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Structural, elastic and magneto-electronic properties of half-metallic $BaNpO_3$ perovskite

Shakeel Ahmad Khandy*, Dinesh C. Gupta

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

HIGHLIGHTS

- The cubic perovskite $BaNpO_3$ is a Half-metallic ferromagnet.
- 100% spin polarization is observed at the Fermi level.
- It is ductile and anisotropic in nature.
- Has high melting temperature of about 1968.71 K.

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ABSTRACT

First principles calculations on structural, electronic, magnetic and elastic properties of $BaNpO_3$ oxide are reported using full potential augmented plane wave method. To achieve the optimized lattice parameters, the local density approximation (LDA) and generalized gradient approximation (GGA) have been used. The calculated values of lattice constant and bulk modulus are found to be in agreement with experimental and other reported results. In addition, Hubbard approximation potential (GGA + U) and modified Becke Johnson approximation (mBJ) are also engaged for the exact prediction of band structure. Half-metallicity along with 100% spin polarization is reflected from the spin resolved band structures as well as densities of states. The ferromagnetic stable configuration of $BaNpO_3$ perovskite is observed from the double cell optimization method as well as the spin-magnetic moment calculations. In addition, elastic constants have been calculated to envisage the mechanical response of this material. From these mechanical parameters, the ductile nature of the material is observed along with a Debye temperature of 356 K and melting temperature of 1968.71 K.

1. Introduction

The density functional theory (DFT) has proven to be one of the most accurate methods for the computation of the electronic structure and other physical properties of solids [1–3]. Perovskites with a general formula ABO_3 has been progressively studied within the framework of the first-principles density functional approach and a lot of research work in this field has been reviewed due to the exhibition of astonishing properties by these oxides. In recent decades, perovskites and their derivatives have gained a lot of attention from researchers worldwide due to their multifaceted and potentially important properties including ferromagnetism [4], superconductivity [5], spin-polarisation [6], colossal magnetoresistance [7], thermoelectricity [8], and from the application point of view, such compounds have revolutionised the technologically important fields like magnetoelectronics, solid-oxide fuel cells, memory devices and spintronics e.g. spin valve generators, magnetoresistive random access memories (MRAMs), read heads for hard disk drives (HDDs), etc. [9–11].

Lanthanide based perovskites especially the oxides of neptunium are potentially the motivating members of the vast Perovskite family due to their complicated electronic structures. We have studied the neptunium based perovskite $BaNpO_3$ to discuss the electronic structure, magnetism and elastic properties which are yet to be explored. The literature of survey reveals a huge gap with a scant experimental information about its cubic structure and lattice constant only [12]. This glaring lack of information about the electronic structure and other physical properties has inspired us to

* Corresponding author.
E-mail addresses: shakeelkhandy11@gmail.com (S.A. Khandy), sosfizix@gmail.com (D.C. Gupta).

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