Translational AI Center (TrAC) Seminar
Fall 2024

Qi An

October 9th at 11:00 AM (US Central Time)

Location and zoom link: https://trac-ai.iastate.edu/event/trac-seminar-series-qi-an/

Understanding Reaction Mechanisms of Ammonia Synthesis through the Combination of Deep Reinforcement Learning and Density Functional Theory

Abstract

The Haber–Bosch (HB) process is the foundation of industrial ammonia (NH_3) production, essential for manufacturing nitrate-based fertilizers and offering potential as a hydrogen carrier. However, the HB process consumes over 2% of global energy annually to produce more than 160 million tons of NH_3, primarily due to the high temperatures and pressures required by iron-based catalysts. In this presentation, we will first present a novel artificial intelligence framework that integrates deep reinforcement learning (DRL) with density functional theory (DFT) simulations to explore and evaluate complex catalytic reaction networks. By transforming first-principles-derived free energy landscapes into a dynamic DRL environment, the model autonomously evolves to identify optimal reaction pathways. Demonstrated through the Haber-Bosch process on the Fe(111) surface, this framework discovers pathways with lower energy barriers than traditional methods. Secondly, to solve the instability of the convergence issue of DRL in the chemical reactions, we introduce a reaction-agnostic framework, HDRL-FP, which combines high-throughput deep reinforcement learning with first principles DFT to explore catalytic reactions. The framework constructs a generalizable representation of reactions from atomic positions, mapping them to potential energy landscapes. HDRL-FP uses thousands of simulations on a single GPU to rapidly and cost-effectively identify optimal reaction pathways. Applied to hydrogen and nitrogen migration in the Haber-Bosch process on the Fe(111) surface, HDRL-FP reveals shared transition states between mechanisms and discovers pathways with lower energy barriers compared to traditional methods. This study presents a pathway for significantly enhancing the understanding of HB catalysts, offering a promising direction for reducing the energy demands of the ammonia synthesis process.

Short Bio

Dr. Qi An is an Associate Professor in the Department of Materials Science and Engineering at Iowa State University. He earned his PhD in Materials Science from Caltech, and his BS from the University of Science and Technology of China. His research focuses on computational materials science, including machine learning, electronic structure calculations, and atomistic simulations. His work specifically targets ammonia synthesis, the mechanical properties of ceramics, semiconductors, and thermoelectric materials, computational alloy design, metallic glasses, material behavior under extreme conditions, and heterogeneous catalysis. Dr. An has authored or co-authored over 210 publications in scientific journals.

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