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Investigating structure, magneto-electronic, elastic and thermoelectric properties of alkaline earth actinide perovskite oxide (BaBkO3) from first principle calculations

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ABSTRACT

First principle calculations with highly precise spin-polarized density functional theory (DFT) have been performed to study the structural stability, mechanical and magneto-electronic properties of cubic perovskite $BaBkO_3$. The properties were studied under the generalized gradient approximation (GGA) and onset Coulomb interaction by WEIN2k package. The DFT and analytically calculated values of Goldschmidt tolerance (GT) factor in addition to stable-phase optimization show stability of the present material in the ferromagnetic cubic phase with a higher magnetic moment of 7 μB. This is because the nature of magnetism of 5f actinide materials ($l = 3$) is governed by the large spin-orbit interaction and the hybridization of 5f electron orbitals with other states. The value of exchange and correlation potential were treated with different approximations: GGA and GGA + U calculations. Contribution of electronic states was studied through total and partial density of states using GGA and GGA + U approach. GGA + U calculations reveal an indirect band gap of 3.15 eV for $BaBkO_3$ in the spin down channel supporting the half metallic nature and spin-polarized electronic band structure encourages complete spin polarization of the material with metallic character in spin up state. Mechanical properties like stability, stiffness, hardness, brittleness and ductility were discussed on the basis of elastic parameters obtained. The oxide perovskite $BaBkO_3$ exhibit higher value of Seebeck coefficient and power factor at room temperature with a value of 150 μVK^{-1} and 5.1×10^{12} $\mu Wcm^{-1}K^{-2}s^{-1}$respectively. The properties of half-metallicity and higher Seebeck coefficient makes this material a promising candidate for thermoelectric and spintronic device applications.

1. Introduction

The perovskite is the nomenclature for all those compounds which adopt the same crystal structure as the mineral calcium titanate ($CaTiO_3$). In the ideal form the crystal structure of cubic perovskite can be described as ABX_3, where the A-site cation is 12-fold coordinated and the B-site cation is 6-fold coordinated with oxygen anions, as simply can be seen in Fig. 1. Atom A is usually alkali, alkaline or rare earth metal while B is likely to be transition, post transition, and non-transition metals and the anion site represented by X are oxides or halides [1–6]. The oxide perovskites (ABO_3) studied extensively have achieved a considerable attention because of their use in a diverse range of applications including superconductors, spintronic devices, thermoelectrics, electro-catalysts, pollution abatement, chemical sensors, memory devices etc. [7–13]. Perovskite oxides also exhibit varied structural phase transition sequences, metal–insulator transitions, pyroelectric behavior, piezoelectricity, and half-metallic ferromagnetism (HMF) or thermoelectric properties, thus making them as promising candidates for multi-functional devices [14,15]. Among them half metallic ferromagnets (HMFs) are a class of materials that have received much interest from the current research community due to its application in spintronic/magneto electronic devices [16]. Such perovskites exhibit spin resolved bands which have special characteristics that; the majority spin band shows metallic

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