

AI for Synthesizable Materials Discovery: From Prediction to Autonomous Design

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Materials informatics uses data-driven models to explore vast chemical spaces and discover new materials with targeted properties. However, many computationally proposed materials fail in practice because synthesizability and processing constraints are often overlooked, leading to costly experimental trial-and-error. In this talk, I will present our recent efforts to develop machine learning models for predicting the synthesizability of inorganic materials and identifying feasible synthesis pathways. I will highlight explainable AI approaches that move beyond black-box predictions by providing interpretable insights into synthesis feasibility. Finally, I will discuss emerging agentic AI frameworks that integrate materials design, synthesis planning, and iterative decision-making to enable autonomous and experimentally actionable materials discovery.

References

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