Journal of Molecular Modeling (2018) 24:131
https://doi.org/10.1007/s00894-018-3666-z

ORIGINAL PAPER

Electronic structure, mechanical and thermodynamic properties of $BaPaO_3$ under pressure

Shakeel Ahmad Khandy[1,2] · Ishtihadah Islam[3] · Dinesh C. Gupta[2] · Amel Laref[4]

Received: 16 February 2018 / Accepted: 17 April 2018

Abstract

Density functional theory (DFT)-based investigations have been put forward on the elastic, mechanical, and thermo-dynamical properties of $BaPaO_3$. The pressure dependence of electronic band structure and other physical properties has been carefully analyzed. The increase in Bulk modulus and decrease in lattice constant is seen on going from 0 to 30 GPa. The predicted lattice constants describe this material as anisotropic and ductile in nature at ambient conditions. Post-DFT calculations using quasi-harmonic Debye model are employed to envisage the pressure-dependent thermodynamic properties like Debye temperature, specific heat capacity, Grüneisen parameter, thermal expansion, etc. Also, the computed Debye temperature and melting temperature of $BaPaO_3$ at 0 K are 523 K and 1764.75 K, respectively.

Keywords Electronic structure · Perovskite · Mechanical and thermal properties

Introduction

Topical advances in bulk and atomic-scale simulations endowed with the technical progress in synthesis of perovskite oxides and their heterostructures have bestowed a productive and new opinion for producing novel, superlative structures with intriguing properties. The designing of structures with promising phenomena can be obtained via different symmetry constraints. Also, the understandings of fundamental physical aspects behind these characteristic properties are liable to be explained by the customary advanced simulative codes available with diverse and appropriate degrees of freedom [1]. Owing to the multifaceted and technologically important properties, perovskites turned out to be an active area of research and therefore symbolize a distinguished class of materials. The various properties for which these oxides are known include superconductivity, charge and spin ordering, ferroelectricity, colossal magnetoresistance, thermoelectricity, and photoconduction, which henceforth make them promising candidates for efficient energy management and other applications [2–5].

Perovskite oxides with actinide element constituents have been principally studied for their chemical instability and structural analysis. Among this family, $BaUO_3$ [6], $BaNpO_3$ [7, 8], and $BaAmO_3$ [9] are reported to be ferromagnetic half-metals. In our previous work, $BaPaO_3$, an important byproduct of fission produce, was studied for structural, electronic, and transport properties [10] and optical properties by Erum et al. [11]. It was therefore found that $BaPaO_3$ can be a potential material for micro as well as nano-electronic devices. However, its experimental study is limited only to structure, thereby a gap for mechanical stability and elastic and thermodynamic properties in the available literature needs to be filled. For that reason, the present work has been undertaken to investigate the undecided elastic response and thermal properties of this material and the effect of pressure on its half-metallic character as well as mechanical properties.

Methods

Density functional theory (DFT) has proven to be the most influential and acceptable and approximate method for

✉ Shakeel Ahmad Khandy
shakeelkhandy11@gmail.com

[1] Department of Physics, Islamic University of Science and Technology, Awantipora, Jammu, Kashmir 192122, India

[2] Condensed Matter Theory Group, School of Studies in Physics, Jiwaji University, Gwalior, MP 474011, India

[3] Department of Physics, Jamia Millia Islamia, New Delhi 110025, India

[4] Department of Physics, College of Science, King Saud University, Riyadh, Saudi Arabia

Published online: 07 May 2018