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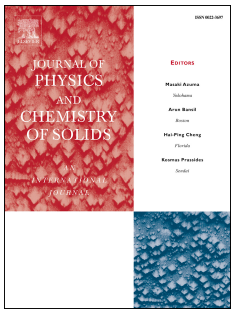

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Mechanical Behavior, Electronic and Phonon Properties of ZrB_{12} under Pressure

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Abstract: The mechanical, phonon and electronic properties of ZrB_{12} under pressure are investigated by first-principles calculations. The research shows that ZrB_{12} is mechanically and dynamically stable up to 100 GPa. The elastic constants, bulk modulus *B*, shear modulus *G*, hardness H_v, *B/G* ratio, Debye temperature under different pressures are systematically investigated. The calculation of electronic properties shows that ZrB_{12} has metallic character. The Zr-d states dominate the DOS at the Fermi level, and the total DOS and PDOS change slightly with the increasing pressure. DOS (E_f) first decreases, then increases with the increasing pressure. At 50 GPa, ZrB_{12} has less electron carriers. The analysis of electron localization function shows that the strong B-B and Zr-B covalent bonds may be responsible for the high hardness and stability.

Keywords: first-principles calculation; mechanical properties, electronic properties; phonon dispersion

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