Chinese Journal of Physics 55 (2017) 1769–1779

Contents lists available at ScienceDirect

Chinese Journal of Physics

journal homepage: www.elsevier.com/locate/cjph

# Temperature and pressure dependent electronic, mechanical and thermal properties of *f*-electron based ferromagnetic barium neptunate

Sajad Ahmad Dar[a], Shakeel Ahmad Khandy[b,*], Ishtihadah Islam[c], Dinesh C Gupta[b], Umesh Kumar Sakalle[a], Vipul Srivastava[d], Khursheed Parrey[c]

[a] Department of Physics, Motilal Vigyan Mahavidyalya College, Bhopal-462008
[b] Condensed Matter Theory Group, School of Studies in Physics, Jiwaji University, Gwalior-474011 (MP), India
[c] Department of Physics, Jamia Millia Islamia New Delhi-110025 India
[d] Department of Physics NRI Institute of Research & Technology, Bhopal-462021 India

ARTICLE INFO

*Article history:*
Received 8 April 2017
Revised 11 July 2017
Accepted 3 August 2017
Available online 4 August 2017

*Keywords:*
Electronic structure
Perovskite
Mechanical and thermodymic properties

ABSTRACT

Overall thermal dependence of electronic, thermodynamic and mechanical properties of $BaNpO_3$ oxide have been investigated via full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). Different approximations such as local density approximation (LDA), generalized gradient approximation (GGA), Hubbard approximation potential (GGA+U) have been employed to achieve the optimized calculation results. The calculated structural, electronic and mechanical parameters are consistent with the available experimental and theoretical data. The elastic parameters at different pressures have also been calculated. Half-metallic nature is reflected from the spin polarized band profile of the present material. Moreover, the temperature and pressure dependent thermodynamic properties including Debye Temperature, specific heat capacity, grueinessien parameter, Entropy, thermal expansion, etc have been calculated via quasiharmonic Debye model.



## 1. Introduction

A great progress in the first-principles approach to work with the ideal Perovskites that have a general prototype structure of $CaTiO_3$ has been reviewed as these materials show remarkable properties [1]. Perovskites especially oxide based and their derivatives have attracted considerable attention from researchers across the globe in recent decades due to their multifunctional properties such as Ferroelectricity [2], piezoelectricity [3], ferromagnetism [4] and from the application point of view they have a great potential usage in devices like solid-oxide fuel cells, transducers, spintronics, gas sensing, sharp memory and thermoelectric devices [5,6]. Predicting new materials and the modification of their desired properties still continues to be an area of great interest.

Neptunium which belongs to actinide series is mostly a by-product of nuclear reactors. Cubic oxides of neptunium are interesting members of Perovskite family due to the presence of highly correlated f-electronic in their structures. Among the

* Corresponding author.
*E-mail address:* shakeelkhandy11@gmail.com (S.A. Khandy).

http://dx.doi.org/10.1016/j.cjph.2017.08.002