SDSU College of Engineering Mechanical Engineering

Mechanical Engineering Seminar Series

February 25, 2025, 11:00AM

Dean's Conference Room, E-203E

Title: Physics-Informed Generative Modelling for Structural Prediction of Amorphous High Entropy Materials

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Abstract: High-entropy materials (HEMs), composed of multiple principal elements, offer transformative potential in catalyst design by leveraging their configurational entropy and cocktail effects. Among these, amorphous HEMs have emerged as particularly promising due to their ability to accommodate diverse elemental mixtures and create highly active, non-equilibrium sites. Recently, surface reconstruction and amorphization have been shown to significantly enhance catalytic performance, particularly for the oxygen evolution reaction. However, searching amorphous materials via random site occupancy is an NP-hard problem and introduces significant challenges in predicting their structures. Strong lattice distortions, arising from structural inhomogeneity and compositional complexity, lead to vast and rugged potential energy landscapes that are difficult to explore with traditional modeling approaches. Capturing the interplay between short-range order (SRO), stability, and catalytic activity in such systems requires advanced methodologies.
This talk presents a physics-guided generative modeling framework for predicting the structure of amorphous high-entropy materials. By incorporating SRO descriptors, our approach integrates density functional theory, machine learning interatomic potentials, and particle swarm optimization to navigate these complex energy landscapes and address the challenges of lattice distortions. This methodology not only accelerates the exploration of compositional spaces but also provides critical insights into the atomic-scale mechanisms that underpin the catalytic superiority of amorphous HEMs, paving the way for next-generation catalyst development in sustainable energy technologies.

Brief Bio: Dr. Wanlu Li is an Assistant Professor in the Aiiso Yufeng Li Family Department of Chemical and Nano Engineering at University of California, San Diego. In 2019, she obtained her Ph.D. from Tsinghua University and completed her postdoctoral research from 2019 to 2023 at University of California, Berkeley and Lawrence Berkeley National Laboratory. In 2021, Dr. Li received the ACS Physical Chemistry Young Investigator Award. In 2023, she obtained the Jacobs School of Engineering Early Career Faculty Development Award and "Faculty Fellowship Program Israel". Dr. Li's research group explores several areas including: (a) Large timescale and length-scale modeling of lithium batteries; (b) Advancing computational modeling and catalyst design under realistic conditions; (c) Investigating the electronic structure and spectroscopy of size-selected nanoclusters and nanoalloys; (d) Developing machine learning frameworks for atomic potentials and materials design. To date, she has published over 65 scientific papers and has received almost 3000 citations, the H-index is 32.