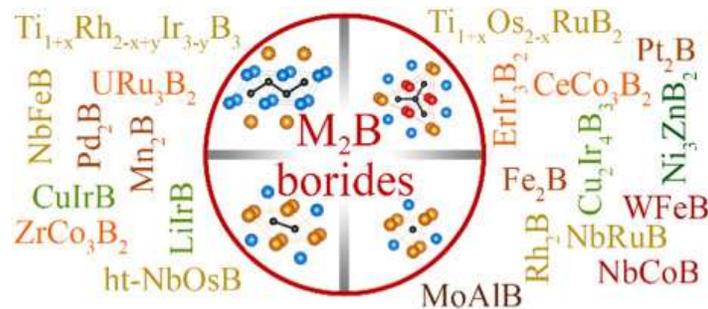# First-Principles Study of Novel Boride Materials for Extreme Conditions: Structural, Electronic, and Mechanical Properties

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Abstract

There has been a consistent need of materials that exhibit multifunctional properties when subjected to varied conditions, physically, electronically, and/or chemically [5]. Studies from recent times have found that boride crystals show promise in this aspect, especially in their mechanical properties in terms of both hardness and toughness [1][2]. Their applications further extend to aerospace, nuclear reactors and many such extreme environments due to properties like thermal stability and chemical inertness [4]. Some boride crystals, due to their lattice structure are expected to be good 2-D materials useful for high-performance coatings [2]. In particular, transition metal borides are being considered competitive substitutes to currently available materials due to their high hardness, distinctive electronic properties and oxidation resistance. Another lucrative aspect of such crystals is the balance they display between hardness and toughness thanks to the presence of both valence electrons and covalent bonding within the lattice [3]. This research aims to investigate novel boride materials using first-principles calculations based on Density Functional Theory (DFT) to predict their structural stability, mechanical behavior, and electronic properties, guiding their potential application in extreme conditions.

Objectives

- To identify new or unexplored boride phases and assess their thermodynamic stability using DFT-based formation energy calculations.
- To predict hardness, elastic moduli, and fracture toughness of selected borides to determine their suitability for super-hard coatings and wear-resistant applications.
- To investigate the electronic band structure, density of states, and thermal conductivity to explore potential applications in high-temperature electronics and thermo-electrics.
- To explore AI-driven computational approaches to accelerate the discovery and screening of promising boride materials.

Methodology

- **Computational Framework:**

    o Utilize Density Functional Theory (DFT) with appropriate exchange-correlation functionals (GGA/PBE, hybrid functionals) for accurate property predictions.
    o Implement beyond-DFT corrections (e.g., GW, DMFT) where necessary for improved electronic structure calculations.

- **Mechanical Property Calculations:**

    o Compute elastic constants via stress-strain methods.
    o Predict Vickers hardness using semi-empirical models.

- **Thermodynamic and Phase Stability Analysis:**

    o Conduct phonon dispersion and ab initio molecular dynamics simulations to assess dynamical stability.
    o Use convex hull construction to determine phase stability in multicomponent boride systems.

- **High-Throughput Screening & AI Integration:**

    o Leverage machine learning models trained on existing boride datasets to predict new candidates with desirable properties.
    o Use Bayesian optimization for efficient material screening.

Impact

- Contribution to high-performance materials design for aerospace, nuclear, and wear-resistant applications.
- Enabling cost-effective material discovery by reducing reliance on trial-and-error synthesis.
- Advancement of computational materials science through AI-enhanced predictive modeling.

References

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