yulia Pushkar**, *Materials design for water oxidation (WOC) and oxygen reduction (ORR): can Fe-based catalysts lead the way?* (pg. 22)

Saturday (Day 2) Afternoon

17. **Junhang Dong**, *2-Dimensional Silicalite Nanosheets Enabled Non-Ionic Polymer Composite Membranes for Efficient Ion Conduction in Electrochemical Cells* (pg. 23)
18. **Ahmed Farghaly**, *Accelerated Discovery of Water Electrolyzers Anode Catalysts: A Closed-Loop Machine Learning and High-Throughput Experimentation Approach.*
19. **Jeff Wu**, *Accelerating the Development of Non-precious Alloy Electrocatalysts for Water Splitting through High-Throughput Experimentation* (pg. 24-25)
20. **Kensaku Kodama**, *Fuel Cell and Water Electrolysis R&D at Toyota Central R&D Labs.* (pg. 26)
21. **Christina Li**, *Electrocatalysis with Functionalized Transition Metal Dichalcogenide Nanomaterials* (pg. 27)

Single atom catalysts and nanocatalysts for photo-& electro-catalytic hydrogen production

Taeghwan Hyeon[1,2]

[1] Center for Nanoparticle Research, Institute for Basic Science (IBS), [2] School of Chemical and Biological Engineering, Seoul National University, Seoul 08826, Republic of Korea. thyeon@snu.ac.kr

We report on the design and synthesis of highly active TiO_2 photocatalysts incorporated with site-specific single copper atoms (Cu/TiO_2) that exhibit reversible and cooperative photoactivation process, and enhancement of photocatalytic hydrogen generation and CO_2 photoreduction activity.[1] We demonstrated a general method for synthesizing atomically dispersed catalysts (ADCs) via photochemical defect tuning for controlling oxygen vacancy dynamics. The optimized Pt-DSA/TiO_2 shows unprecedentedly high photocatalytic hydrogen evolution activity.[2] We presented a floatable photocatalytic platform constructed from elastomer-hydrogel nanocomposites, demonstrating its superiority over conventional systems in solar hydrogen production.[3] We propose a strategy involving polymeric stabilization of photocatalytic centers uniquely localized at the gas-liquid interface, substantially enhancing both catalytic activity and stability.[4] We designed of a structurally tuned metal-organic framework (MOF) photocatalyst that incorporates cooperative Brønsted acid-single cobalt atom catalytic sites, achieving an excellent visible-light-activated photocatalytic H_2 production.[5]

The electrocatalytic oxygen evolution reaction (OER) plays a pivotal role in the mass production of hydrogen fuel and chemical feedstocks by various electrochemical reactions. We report that early transition metals with vacant *d* orbitals (d^0-oxoanions) directly participate in and accelerate the alkaline OER via a redox cycle associated with early transition metal–peroxo species.[6] We report that doping aluminum (Al) into RuO_2 (Ir-free) and $RuIrO_x$ (low-Ir) leads to outstanding activity and excellent durability for OER at a high current density.[7] We report on the activation of Ir-doped $CoMn_2O_4$ in acidic electrolyte, leading to enhanced activity and stability in acidic OER for long-term PEMWE operation.[8] We demonstrated that Ta-doped Co_3O_4 exhibits low overpotential, while maintaining high catalytic activity for over 140 hours in acidic OER.[9] We demonstrate that active machine-learning on even small datasets – but supplemented by informative structural-characterization data and coupled with close-loop experimentation – can discover a “champion” four-metal perovskite oxide OER catalyst.[10]

1. “Reversible and cooperative photoactivation of single-atom Cu/TiO_2 photocatalysts,” *Nature Mater.* **2019**, 18, 620; “Electronic interaction between transition metal single-atoms and anatase TiO_2 boosts CO_2 photoreduction with H_2O,” *Energy Environ. Sci.* **2022**, *15*, 601.
2. “Photochemical tuning of dynamic defects for high-performance atomically dispersed catalysts,” *Nature Mater.* **2024**, 23, 552.
3. “Floatable photocatalytic hydrogel nanocomposites for large-scale solar H_2 production,” *Nature Nanotech.* **2023**, 18, 754.
4. “Polymeric stabilization at gas-liquid interface enables high-performance durable photocatalysis,” *Nature Nanotech.* **2025,** *20*, NNANO-24092963.
5. “Cooperative Brønsted acid-single atom photocatalysis in metal-organic framework,” *J. Am. Chem. Soc.* **2025,** 147, 1740 -1748.
6. “Electrochemically generated electrophilic peroxo species accelerates alkaline OER,” *Joule* **2023**, *7,* 1902.
7. “Modulating the valence electronic structure using earth-abundant aluminum for high performance acidic oxygen evolution reaction,” *Chem* **2023,** 9, 3600.
8. “Controlled Structural Activation of Iridium Single Atom Catalyst for High-performance Proton Exchange Membrane Water Electrolysis,” *J. Am. Chem. Soc.* **2025,** *147,* 2369.
9. “Tailoring cobalt spinel oxide with site-specific single atom incorporation for high-performance electrocatalysis,” *Energy Environ. Sci.* **2024**, *17*, 3628.
10. “Active learning guides discovery of a champion four-metal perovskite oxide for oxygen evolution electrocatalysis,” *Nature Mater.* **2024,** *23,* 108.

Keywords: nanocatalysts, single atom catalysts, electrocatalysis, photocatalysis, hydrogen production

Engineering Surface and Interface Structures for Efficient and Durable Water Electrolysis Electrodes

Naoto Todoroki
Graduate School of Environmental Studies, Tohoku University, Sendai, Japan
Email: naoto.todoroki.b1@tohoku.ac.jp

The oxygen evolution reaction (OER) is a key electrocatalytic process in water electrolysis, primarily due to its significantly higher overpotential compared to the hydrogen evolution reaction (HER). Catalysts and electrodes for OER face various technical challenges, including electrode degradation and reliance on scarce noble metals. To overcome these material-specific limitations and achieve long-term stability and high catalytic performance, precise engineering of both surface and interfacial structures is essential. In this talk, I will present two case studies that address these challenges through model electrode studies and interface control strategies.

Metal-doped Ru oxides have attracted significant attention as alternative OER catalysts to Ir oxides for polymer electrolyte membrane water electrolysis (PEMWE). In this study, we investigated the effects of Ti doping on $RuO_2(110)$ thin films prepared by arc plasma deposition for OER in acidic media. Ti was uniformly incorporated up to 5 at% without disrupting surface symmetry, though surface TiO_2 segregation and accompanying surface structural change occurred at higher concentrations. Ti doping improved OER activity, enhanced surface area, and suppressed overpotential increase and Ru dissolution. Structural analyses showed that doping induced anisotropic lattice strain and electronic structure modification, collectively boosting activity, stability, and corrosion resistance.(1)

Alkaline water electrolysis (AWE) systems often suffer from catalyst layer (CL) detachment under intermittent operation, which significantly limits electrode durability.(2) We found that post-annealing $NiCo_2O_4$-coated Ni electrodes effectively eliminates nanoscale voids at the CL/substrate interface and induces the formation of a epitaxially aligned Co-doped NiO interlayer. This modification substantially improves adhesion and structural robustness. Despite a modest initial drop in OER activity, the electrodes showed enhanced performance and negligible degradation during simulated start-stop cycles. These results demonstrate how interfacial microstructure modulation can mitigate mechanical degradation and enhance long-term electrode stability in dynamic electrolysis environments.(3)

(1) N. Naraki, Y. Okayama, T. Watanabe, T. Uchiyama and N. Todoroki, *under review*.
(2) H. Kojima, K. Nagasawa, N. Todoroki, Y. Ito, T. Matsui and R. Nakajima: Int. J. Hydrog. Energy, **48**, (2023), 4572-4593.
(3) N. Todoroki, K. Nagasawa, H. Enjoji and S. Mitsushima: ACS Appl. Mater., **15**, (2023), 24399-24407.

Accelerating PEMFC Technology toward Commercial Applications: ORR Catalysts for LT and HT PEMFCs

Liang Wang

Toyota Research Institute of North America

The commercialization of polymer electrolyte membrane fuel cells (PEMFCs) hinges on overcoming catalyst performance and durability limitations under both low- and high-temperature operating conditions. This presentation will introduce interface-engineered Pt-based catalysts modified with ionic liquids, which enhance oxygen reduction reaction (ORR) activity and phosphate tolerance by tailoring local surface environments. We will discuss how this strategy accelerates performance improvements for both LT- and HT-PEMFC platforms. These advancements support Toyota’s broader hydrogen energy roadmap, highlighting how fundamental materials innovations can directly address commercialization challenges in mobility and distributed energy applications.

Engineering Fuel Cell Catalysts, Supports, and Electrodes for Heavy Duty Trucking and Beyond

Jacob Spendelow, Los Alamos National Laboratory

Electrochemical systems such as fuel cells, electrolyzers, and reversible fuel cells require complex multiphase transport and reaction at poorly defined interfaces. This presentation will describe new approaches to design both catalysts and electrodes for faster transport and reaction. We have recently demonstrated that the use of intermetallic nanoparticle catalysts such as $L1_0$-PtCo can enable significant improvements in long-term performance due to improved stabilization of base metal in the ordered lattice, while use of carbon supports with controlled pore size distribution provides further advantages by protecting metal nanoparticles from degradation or poisoning by ionomer. Recent results and future directions for this catalyst research will be discussed. While kinetic performance and durability of these catalysts is promising, performance at high power densities continues to be limited by slow O_2 transport. Several factors, including slow diffusion through ionomer films, Knudsen diffusion through micropores, and pore blockage by liquid H_2O contribute to these transport limitations. Design of unconventional electrode structures that can minimize these limitations is needed to enable full utilization of cathode catalysts. New hierarchical electrode structures capable of reducing these transport losses will be presented.

“First principles treatments of oxygenate electrooxidation – structure sensitivity and influence of solvent on chemically diverse elementary reaction steps”

Zhenhua Zeng, Siddharth Deshpande, Brady Dupleiss, Anwin John, and Jeffrey Greeley

Purdue University

Advances in the theoretical understanding of electrochemical systems have, over the past decade, led to growing use of periodic Density Functional Theory (DFT) studies to treat a surprisingly large ensemble of electrocatalytic reactions, ranging from carbon dioxide electroreduction to oxygen evolution. Many such studies have employed simplified models of the electrochemical environment to determine reactivity trends across a broad space of catalytic materials, while other efforts have focused on developing detailed descriptions of electrochemical phenomena, such as the structure of electrochemical double layers, on model catalyst structures. An emerging challenge is to combine these approaches to ultimately enable theoretical design of electrocatalysts for reactions of significantly expanded chemical and materials complexity.

In this talk, we begin by discussing how we develop and apply DFT-based methods to study the electrooxidation of ethanol and related oxygenated species on Pt surfaces. We show how explicit double layer models and *ab initio* molecular dynamics provide exciting insights beyond the traditional computational hydrogen electrode treatments, leading to improved descriptions of elementary reaction steps involving adsorption/desorption of reaction intermediates and proton-coupled electron transfer processes. By combining the aggregate results with detailed microkinetic models and explicit descriptions of adsorbate-adsorbate interactions, we further demonstrate how these effects can influence both the predicted overpotentials and the selectivities to acetic acid, acetaldehyde, and carbon dioxide. We conclude with some perspectives on how these insights may be used to enhance the search for improved oxygenate electrooxidation catalysts.

Designing Advanced Low-PGM Electrocatalysts using Nitride-based Cores/Supports for Fuel Cells and Electrolyzers

Kotaro Sasaki

Chemistry Department, Brookhaven National Laboratory, Upton, NY, 1197, USA

The low-content Pt-based core-shell catalysts potentially alleviate the drawback in the existing Pt catalysts including high cost, slow kinetics, and poor stability; they could further improve the oxygen reduction reaction (ORR) activity and stability for the proton exchange membrane fuel cells (PEMFCs). There have been remarkable advances in both the development of promising core−shell catalysts and the understanding of the fundamental catalytic mechanisms, and it is clear that some of the low platinum-group-metal (PGM) core−shell catalysts with enhanced activity and stability have great potential for use in PEMFCs. Nevertheless, various issues still need to be clearly addressed for the advanced core−shell catalysts of the future. On the other hand, PEM electrolyzers (ELs) are desirable large-scale energy devices to produce *green hydrogen* toward a net-zero carbon economy. The technologies require the availability of effective catalysts, particularly for the oxygen evolution reaction (OER). Ir- and Ru-based catalysts are currently the best-performing OER catalysts; however, their cost and limited availability hamper the widespread commercialization/deployment of PEMELs. Therefore, there is also an urgent need for developing highly durable and inexpensive catalysts for the OER. This talk first focuses on synthetic strategies, catalytic mechanisms, and influencing factors of Pt- and Ir-based catalysts used for PEMFCs and PEMELs. We will then discuss effective and solid strategies/designs to employ nitride-based cores/supports for the development of highly advanced low-PGM catalysts for the ORR, particularly in heavy-duty vehicle (HDV) PEMFC applications, and for the OER in PEMEL applications.

Sub-nanometer Cobalt on Tungsten Titanium Carbide MXene ($W_2TiC_2T_x$): An Electrocatalyst for Highly Efficient and Stable Alkaline Hydrogen Evolution at Industrial-Scale Current Density

Yue Wu

Department of Chemical and Biological Engineering, Iowa State University, Ames, Iowa 50011, United States, E-mail: yuewu@iastate.edu; Tel: +1-515-294-0702

ABSTRACT

Electrocatalysis plays a central role in enabling large-scale green hydrogen production from water electrolysis. It is important to develop efficient, durable, and earth-abundant catalysts that operate at industrially relevant realistic operating conditions. Here, we reported a new type of 2D metal carbide (MXene) – tungsten titanium carbide ($W_2TiC_2T_x$, T stands for surface termination groups) synthesized for the first time from a novel MAX precursor route. By loading cobalt (Co) onto the surface of $W_2TiC_2T_x$ and rationally designing of the local atomic and interface configurations, we developed a highly effective and stable catalyst for alkaline hydrogen evolution reaction (HER). The optimized Co/W_2TiC_2 catalyst exhibits small overpotentials of 63 mV and 191 mV at 10 and 100 mA cm^{-2}, respectively, and achieves outstanding long-term operational durability, maintaining stable hydrogen production at 4000 A cm^{-2} for over 1000 hours. In a flowcell MEA electrolyzer, it delivers near-unity hydrogen Faradaic efficiency over a wide current range (50 - 400 mA cm^{-2}), while requiring significantly lower cell voltages than the commercial Pt/C electrode under same conditions. Comprehensive structural analysis with in-situ X-ray photoelectron spectroscopy (XPS), X-ray absorption near edge structure (XANES), and extended X-ray absorption fine structure spectroscopy (EXAFS) reveal that thermal modulation induces a transformation of Co from isolated atoms and large nanoparticles (NPs) into uniform subnanometer particles anchored on the tungsten outer layers. Density functional theory (DFT) calculations reveal that the HER activity was sensitive to the coordination environment of Co on W_2TiC_2 and identify Co-W interfacial sites as the primary active centers. This work demonstrates a structurally well defined, non-precious HER catalyst capable of operating under harsh industrial conditions. It sheds light on structure design and utilization of metal-support interaction (MSI) in MXene-supported metal catalysts for the efficient electrochemical water splitting.

Theoretical Insights into Material Discovery and Design for Oxygen Electrocatalysis

G. T. Kasun Kalhara Gunasooriya*

Proton exchange membrane (PEM) fuel cells and electrolyzers are promising renewable electrochemical energy storage and conversion technologies. The energy efficiencies of these technologies have been hampered by the sluggish kinetics of oxygen-based (oxygen evolution reaction-OER and oxygen reduction reaction-ORR) electrochemical reactions and consequently demand a high overpotential to drive these reactions, even when using state–of– the–art oxygen electrocatalysts. Moreover, the stability of these materials should be on par with their catalytic activity to develop electrocatalysts for practical applications. In this presentation, I will discuss our efforts in (i) discovering stable, active and selective ORR and OER catalysts, and (ii) understating acid electrolyte and pH effects. Based on theoretical and experimental findings, rational catalyst design principles for next-generation oxygen electrocatalysts are established.

James Wortman, *Improved durability of PEMFC cathode enabled by engineering ionomer-catalyst interactions and catalyst agglomeration*

In heavy duty vehicle (HDV) applications for proton exchange membrane fuel cells (PEMFCs), efficiency in H_2 fuel consumption over the long application lifetime becomes increasingly important compared to light duty applications. This places added importance on sustained performance and durability, especially of the cathode catalyst layer.

Several strategies exist for improving upon the durability of the state-of-the-art Pt/C cathode electrode. One important route for improvement involves design of the catalyst itself - for example, shell-protected catalysts, anchored catalysts and ordered PtCo intermetallic alloys are some of the catalyst design strategies evaluated by General Motors. However, the interaction of the catalyst with the surrounding electrode environment (namely, perfluorosulfonic acid ionomer) also plays a key role in durability.

In recent work, General Motors has found that incorporating a small fluorocarbon molecule (methoxy-nonaflurorobutane, NFB) onto the surface of a Pt/high surface area carbon catalyst (Pt/HSC) greatly impacted ink and electrode properties. It was discovered that NFB treatment allows for a 25-50% decrease in ionomer content without sacrificing initial performance. Interestingly, this decrease in ionomer content also led to an increase in Pt electrochemical surface area retention after accelerated testing. This improved durability is likely due to the lowered ionomer content, which led to lowered Pt dissolution and/or diffusion rates. In this presentation, several ex-situ characterization methods and in-situ MEA diagnostics will be used to elucidate the mechanism of NFB-mediated changes to ionomer-catalyst interactions, which help facilitate a less corrosive microenvironment around Pt without sacrificing performance. Overall, this study will give insight into electrode design parameters for engineering advanced PEMFC cathode electrodes with improved durability for HDV applications.

Acknowledgements: This work is partially supported by U.S Department of Energy, Hydrogen and Fuel Cell Technologies Office under grant DE-EE0010749.

Super Stable and Highly Active Pt and Pt Alloy Catalysts over Nanostructured Single-Pt-Atomic-Site Support for PEMFCs

Jian Xie, PhD Professor
School of Mechanical Engineering School of Materials Engineering Purdue University, West Lafayette

Polymer electrolyte membrane fuel cells (PEMFCs) for heavy-duty vehicle (HDV) applications require the membrane electrode assemblies (MEAs) with high durability and efficiency, which directly associate with the activity and stability of the cathode catalysts for the oxygen reduction reaction (ORR). We are developing the innovative single-Pt-atomic-site Pt-N-C supports and the new class of platinum group metal (PGM) catalysts over such supports to achieve enhanced activity and super strong stability, in combination with an ingeniously designed ionomer/catalyst interface into an ideal nanostructured MEA for HDV applications. For traditional PGM catalyst with non- or functionalized supports (carbon black, nanotube, graphene, metal oxides etc.), severe particle surface migration due to the physically weak/non interaction between PGM nanoparticles (NPs) is mainly responsible for the catalyst degradation in PEMFC operation. To overcome this nanoparticle migration, we developed the single Pt atomic sited Pt-N-C structured supports which uniformly distributes on and embeds on the single Pt atoms on the surface of carbon support at a very low Pt content (up to 1 wt.%Pt) but with extremely high site density, which enables the establishment of the strong Pt-Pt bonds between Pt atoms in the Pt NPs and the single Pt sites on the support surface after the catalyst synthesized. Such catalysts show superior stability and activity,1.07 A/cm$_2$ after 300,000 accelerated stress test (AST) cycles, which successfully exceeds the DOE 2025 targets, 1.07 A/cm$_2$ at 0.7V, 150k AST cycles, with 2.0X performance of targets.

About the Speaker: Dr. Xie is a professor at the School of Mechanical Engineering and School of Materials Engineering, Purdue University. His research focuses on the materials chemistry and devices with research theme on energy, analysis, origins, synthesis and catalysis. Additionally, 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 has published more than 80 journal papers including *Nature Energy*, *Nature Catalysis* and *Nature Communications*, and 2 book chapters, has 27 patents (14 issued). He serves as a panelist for US National Science Foundation, Advanced Research Project AgencyEnergy (ARPAE), Fuel Cell Technology Office, US Department of Energy Office of Technology Transfer, and the Canadian National Science Foundation. Before joining academia, he conducted research at Battelle Memorial Institute (fuel cells, 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 in 1999 and a BS in chemical engineering (emphasis on electrochemical engineering) from Tianjin University, China in 1982

Defect Engineering in Complex Oxides as High-Performing Electrocatalysts for Oxygen Evolution Reaction

Hong Yang
Department of Chemical and Biomolecular Engineering
University of Illinois at Urbana-Champaign
206 Roger Adams Laboratory, MC 712
600 S. Mathews Avenue, Urbana, IL 61801
E-mail: hy66@Illinois.edu

Oxygen reduction reaction (OER) occurs in a range of electrochemical and electrocatalytic processes, such as electrolyzers for water splitting and carbon dioxide utilizations. High-level control of atomic and surface structures is critical for the development of high-performance OER electrocatalysts and both bulk and surface properties are important in determining the activity and stability. This is because both adsorbate evolution mechanism (AEM) and lattice oxygen mechanism (LOM) may be involved in the electrocatalytic cycle. In this presentation, I will discuss the synthesis-structure-electrocatalytic property relationship of complex oxides that can be described in a generic formula of $A_xB_yO_z$, where A and B can be a single metal cation, or mixed cations located at a given lattice site. I will present several archetypes of oxide structures, including perovskite, pyrochlore, spinel, and Ruddlesden-Popper (RP) phase compounds and their site-mixed solids, all of which are found to be active for OER under acid conditions. Our results indicate defect engineering is particularly important for OER catalysis in these solids. Thus, it is essential, besides understanding heterogeneous catalysis, solid-state chemistry approach is often needed to uncover the design strategy for optimal performance. In addition, the dynamics of electrocatalysts occurring during OER suggest the need to re-examine how to regulate the cation sites and oxygen defect chemistry for enhancing the bond and lattice stability of key structural constituents.

Hydrothermally Synthesized Nano-Sized High-Entropy Spinel Oxide Particles as Oxygen Evolution Electrocatalysts

Kazuyuki Iwase[1]
[1] *Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai, Japan*

e-mail address: kazuyuki.iwase.a6@tohoku.ac.jp

High-entropy oxides (HEOs), consisting of multiple metal cations homogeneously distributed within a single-phase crystal structure, have emerged as promising candidates for electrocatalysis owing to their unique electronic structures and tunable compositions.1) In particular, spinel-type HEOs (HE-SOs) incorporating transition metals have been studied as electrocatalysts for the oxygen evolution reaction (OER) under alkaline conditions. However, many HEOs reported to date have been synthesized via hightemperature solid-state routes, resulting in large particle sizes and low surface areas, which limit their catalytic activity. To address this issue, we have developed a solution-based synthesis strategy using supercritical hydrothermal processing to produce nano-sized HE-SO particles.

Aqueous solutions containing Mn, Fe, Co, Ni, and Zn precursors were reacted under supercritical water conditions, yielding spinel-type HEO nanoparticles with an average size of approximately 18.6 nm. XRD patterns confirmed the formation of a single-phase cubic spinel structure, and STEM–EDX mapping revealed homogeneous elemental distribution, indicating the successful formation of a multicomponent solid solution. Electrochemical measurements in O_2-saturated 1 M KOH electrolyte demonstrated that the synthesized HE-SO nanoparticles exhibit OER activity, with an overpotential of 330 mV at 10 mA cm^{-2} and a Tafel slope of 36.7 mV dec^{-1}. 2)

To further enhance the OER activity, we explored particle size tuning through surface modification by introducing organic molecules during the synthesis. Specifically, catechol was added to the precursor solution as a capping agent to modulate nucleation and growth under subcritical hydrothermal conditions. TEM and XRD analyses confirmed that the average particle size could be reduced from 19.3 nm to 6.8 nm without disrupting the spinel oxide structure. TG-DTA analyses further revealed the stable binding of catechol molecules to the nanoparticle surface, suggesting its role in controlling the particle size. OER activity measurements demonstrated that the reduced particle size led to improved OER activity, with the current density at 1.65 V vs. RHE increased from 109 to 190 mA cm^{-2} and a decrease in overpotential from 342 to 327 mV. The Tafel slope value remained nearly constant, indicating that the rate-determining step was unchanged. This suggests that the enhancement is primarily attributable to the increased surface area. These findings highlight the effectiveness of organic surface modifiers for size tuning in HEOs.3)

This work establishes a general strategy for the design of nano-sized HEO electrocatalysts. Further details on structural and electrochemical analyses will be presented at the presentation.

1) C. Oses, C. Toher and S. Curtarolos *Nat. Rev. Mater*., 2020, 5 , 4, 295-309.
2) **K. Iwase** *et al*., *ACS Appl. Energy Mater*., 2022, 5, 8, 9292-9296.
3) **K. Iwase** *et al*., *in preparation*

Overview of Catalyst and Electrode Development Efforts Targeting Improved Fuel Cell Performance and Durability

Venkata Yarlagadda[1] *and Swami Kumaraguru*[1]

[1] *Fuel Cell Activities, General Motors Company*

Abstract

In a PEM fuel cell, the catalyst support plays a key role in determining the catalyst nanoparticle distribution thus having an impact on the activity and durability of Pt and Pt-alloy based catalysts. At General Motors, we have explored various carbon supports over the years that can enable electrodes with improved fuel cell performance and durability over state-of-the art high surface area carbon (Ketjen black) supported catalyst-based electrodes.

In this talk, we will primarily discuss two carbon supports that showed promising potential in terms of enabling durable and high performing cathodes. The first one is a mesoporous carbon support with ordered pore structure that can support higher weight percent of platinum (Pt). The accessible pores present in mesoporous carbon can host Pt that has reasonable access to proton and oxygen while being shielded from direct ionomer adsorption. However, the templated synthesis of these mesoporous carbons often results in larger primary particle sizes that can negatively impact proton transport under sub-saturated operating conditions and need to be addressed. The second carbon support of interest is a sulfonated carbon support that enables lower ionomer usage in the fuel cell electrode. The lower ionomer volume fraction in the electrode reduces Pt dissolution and restricts Pt^{2+} diffusion. We have explored the sulfonated carbon support both in terms of fabricating low-ionomer content and completely ionomer-free electrodes. The advantages and limitations of the aforementioned sulfonated carbon-based electrodes will be discussed in this talk.

This work was partially supported by the U.S. Department of Energy, ARPA E project number DE-AR0001550

Electric Aviation: Triple-Breakthrough Fuel Cells for Lightness, Power, and Fuel Flexibility

Xiao-Dong Zhou
Chemical and Biomolecular Engineering, Materials Science and Engineering, and Mechanical Engineering Departments
Center for Clean Energy Engineering University of Connecticut, Storrs, CT 06269
xiao-dong.zhou@uconn.edu

Researchers at the University of Connecticut is advancing the future of electric aviation through the development of next-generation fuel cell systems. In this talk, I will discuss our recent progress toward a triple breakthrough in fuel cell design: achieving **ultra-lightweight structures**, **unprecedented specific power**, and **high fuel flexibility**. These innovations are essential to enabling high-performance, scalable electric propulsion platforms.

Our team has developed novel fuel cell architectures for integration into RC airplanes that are designed, built, and flown by students. This includes ground and flight testing of solid oxide and polymer electrolyte fuel cell systems under real-world conditions. In addition, I will briefly elaborate the activities in hydrogen production and carbon management.

This work is supported by the U.S. Department of Energy ARPA-E's Range Extenders for Electric Aviation with Low Carbon and High Efficiency (REEACH) Program under the contract: DE-AR0001774

Emerging Electrochemical Routes for Green Hydrogen: Water and Hydrogen Sulfide Electrolysis

Samira Siahrostami
Department of Chemistry, Simon Fraser University
8888 University Drive, Burnaby, B.C. V5A 1S6, Canada
email:(ssiahros@sfu.ca)

The development of sustainable hydrogen production pathways is critical for decarbonizing energy systems and advancing a circular, low-carbon economy. In this talk, I will highlight two emerging electrochemical routes for hydrogen generation that also provide added environmental and chemical valorization benefits.

First, I will discuss water electrolysis not only as a green hydrogen production process but also as a tunable platform for the selective generation of hydrogen peroxide (H_2O_2) via the two-electron water oxidation pathway. This dual-product strategy enables the decentralized and clean production of H_2 for energy storage while simultaneously generating H_2O_2, a valuable chemical for water treatment and industrial processes, offering a sustainable alternative to the energy-intensive anthraquinone process.[1,2]

Second, I will present hydrogen sulfide (H_2S) electrolysis as a zero-emission approach for hydrogen production while addressing the pervasive environmental challenge of H_2S emissions from oil and gas refineries. Through combined experimental studies and density functional theory (DFT) calculations, we elucidate the hydrogen sulfide oxidation reaction (H_2SOR) mechanisms over various metal oxides and sulfides, identifying sulfur-tolerant catalysts such as TiO_2 that enable efficient and durable H_2S electrolysis while mitigating sulfur poisoning.[3]

By integrating mechanistic insights and catalyst design principles, these electrochemical strategies establish new, leverageable routes for sustainable hydrogen production. They not only contribute to global hydrogen supply but also align with environmental remediation and green chemical manufacturing goals, moving us closer to scalable, efficient, and circular energy solutions.

References:

1. Baek, J.; Jin, Q.; Johnson, N.S.; Jiang, Y.; Ning, R.; Mehta, A.; Siahrostami, S., Zheng, X. Discovery of $LaAlO_3$ as an efficient catalyst for two-electron water electrolysis towards hydrogen peroxide. *Nat. Commun*. **2022**, 13, 7265.
2. Siahrostami, S. H_2O_2 electrosynthesis and emerging applications, challenges, and opportunities: A computational perspective. *Chem Catal*. **2023**, 3(3).
3. Siahrostami, S.; Baratifar, S. Hydrogen Recovery from H_2S Electrochemical Oxidation: A DFT Study. *Phys. Chem. C* **2024**, 128, 15277.

Materials design for water oxidation (WOC) and oxygen reduction (ORR): can Fe-based catalysts lead the way?

Jully Patel[†], Naduvile Purayil Dileep[†], Anurupa Naskar[‡], Jeremy M. Smith[‡], Yulia Pushkar[†]

[†] *Department of Physics, Purdue University, 525 Northwestern Ave, West Lafayette IN*

[‡] *Department of Chemistry, Indiana University, 800 E. Kirkwood Avenue, Bloomington IN*
E-mail: ypushkar@purdue.edu

Green hydrogen can be produced via artificial photosynthesis where water is split by energy input of sunlight. Hydrogen can be later used in fuel cells. All these applications require new, electrochemically active materials and catalysts which utilize earth abundant elements. While in natural photosynthesis water oxidation is accomplished at the oxygen evolving complex of Photosystem II, which is Mn and Ca based[1], modern electrolyzes use IrOx to facilitate water oxidation at the anode. Biological systems can also activate oxygen using Fe and Cu-based active centers, while modern fuel cells require high loading of Pt at the cathode for oxygen activation. Thus, further investigations of earth abundant systems for WOC and ORR are required.

We discovered that Fe- and Fe-Mn-triazole ($Fe(ta)_2$, $Fe\text{-}Mn(ta)_2$) Metal-Organic Frameworks (MOFs) perform as dual-function materials for photo-absorption and water oxidation in acidic media. $Fe(ta)_2$ or $Fe\text{-}Mn(ta)_2$ were found to be highly active and stable in chemical and photochemical water oxidation, and in addition function as photoanodes, with photo-electrocatalytic currents (~2.00×10^{-3} Acm^{-2} at +1.4 V *vs.* Ag/AgCl) at *pH*=1. DFT demonstrated the possibility of a unique catalytic mechanism where O-O bond formation is possible from the coupling of two adjacent $Fe^{IV}=O$ fragments. This mechanism prompted us to investigate whether at some conditions closely positioned Fe centers in $Fe(ta)_2$ can also activate O_2 in ORR process. $Fe(ta)_2$ was found to be active in ORR in the range of pH=1-7 with the onset potential of ~0.4 V vs RHE and high conversion efficiency. Further electrochemical stabilization of material was demonstrated for $Fe(ta)_2$ prepared with 1-5% of carbon nanotubes.

References:

1. Jensen, S., Sullivan, B.T., Hartzler, D.A., Kosheleva, I., Henning, R.W., Page, A., and Pushkar, Y. (2025). Challenges of observing O-O bond formation in the Mn4Ca cluster of photosystem II. Chem. 10.1016/j.chempr.2025.102448.

2-Dimensional Silicalite Nanosheets Enabled Non-Ionic Polymer Composite Membranes for Efficient Ion Conduction in Electrochemical Cells

Junhang Dong (jdong@ucmail.uc.edu)
Department of Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH 45221

The ion exchange membranes (IEMs) are critical to the performance of various electrochemical cells including fuel cells (FCs), redox flow batteries (RFBs), and water and CO_2 electrolyzers, etc. Over the past decade, our group has been investigating the highly selective ion transport in zeolite structures and developing zeolite-based membranes as alternative proton exchange membranes (PEMs) and anion exchange membranes (AEMs). Our IEM development has been primarily directed towards applications in aqueous RFBs and alkaline water electrolyzers (AWEs). In this presentation, we will give a brief overview of our work on the polymer supported silicalite nanosheet (SN) laminated membranes (SNLMs) as PEMs for RFBs. The presentation will focus on the recent demonstration of SNs with surfaced quaternary ammonium cations (QAC) as a new type of anionic building block for high-performance AEMs. The SNs with surfaced QAC groups have been synthesized to fabricate both anionic SN-tiled membranes (SNTMs) on porous non-ionic PVDF substrates (SNLM-PVDF) and unsupported SN-PBI mixed matrix membranes (MMMs) for AWE applications. These SN-based AEMs exhibited low ASR for anion conduction and outperformed the commercial FAA3-50 AEM in AWE with enhanced current density at lower operation voltage. The results demonstrate that the QAC-templated SNs can be a new class of building blocks for high-performing AEMs for AWE for green hydrogen production using renewable energy.

Accelerating the Development of Non-precious Alloy Electrocatalysts for Water Splitting through High-Throughput Experimentation

Dr. Jeff Wu*, Dr. Uzoma Nwabara, Dr. Jorge Gonzalez, Dr. Stuart Miller*

Materials Discovery Research Institute, UL Research Institutes

Skokie, Illinois, 60077, USA

**stuart.miller@ul.org, jeff.wu@ul.org*

Hydrogen energy is recognized as a clean, innovative, and highly efficient energy source that plays a crucial role in efforts to decarbonize and promote a sustainable, carbon-neutral economy. However, challenges remain, particularly regarding the high energy requirements and costs associated with producing green hydrogen through water electrolysis. While precious metals are currently the most effective electrocatalysts for green hydrogen production, their widespread industrial application is limited due to their scarcity and high prices. As a result, a significant challenge lies in developing non-precious electrocatalysts for both the HER and the OER that are abundant in resources and provide higher activity at lower costs.

At UL Research Institutes, the Materials Discovery Research Institute (MDRI) is dedicated to developing novel non-precious alloy electrocatalysts for HER and OER through high-throughput experimentation and computation. This process employs high-throughput DFT computation and machine learning, along with comprehensive experimental methodologies that include alloy and compound synthesis, property characterization, and performance evaluation, as illustrated in Figure 1.

The nanoprinter at MDRI uses physical vapor deposition to vaporize different pairs of metals into nanoparticles. This technology enables the creation and printing of various metals or metal alloys by combining, generating, and depositing nanoparticles in a single automated workflow. Using this nanoprinter, we are accelerating the synthesis of non-precious metallic alloy electrocatalysts based on Ni, Co, Fe, and other metals. Additionally, we are systematically characterizing the physical properties of the printed metal electrocatalysts, including thickness, composition, and microstructures, along with the electrochemical activity of the printed samples in a high-throughput manner. This integrated workflow, which combines computational and experimental approaches, will significantly expedite the discovery process, reducing development time from years to just months.

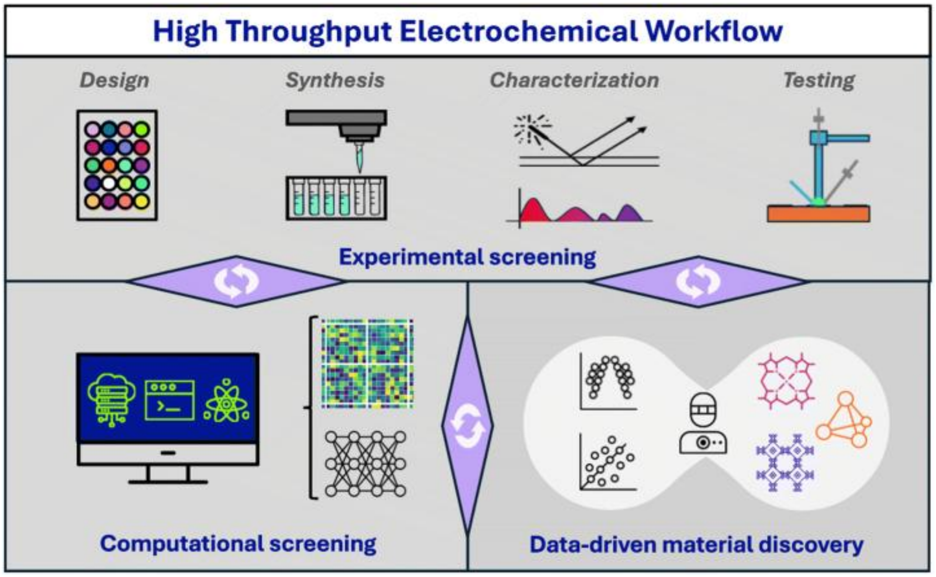


Figure 1. Workflow for accelerating the development of non-precious alloy electrocatalysts for water splitting through high-throughput computation and experimentation. Figure reprinted with permission from ref. [1]. Copyright 2025 Royal Society of Chemistry

References

[1] U. Nwabara, K. Yang, A. Talekara, et al., High throughput computational and experimental methods for accelerated electrochemical materials discovery, J. Mater Chem. A, https://doi.org/10.1039/D5TA00331H.

Fuel Cell and Water Electrolysis R&D at Toyota Central R&D Labs.

Kensaku Kodama[a]
[a]*Toyota Central R&D Labs., Inc.*,
[a]*Nagakute 480-1192, Japan,*
kkodama@mosk.tytlabs.co.jp

In the face of growing concerns over the serious impacts of global warming, hydrogen is expected to be a promising energy carrier for maximizing the benefits of renewable energy. Fuel cells and water electrolysis are essential technologies for the large-scale and widespread production and utilization of green hydrogen, and have been actively studied in both academia and industry.

Toyota Motor Corporation (TMC) launched its fuel cell passenger vehicles, MIRAI, in 2014 and 2020, and is now working to expand the application of this technology to a broader range of fields, including heavy-duty vehicles. Furthermore, taking advantage of the significant overlap in components between fuel cells and water electrolyzers, TMC is also applying its fuel cell technologies to the development of water electrolysis systems. However, there are still considerable challenges in deploying these devices at a global societal scale.

Toyota Central R&D Labs., Inc. (TCRDL), the core research institute of the Toyota Group, has made contributions to the development of fuel cell and water electrolyzer stacks at TMC, particularly through fundamental research spanning from system-level to materials-level approaches.[1, 2] In this presentation, we will introduce the past and future research and development activities on fuel cell and water electrolysis technologies at TCRDL.

Reference

(1) Watanabe, T. et al., Setting Development Targets for Fuel Cells and Systems for Heavy-Duty Trucks Using a Comprehensive Model-Based Approach. *Electrochemical Society Meeting Abstracts* 2022 **242** (40), 1468-1468.
(2) Inaba, M. et al., Synthesis of a Mesoporous SnO_2 Catalyst Support and the Effect of Its Pore Size on the Performance of Polymer Electrolyte Fuel Cells. *ACS Applied Materials & Interfaces* 2024 **16** (8), 10295-10306

Electrocatalysis with Functionalized Transition Metal Dichalcogenide Nanomaterials

Christina Li

Tarpo Department of Chemistry, Purdue University

Supported metal atoms are found ubiquitously as heterogeneous catalysts for a wide variety of industrial, organic, and energy catalytic processes. The electronic and steric environment at the nanomaterial surface has a huge impact on the reactivity and selectivity of catalytic transformations occurring at surface active sites, but these properties are difficult to independently control through conventional materials synthetic methods. In this work, we develop molecularly-precise surface functionalization strategies in order to precisely tune both the ensemble geometry and redox properties of active site metal atoms. We focus on tuning the defect chemistry and metal–sulfur coordination environment of intercalated and doped metal atoms on metal chalcogenide nanosheets for electrochemical catalysis and optoelectronic applications. Our synthetic strategies enable modulation the surface active site environment in order to access more reactive and selective nanomaterial catalysts.