Bridging First-Principles Calculations and AI Predictions for Materials Synthesizability

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“Materials design on demands” is one of the final goals of materials science. Over the past decades, first-principles calculations have played a pivotal role in guiding new materials development, evolving from simple property predictions in the early stages to more complex, high-throughput computational designs as computing power has grown. However, the gap between theoretically predicted stability and practical feasibility often leads to significant challenges in synthesizing these predicted compounds, thereby highlighting the critical importance of “synthesizability prediction.” In this talk, we introduce potential solutions to this challenge through two avenues: constructing a chemical reaction network and leveraging large language models (LLMs) and Natural Language Processing (NLP) for recipe generation via natural language processing. By integrating these approaches, we aim to pave the way toward more efficient, AI-driven materials research that bridges the gap between theory and experiments.