

Machine Learning in Chemistry: From Structure Prediction to Ion Dynamics

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What to learn and what to predict are central questions facing chemists as we seek to leverage recent advances in machine learning for our research. In this talk, I will discuss how my group addresses these questions in the area of computational materials chemistry, with a focus on nanocatalysis and energy storage. Through two case studies, I will illustrate the power of machine learning: first, how deep neural networks can locate hydrides in copper–hydride nanoclusters in lieu of neutron scattering to solve their total structures, which allows us to establish the structure-activity-selectivity relationships in their unique capabilities in reduction reactions such as CO₂ reduction; and second, how machine learning interatomic potentials or force fields enable us to probe superionic Li transport in amorphous materials and to predict new solid electrolytes for solid-state Li batteries. Across these two examples, you will see the close interplay of experiment, density functional theory, and machine learning. I argue, and hope to convince you, that this trinity will shape the next decade of predictive modeling in chemistry.