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Machine Learning Algorithms and FAIR (Findable, Accessible, Interoperable, and Reusable) Materials Databases to Design Inorganic Heterostructures with Exceptional Accuracy and Efficiency

Abstract

The design of crystalline materials with specific properties is a critical challenge in materials science, and recent developments in computational approaches offer promising solutions. In particular, the use of machine learning algorithms and FAIR (Findable, Accessible, Interoperable, and Reusable) materials databases have enabled design of inorganic materials with exceptional accuracy and efficiency. Magnetic materials are of particular interest due to their broad range of existing and potential applications, such as data storage, spintronic devices, and permanent magnets. Moreover, magnetic materials exhibit a diverse range of fundamental physical properties, including the relation between magnetic order and superconductivity, lattice properties, multiferroic systems, skyrmions, and altermagnetic systems, making them attractive for both applied and basic research. However, designing magnetic materials with unconventional properties, i.e. beyond coplanar order, remains a significant challenge. The energy landscape of these materials is complex and rough, with multiple free energy minima that hinder the identification of the ground state of a material from first principles. Despite this challenge, recent advances in computational materials design have shown promising results [6]. We propose to transform the

current computational magnetic materials design workflow by developing a symmetry-driven search of complex inorganic magnetic and nearly magnetic materials based on borides and chiral chalcogenides. This approach leverages the unique structural features of these materials to enable the discovery of novel magnetic systems with tailored properties. Our vision is to combine two synergistic computational methodologies that will target the class of novel borides and chiral chalcogenides materials. The methodology involves a high-throughput search of stable/metastable structures in underexplored ternary and quaternary boride systems that are anticipated to exhibit a subset of structures with symmetry requirements for (i) unconventional magnetic properties (chiral, broken inversion, parity symmetry and related), as well as (ii) conventional magnetic, superconducting, magnetoelastic, and magnetocaloric applications, followed by a high-throughput search of stable structures in systems composed of chemically similar elements (including alloying). The systems that demonstrate promising magnetic or superconducting properties and predicted to have low free energy (thermodynamically stable and kinetically stabilized metastable) will be synthesized, and their transport properties will be characterized.