Predicting the Chemical (Dis)order in Multicomponent Materials with High-Throughput Simulations and Representation Learning

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1. Introduction

The vast structural tunability and compositional diversity of multicomponent materials make them promising for a range of applications, yet the complexity of atomic ordering in such multinary materials, all the way from highly ordered elemental arrangements to fully disordered solid solutions, poses significant challenges in the rational design, rigorous discovery, and global optimization of materials with desired properties [1,2].

2. Substantial section

This presentation will explore our recent advancements in leveraging physics-informed, data-driven approaches to predict the chemical dis(order) in these complex materials, offering a new lens to reconcile theoretical, machine learning, and experimental perspectives (Fig. 1). Through high-throughput atomistic simulations with physics-driven machine learning, we establish and evaluate data-driven, physics-informed descriptors to universally and accurately predict experimental cation ordering in multicomponent perovskite oxides, providing systematic benchmarks between machine learning, theory, and experiments [3].

More importantly, we examine an overlooked question in designing graph convolutional neural networks—whether these state-of-the-art architectures can learn the dependence of key materials properties on chemical compositions and atomic orderings equally accurately. We demonstrate that although these models can generally capture composition-dependent properties across the periodic table, building ordering-sensitive graph neural networks requires symmetry-aware architectures that can inherently preserve and differentiate the distinct crystallographic symmetries of various inequivalent atomic orderings [4,5].

Together, our work formalizes standing challenges and pinpoints promising paths for more rigorous AI-driven materials design, where the critical role of chemical (dis)order can be accurately captured.

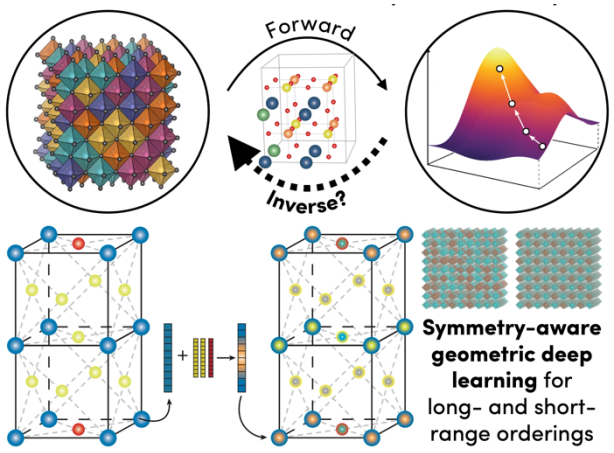

Fig. 1: Reimagining physics-driven atomistic machine learning for the differentiable inverse design of multinary compositions and chemical disorders.

References

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