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Case Studies of Machine Learning in Nano and Materials Sciences

What to learn and predict is a question facing domain scientists when they would like to leverage the advances in machine learning to their specific areas of research. In this talk, I will discuss how my group is answering this question in my research interest of computational materials chemistry for nanocatalysis and energy storage. Through two case studies, I will show the power of deep neural networks in locating hydrides in copper nanoparticles (highly relevant to neutron scattering) and machine learning potentials in understanding superionic Li transport in amorphous materials. I hope to convince you that machine learning is now a key approach in predictive modeling in nano and materials sciences.

Topical Area

AI and data science

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