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Structural, elastic, thermodynamic, and electronic properties of BaHfO₃: a first-principles study using GGA-PBEsol + TB-mBJ approach

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Abstract

The structural, elastic, thermodynamic, and electronic properties of cubic perovskite BaHfO₃ are calculated by means of the full-potential linearized augmented plane wave (FP-LAPW) method and the quasi-harmonic Debye model. Accurate structural and elastic parameters are obtained by using the GGA-PBEsol scheme of the generalized gradient approximation (GGA) to describe the exchange-correlation potential. BaHfO₃ is found brittle, mechanically stable, and elastically anisotropic, with a predominance of directional bonding. First predictions of the Grüneisen parameter, the specific heat at constant volume, the isothermal bulk modulus, and the adiabatic bulk modulus are given. BaHfO₃ has high thermal expansion coefficient. The effects of pressure and temperature on the thermodynamic parameters are also investigated. The electronic properties are calculated using the Tran-Blaha modified Becke-Johnson (TB-mBJ) exchange-correlation potential. BaHfO₃ has an indirect band gap R-Γ of 5.66 eV. The top of the valence band is due essentially to O 2p states while the bottom of the conduction band results mainly from Ba *d* and Hf *d t_{2g}* states. The Hf-O bonds have an ionic-covalent character while the Ba-O bonds are ionic.

Keywords:

first-principles; GGA-PBEsol; TB-mBJ; elastic parameters; thermodynamic properties; band structure

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