Membranes, superionic conductors, and nanocatalysts: From design to deep learning

De-en Jiang
Department of Chemical and Biomolecular Engineering
Department of Chemistry
Vanderbilt University

Abstract: My group is interested in both knowledge- and data-driven design of functional molecules and materials in chemical separations, electric energy storage, and nanocatalysis, from a computational perspective. In this talk, I will first discuss several design approaches to tune and control pore size to achieve desired gas separation performances via graphene and fullerene membranes. Concepts of ion-gating and entropic selectivity will be demonstrated via molecular simulations. Next, I will introduce a new mechanism of superionic Li transport in glassy LiTaCl$_6$, enabled by anion vibrations and revealed by molecular dynamics simulations via machine-learning force fields. In the third topic, I will show an exciting progress in atomically precise metal-hydride nanocluster catalysts where the challenge to locate the hydrides was addressed by deep neural networks. In each of the studies, one will see a close interplay between computation and experiment, demonstrating that computation or an experiment in silico is now a valuable tool to drive advances in chemical separations, battery materials, and nanocatalysis.

Bio: De-en Jiang is a Professor in Department of Chemical and Biomolecular Engineering, with a secondary appointment in Department of Chemistry, at Vanderbilt University. He received his BS and MS degrees from Peking University and PhD degree from UCLA, all in chemistry. He worked at Oak Ridge National Laboratory first as a postdoc and then as a staff scientist before joining University of California Riverside (UCR) in 2014. He was a Professor of Chemistry at UCR, as well as a cooperating faculty member of Chemical & Environmental Engineering and Materials Science and Engineering before moving to Vanderbilt in July 2022. His research focuses on computational materials and chemistry for energy and the environment. He received the DOE Early Career Award and the Presidential Early Career Awards for Scientists and Engineers. He was an elected Fellow of the American Association for the Advancement of Science. According to Google Scholar, his 360+ peer-reviewed publications have been cited over 28,700 times with an H-index of 90.