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ORIGINAL PAPER

A DFT Study on Structural, Electronic Mechanical and Thermodynamic Properties of 5f-Electron System $BaAmO_3$

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Abstract The structural, electronic, mechanical and thermodynamic properties of the perovskite oxide $BaAmO_3$ have been predicted using the full-potential linearized augmented plane wave (FP-LAPW) method. The equilibrium lattice constant, bulk modulus and pressure derivative were computed using different exchange correlations. The optimization of structure was carried out in ferromagnetic, anti-ferromagnetic and non-magnetic states, and the compound was found to be stable in the ferromagnetic state. A systematic study on the band structure and density of states was accomplished using generalized gradient approximation (GGA), Hubbard approximation (GGA+U) and modified Becke–Johnson exchange potential (mBJ),and the compound was found to have a half-metallic nature in all the approximations. The calculated total spin magnetic moment was found to be 5 μ_B in all the approximations used. The second-order elastic constants, Young modulus, shear modulus, Poisson ratio and anisotropic factor have also been calculated. In order to have a complete understanding of $BaAmO_3$, the thermodynamic properties were studied in the pressure range of 0 to 40 GPa and the temperature range extending from 0 to 600 K.

Keywords Perovskite · Elastic properties · Ferromagnetism · Thermodynamic properties

1 Introduction

Great attention towards perovskites, especially oxide based, has been paid in the recent past because of their countless different applications and device fabrication [1–4]. Perovskite oxides particularly with ABO_3 composition containing f-electrons are very important, because of the properties that result from their highly correlated electron systems. These perovskite oxides are extensively investigated in several technological domains, and these are considered as the best candidate for multiferroic materials, spintronic devices and solid oxide fuel cells [5, 6]. $BaAmO_3$ is one of the ABO_3-type perovskite oxides, crystallizes in cubic form with the space group *pm-3m* (221). The divalent cation (Ba) is located at the (0, 0, 0) position; (O) at the (0.5, 0.5, 0), (0.5, 0, 0.5) and (0, 0.5, 0.5) positions; and (Am) at the body-centred position (0.5, 0.5, 0.5) of the cubic unit cell. The molar enthalpy of formation was found to be −15,446.6 kJ mol^{-1} [7]. Extensive theoretical studies have been made using first-principles calculations for closely related compounds like $BaMO_3$ (M = Pr, Th, U) and $SrUO_3$ perovskites [8–10]. As far as the previous literature study is concerned, not much attention has so far been paid to understand the physical behaviour of such a highly correlated f electron system, $BaAmO_3$. This glaring lack of information on the physical behaviour of $BaAmO_3$ and the absence of

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