Data-Driven Crystal Structure Prediction for Ternary Metal Chalcogenides

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Abstract

The efficient design and discovery of stable inorganic crystal structures is central to materials innovation. Here, we compare data-driven approaches for accelerated crystal structure prediction: substitution into known prototype structures, generative artificial intelligence (GenAI) using denoising diffusion as implemented in *Chemeleon*, and an evolutionary global optimisation search[1]. Candidate structures are optimized using an ensemble of machine-learned interatomic potentials, providing both energy estimates and uncertainty quantification. Applied to a large set of known and hypothetical ternary metal chalcogenide compositions, including technologically relevant sulfides such as Na_2SiS_3, $RbPS_3$, and KMo_2S_4, our analysis reveals that the GenAI approach not only matches but can surpass traditional methods in identifying diverse, low-energy structures. These findings highlight the promise of generative models for scalable structural exploration of inorganic materials space. At the end of the talk, I will briefly introduce our recent work on GenAI-driven discovery of disorder-stabilized ground states.

References

[1] Tianshu Li, Hyunsoo Park, Aron Walsh* Chem. Mater. 2026, 38, 1, 161–170.

Figures

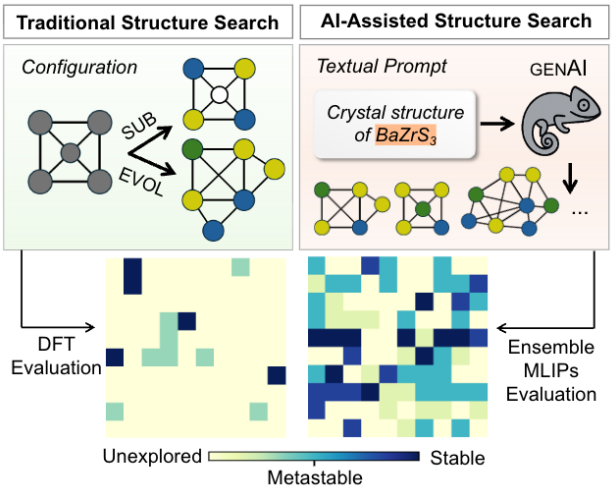

Figure 1. Table of Contents