THE OHIO STATE UNIVERSITY

The William G. Lowrie Department of Chemical and Biomolecular Engineering Graduate Program Cordially invites you to attend a seminar on

Bridging Physics-Informed and Data-Driven Materials Designs to Catalyze Deep Decarbonization

Dr. Jiayu Peng

Postdoctoral Associate

Massachusetts Institute of Technology

February 8, 2024, 11:30 AM

130 Koffolt Lab, CBEC 151 W Woodruff Ave

Reception at 11:00 AM - CBEC Lobby

Bio

Jiayu Peng is a postdoctoral associate in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology, supervised by Prof. Rafael Gómez-Bombarelli. He obtained his Ph.D. in Materials Science and Engineering in 2022 from the same department working with Prof. Yang Shao-Horn. His research bridges the physics-informed and data-driven designs of new catalyst materials to decarbonize chemical transformations through the combination of atomistic simulations, advanced characterization, and machine learning. Jiayu has been awarded a Graduate Student Award from the Materials Research Society, the ENFL Future Investigator Spotlight from the Energy and Fuels Division of the American Chemical Society, and the IUPAC-Zhejiang NHU International Award for Advancements in Green Chemistry for Young Chemists from the International Union of Pure and Applied Chemistry.

Abstract

Electrifying and decarbonizing key industrial sectors, including chemical and materials industries, as well as transportation and aviation, is a pressing mission of our time. Industrial players and governments worldwide have set ambitious targets to reduce carbon emissions, which need to be decreased to net-zero around mid-century in order to address global warming and climate change. For such deep decarbonization, it is crucial to develop unprecedented materials, such as electrocatalysts that can efficiently and steadily produce green chemicals and fuels at scale and generate renewable electricity on demand. In this seminar, I will introduce how a joint computational–experimental approach can be established to accelerate catalyst materials design using first-principles atomistic simulations, synchrotron X-ray spectroscopies, and physics-inspired machine learning. I will highlight how mechanistically elucidating and quantitatively controlling the electronic structure of transition metal compounds can effectively alter their chemical bondings, modulate key reaction barriers toward dissolution and electrocatalysis, and thus influence their durability and reactivity, respectively, offering physics-driven guiding principles for optimizing their catalytic performance. Moreover, I will demonstrate how combining machine learning with materials physics can accelerate the discovery of multicomponent oxides—a new class of materials with too-complicated atomic orderings for an exhaustive investigation—through the development of machine-learning models that accurately predict ordering-dependent materials properties by capturing intrinsic symmetries. To conclude, I will discuss new opportunities for fully unlocking transformative physics-informed, data-driven materials design for sustainability and decarbonization.