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Physical properties of cubic $BaGeO_3$ perovskite at various pressure using first-principle calculations for energy renewable devices

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ABSTRACT

The electronic, optical and thermoelectric analyses of $BaGeO_3$ perovskite have been done by using density functional theory (DFT) based Trans and Blaha modified Becke and Johnson (TB-mBJ) approach. The applied pressure (up to 30 GPa) has been found tailoring the band gap from indirect to direct bandgap (at 20 GPa), within the visible region, revealing renewable energy applications of the studied perovskite. The applied pressure improves mechanical stability by increasing ductility. Furthermore, optical properties are illustrated by computing dielectric constants, refraction, absorption, optical conductivity and optical loss factor for suggesting optoelectronic applications. The maximum peaks shifting to higher energy, due to increasing pressure indicate a blue shift. Finally, the calculated thermal and electrical conductivities, See-beck coefficient, power factor, Hall coefficient, specific heat capacity, susceptibility and electron densities are also elaborated for thermoelectric applications by using BoltzTraP code.

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1. Introduction

With the evolution of modern technology, various devices exhibiting amazing functionalities have been introduced [1]. The devices designed for the wonderful commercial utilities primarily rely on the nature of the underlying materials. Therefore, the role of material science for understanding and optimizing the materials, to achieve the desired material parameters, becomes significant. The crystallographic structures of the grown materials are the main factors those prominently affect the exhibited properties [2–4]. Moreover, the practical devices are mostly vulnerable to various environmental conditions i.e., temperature, pressure etc., and this fact also invites investigations to reveal the impact of such varying parameters on the illustrated structural parameters to know in advance the corresponding physical properties. For example, $MAPbI_3$ (MA = methyl ammonium) perovskite has been demonstrated to exhibit cubic to orthorhombic transition at 2.7 GPa, and beyond 4.7 GPa, crystalline and amorphous contributions become separated, indicating the possibilities to tune the material parameters [5]. Similarly, Noor et al. [6], have illustrated pressure induced tuning of the optical band gap nature of $CaTiO_3$perovskite from indirect to direct to vary the optical and thermoelectric parameters. Similarly, a mixed $PrAlO_3$–$SrTiO_3$ system of two binaries has been illustrated to exhibit a rhombohedral to cubic phase transition at 930 K that is found much lower than 1770 K (for the perovskite $PrAlO_3$) [7].

In addition, the research interests for finding the efficient devices not only involve optimizations of the existing materials but also include the efforts to look for the novel or very less explored materials. Sometimes, even new phases are required to be stabilized, which in fact do not exist in nature, e.g., the non-equilibrium growth techniques are designed to stabilize the naturally unstable phases. The hexagonal Si and Ge have been reported to be stabilized, which show possibilities to realize novel properties from these well understood cubic semiconductors [8,9]. Hence, similar materials stabilizing in two different crystallographic structures show attractive technological applications. Similarly, it has been already suggested that surface stabilization for an unstable phase and the vice versa are possible [10].

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In the present study, we investigate the very less explored $BaGeO_3$ perovskite, which exhibits low and high temperature hexagonal (pseudowollastonite-type)and orthorhombic (pyroxene-type) structures, respectively, and stabilized structures has been reported highly sensitive to the additives applied during the growth [11–14]. A low temperature monoclinic phase of $BaGeO_3$ has been also reported [15]. Owing to the simplicity, the cubic structures are considered highly demanding for the device applications. These properties of $BaGeO_3$ in stable cubic perovskite, till now have not been studied to our knowledge. This study is therefore believed to be fruitful in the formation optical and thermoelectric devices based on $BaGeO_3$. The cubic phase of GaN, InN, AlN are being investigated because of their capabilities to overcome the polarization effects those limit the optoelectronic devices applications [16]. Therefore, motivated from the technological significance of the cubic phase and scarcity of the literature about $BaGeO_3$, we have investigated the electronic structure and optical properties exhibited by the cubic phase under the influence of applied pressure. Moreover, the pressured induced tuning of the band gap magnitude and nature (indirect to direct) inspires us to explore the corresponding thermoelectric properties as well.

2. Method of calculations

In the present article, cubic structure of $BaGeO_3$ with space group 221-Pm3 m (see Fig. 1(a)) has been relaxed to minimize the forces using PBEsol approximation. The fully relaxed structure is optimized (see Fig. 1(b)) for extracting the ground state parameters, such as lattice constant, bulk modulus and the ground state energy. The self-consistent field is applied for converging the total energy, and PBEsol + TB-mBJ potential [17,18] is employed for executing the precise electronic and optical calculations. The TB-mBJ potential determines comparatively improved band gap compared with that by local density approximation (LDA), PBEsol [17], generalized gradient approximation (GGA) [19], etc. In TB-mBJ scheme [18], Trans and Blaha have used average lattice constants in LDA, GGA and revised the convergence parameter. The mathematical expressions for mBJ potential and convergence parameter are given as Eq. (1) and Eq. (2), respectively.

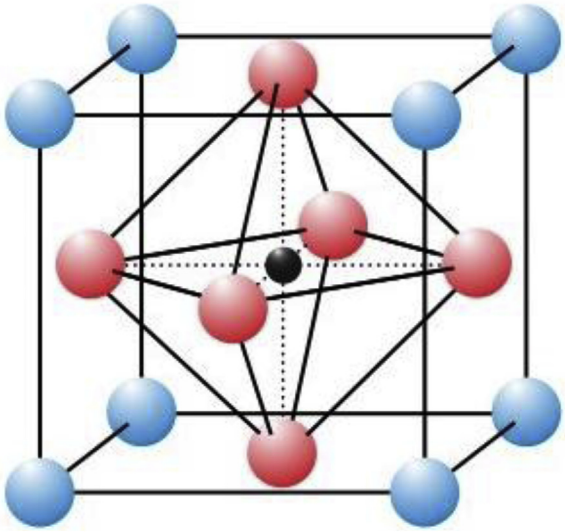

Fig. 1a. the structure of BaGeO3 by using xcrysden (O is pink, Ba is black, Ge is blue).

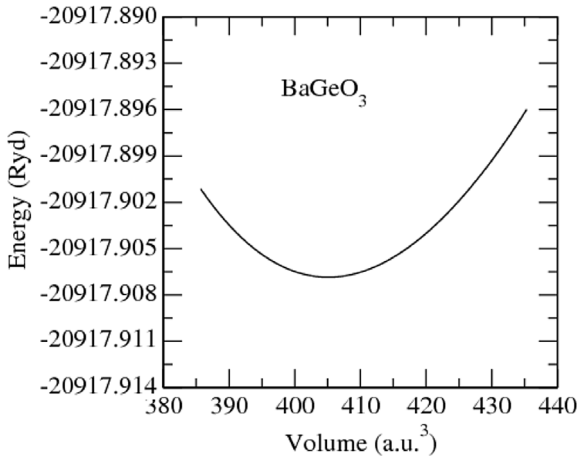

Fig. 1b. The optimized plot energy verse volume at pressure 0 GPa.

$$V_{x,\sigma}^{mBJ}(r) = cV_{x,\sigma}^{BR}(r) + (3c-2)\frac{1}{\pi}\frac{\sqrt{5}}{12}\frac{\sqrt{2t_\sigma(r)}}{\rho_\sigma(r)} \quad (1)$$

$$c = \alpha + \left(\beta\frac{1}{V_{cell}}\int d^3r\frac{|\nabla\rho(r)|}{\rho(r)}\right)^{1/2} \quad (2)$$

Here, $\rho_\sigma(r)$, $t_\sigma(r)$ and $V_{x,\sigma}^{mBR}(r)$ are the density of states, kinetic energy density and modified form of Becke-Roussel potential (mBR), respectively. The α and β are adjusted into Wien2k code [20] as $\alpha = -0.012$ and $\beta = 1.023$ $Bohr^{1/2}$. In Wien2k code, FP-LAPW is implemented in which the potential inside the muffin-tin and interstitial regions is evaluated to simplify the calculations. The parameters $R_{MT}\times k_{max}$(controls basis vector size), G_{max} and l_{max}(-angular momentum vector) are taken as 8, 12 and 10, respectively. For best convergence, a k-mesh of order $10\times10\times10$ is used inside the irreducible first Brillion zone. The self-consistent iterations have been stopped as the energy difference between the iterations reduces to 0.0001 Ry.

For calculating the thermoelectric parameters, the electronic structures computed by applying TB-mBJ potential are inserted in BoltzTraP code [21]. The electrical conductivity and See-beck coefficient are calculated by using the following equations.

$$\sigma_{\alpha\beta}(\alpha,\mu) = \frac{1}{\Omega}\int\sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right]d\varepsilon \quad (3)$$

$$S_{\alpha\beta}(T,\mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T,\mu)}\int\sigma_{\alpha\beta}(\varepsilon)(\varepsilon-\mu)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right]d\varepsilon \quad (4)$$

Where N is the number of electrons, τ is the relaxation time, μ is the chemical potential,$f_0$isFermi–Dirac distribution function,

In terms of equations (3) and (4), energy project transport distribution function $\sigma_{\alpha\beta}(\varepsilon)$ defined as

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N}\sum_{i,k}\sigma_{\alpha\beta}(i,k)\frac{\delta(\varepsilon-\varepsilon_{i,k})}{\delta(\varepsilon)} \quad (5)$$

$\nu_\alpha(i,k)$ is the component of group velocity.

3. Results and discussion

The analysis of the impact of external pressure on various physical properties of the investigated perovskite is performed by

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