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First Principles study of Electronic Properties of $BaPbO_3$ Simple Perovskite

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Abstract

The structural electronic and magnetic properties of simple perovskite $BaPbO_3$ is carried out using the density functional theory calculation method. The structural parameters define the cubic phase as the stable phase group with space group of Pm-3m (221). The optimized lattice parameter comes out as 4.29 Å. The band profile simulation define the spin-polarized character of bands with semiconducting bands in minority spin channel, while as the metallic character in the majority channel. The bands along the Fermi level comes out from the hybridization between the O-Pb below the fermi level, while as Ba-Pb hybridizations leads to occupation of bands above the Fermi level.

Keywords: Density Functional theory; Perovskites; Electronic structure.

1. Introduction

Electronic structure plays an important role in defining the materials applications for future technologies like as spintronics, magneto electronics, tunnel junctions, spin-caloritronics etc. [1]. The behaviors of the materials for the desired kind of application presides on its electron behavior along the Fermi level. The material science simulation has been emerged as an important field in this category, because they can easily avail the information about the possible outcomes of the properties prior to their synthesis. Furthermore, in order to hunt for the material candidate for the desired application, this simulation technique helps us in determining the path of the quest. Perovskites [2-7] for the beginning has proved to be an emerging field in the spintronics as well, as the magneto electronics due to their easy preparation and manipulation. They have been used in solar cells, as they are less toxic in nature from the conventional lead based solar cells [8]. The motivation for current research has been got from their astonished band profile along the Fermi level. The whole manuscript is divided into three sections. Sections I defines the method of computation of the various properties, section II is for the discussion of the various results, section III gives the conclusion of the various reported results.

2. Computational Method

Using the basic density functional theory, we have established the ground state properties BaPbO3 simple perovskite, under the full potential linearized augmented plane wave method [9]. The correlation effects are adjusted using the generalized gradient approximation under Perdew-Burke-Erenzof approximation [10]. The method is based on the fact of dividing the whole crystal lattice

into two regions as muffin tin spheres and the remaining as interstitials. The radius for the muffin tin spheres of Ba, Pb and O are 2.11, 2.3, 1.7 a.u., respectively. The calculations are guaranteed through the convergence criteria for charge and energy as 10^{-4}e/a.u. and 10^{-4} Ry, respectively. For Brillouin zone sampling, we use a dense mesh of 2000 *k*-points to exactly simulate the nature of electrons in the First Brillouin zone.

3. Results and Discussion

The theory behind the occurrence of various results are discussed under various headings as

3.1 Structural and electronic properties

The present materials exhibit the perovskite type structure with a chemical formula ABO_3, wherethe oxygen atoms form a regular octahedron surrounding the B atom, as also proved experimentally [11]. The crystal structure is shown in Fig. 1, which belongs to the space group Pm-3m (221).

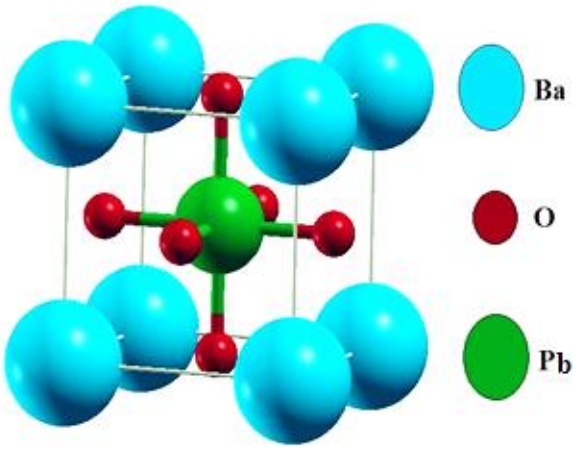

Fig. 1. Crystal structure of $BaPbO_3$.

For enquiring about the ground state properties, we have investigated the structural optimization in the magnetic configuration, with variation of crystal lattice energy versus volume shown in Fig. 2. The data predicts the ferromagnetic state as the optimized ground state with perfect half-metallic nature.

Next, we predict its band structure character along the Fermi level, where in one spin channel a intercrossing of bands of conduction band and valence band occurs. This is generally shown by metallic systems. The other spin channel show a perfect band gap, depicting its semiconducting nature. The two type of bands in two spin orientations of the compounds categories it in the half-metallic family, which have a 100% spin polarization along the Fermi level. The band structure is shown in Fig. 2 below

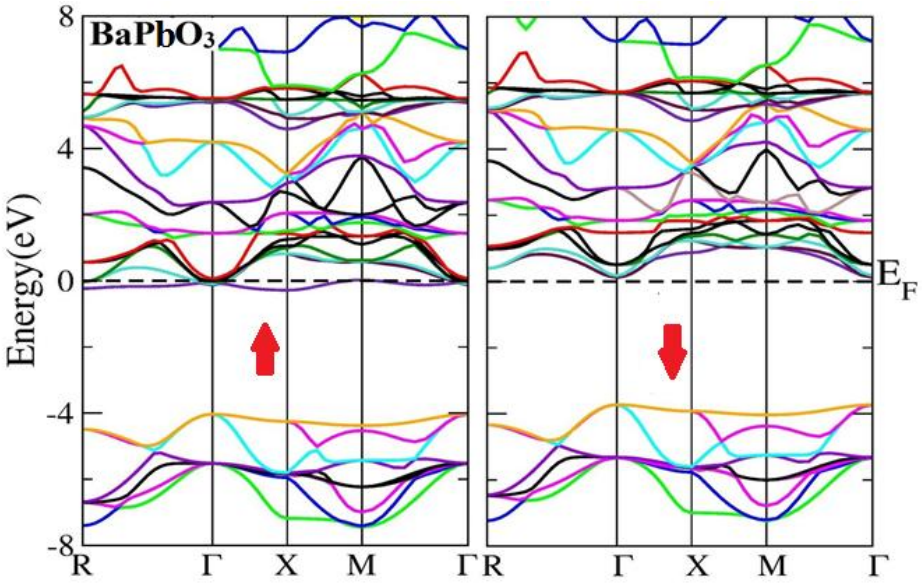

Fig. 2. Band structure along the high symmetry points of $BaPbO_3$ simple perovskite.

From the band structure distribution plot, the sharing of electrons between Pb atom and O is seen and thus it reveals the covalent nature of the bond between them. The electronic charge sharing of the Ba and Pb convey that there is ionic nature of bonds. The shifting of the bands in the spin down channel is because of the covalent nature of bonding the Ba-Pb atoms.

3.2Conclusion

We successfully utilized the FPLAPW method, to study the electronic structure of the simple $BaPbO_3$ perovskite. The optimization of crystal structure show, ferromagnetic state as the stable phase. While discussing the band structure, a perfect half-metallic character is seen where one spin channel show a metallic nature while as the other spin as semiconducting. This shows the 100% spin polarization of the electrons along the Fermi level. Further, the hybridization between the constituent atoms is responsible for occurrence of such behavior along the Fermi level.

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