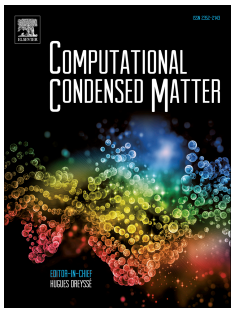
Accepted Manuscript



Structural, elastic, thermodynamic, and electronic properties of $BaHfO_3$: A first-principles study using GGA-PBEsol + TB-mBJ approach

Mohamed Benatia, Fatima-Zohra Driss-Khodja, Fatiha Saadaoui, Mohammed Driss-Khodja, Abdelkader Boudali

PII: S2352-2143(18)30060-1

DOI: 10.1016/j.cocom.2018.e00296

Reference: COCOM 296

To appear in: *Computational Condensed Matter*

Received Date: 6 March 2018

Revised Date: 13 April 2018

Accepted Date: 18 April 2018

Please cite this article as: M. Benatia, F.-Z. Driss-Khodja, F. Saadaoui, M. Driss-Khodja, A. Boudali, Structural, elastic, thermodynamic, and electronic properties of $BaHfO_3$: A first-principles study using GGA-PBEsol + TB-mBJ approach, *Computational Condensed Matter* (2018), doi: 10.1016/j.cocom.2018.e00296.

Structural, elastic, thermodynamic, and electronic properties of $BaHfO_3$: a first-principles study using GGA-PBEsol + TB-mBJ approach

Mohamed BENATIA, Fatima-Zohra DRISS-KHODJA, Fatiha SAADAOUI,
Mohammed DRISS-KHODJA*, and Abdelkader BOUDALI

Laboratoire d'Etudes Physico-Chimiques, Université de Saïda, 20000 Saïda, Algérie

Abstract

The structural, elastic, thermodynamic, and electronic properties of cubic perovskite $BaHfO_3$ 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. $BaHfO_3$ 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. $BaHfO_3$ 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. $BaHfO_3$ has an indirect band gap R-Γ of 5.66 eV. The top of the valence band is due essentially to O 2*p* 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 iono-covalent character while the Ba-O bonds are ionic.

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

* Corresponding author. Tel.:+213661541669 Fax: +21348477697

E-mail address: drisskhodjam@yahoo.com (M. Driss-Khodja)