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Study of Electronic Properties of Fluoride Perovskite $BaLiF_3$ Using FP-LAPW Method

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Abstract: We have studied the electronic properties of cubical perovskite $BaLiF_3$, by using the first principles method within the full potential linearized augmented plane wave (FP-LAPW). Here the exchange correlation effects are included through the generalized gradient approximation (GGA) exchange potential on the basis of density functional theory (DFT). The calculated structural properties such as equilibrium lattice constant, the bulk modulus and its pressure derivative are in agreement with the published results of other authors. We have found that the band gap of $BaLiF_3$ is 6.8 eV which indicates that the insulating behavior perovskite $BaLiF_3$.

Key words: DFT, GGA, FP-LAPW, DOS (density of state), band structure.

1. Introduction

The ternary fluoro-perovskite like $BaLiF_3$ has great potential for a variety of device applications in optical, ferroelectric, antiferromagnetic systems due to their wide band gaps [1]. It is always an advantage to know the physical and electronic properties of such order to understand their possible applications. Perovskites are well known for their applications in different fields of science and technology because of their wide range of electro-optic, mechanical, semiconducting and insulating behavior. $BaLiF_3$ is used as a vacuum-ultraviolet-transparent material for lenses in optical lithography steppers in electro-optical applications [2-3]. This shows photo-luminescence properties when it is doped with lanthanide ions . It is therefore desirable for scintillators and radiation dosimeters when it is doped approximately [4].

In this paper, we will do the theoretical investigations of the structural and electronic properties of fluoride type perovskite $BaLiF_3$. In this work, for exchange correlation potentials, the GGA (generalized gradient approximation) is employed which is implemented in WIEN2k code [5].

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2. Computational Details

The unit cell of fluoro-perovskite $BaLiF_3$ with space group (P m-3 m) contains three atoms that form the cubical structure. The atoms of $BaLiF_3$ are located at the Wyckoff positions Ba (0, 0, 0), Li (0.5, 0.5, 0.5), F (0, 0.5, 0.5) [6] to form the crystal structure. For volume optimization of $BaLiF_3$, we have used at first the calculated lattice constant a = 4.04Å [7] followed by the theoretically obtained optimized lattice constant to study the DOS (density of state) and band energy of $BaLiF_3$. Non spherical contributions to the charge density and potential within the MT (muffin tin) spheres are considered andthe cut-off parameter is $R_{MT} \times K_{max} = 7$ where K_{max} is the maximum value of the reciprocal lattice vector in the plane wave expansion and R_{MT} is the smallest atomic sphere radii of all atomic spheres. In the interstitial region, the charge density and potential are expanded as a Fourier series with wave vectors up to G_{max} =12 $a{\cdot}u^{-1}$. The number of k-points used in the irreducible part of the Brillouin zone is 1,000. The criterion for the convergence of the self-consistent density functional theory (DFT) calculation is 0.0001 Ry in total energy.

However the core states are treated relativistically, the semi-core states are treated semi-relativistically by ignoring the SO (spin-orbit) coupling.

3. Results and Discussions

3.1 DOS and Band Structures

Fig. 1 shows the plot of total DOS in the case of $BaLiF_3$ and individual atoms Ba, Li and F respectively. We have found a maximum peak at -1.11 eV below the Fermi level due to the main contribution by F atom and very less contribution of Ba atom. Similarly we have observed other narrow peaks from -2.5 eV to 0 eV below the Fermi level. In the conduction region above the Fermi level, we have found a maximum peak at 13.36 eV due to the main contribution by Ba atom.

From the partial DOS plots of Ba atom as shown in Fig. 2, we have found a very small peak in the valence band due to the contributions of only *p* and *d* state electrons of Ba atom. However, in the conduction band, *d* state electron contributes mainly up to 11.25 eV and *f* state electron contributes above 11.25 eV. In the conduction band in the Fig. 2, we have observed a maximum peak at 13.36 eV due to the main contribution ofBa-*f*state electrons.

We have observed very small peaks in the range of -2.5 eV to 0 eV below Fermi level for the partial DOS plots of Li atom as shown in Fig. 3. In the valence band, the main contributions are by *s*, *p* and *d* state electrons. However, in the conduction band, we have observed a sharp narrow peak at 17.06 due to the hybridization of *s* and *d* state electrons and other small peaks are observed due to the contribution by *s*, *p* and *d* state electrons of Li atom.

Fig. 4 shows the plot of total and partial DOS of F atom. In the valence band, there is a sharp peak occurring at -1.11 eV and other small peaks are observed from -2.5 ev to 0 eV below the Fermi level due to the contribution of *p* state electrons and virtually with no contribution by *s* and *d* state electrons. However, in the conduction band small peaks occur due to the *p* and *d* state electrons.

The calculated electronic band structure for fluoro-perovskites $BaLiF_3$ along the high-symmetry directions of the Brillouin zone is shown in Fig. 5. In the valence band (Fig. 5), the lowest lying band has been found to occur at 9.0 eV below Fermi level due to the core state electrons of Ba, Li and F atoms. We also observe from Fig. 5 that the maximum band energy occurs at the Fermi level at the symmetry point R.In the conduction band, minimum in energy occurs at 6.8 eV above the Fermi level at the point symmetry Γ and from this plot in Fig. 5, we find that it is an indirect type of transition which takes place along R-Γ symmetry directions.

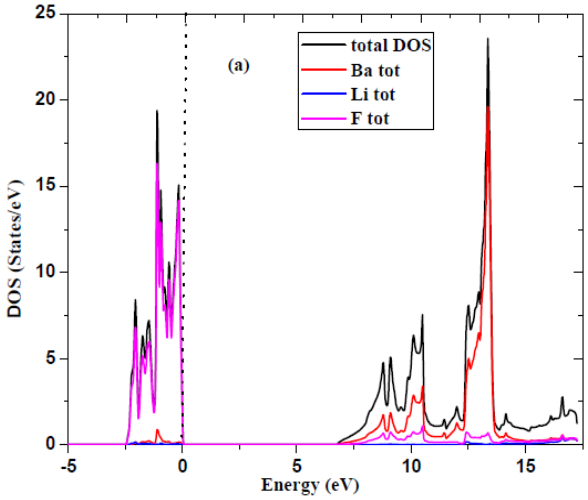

Fig. 1 Total DOS of $BaLiF_3$, Ba, Li and F.

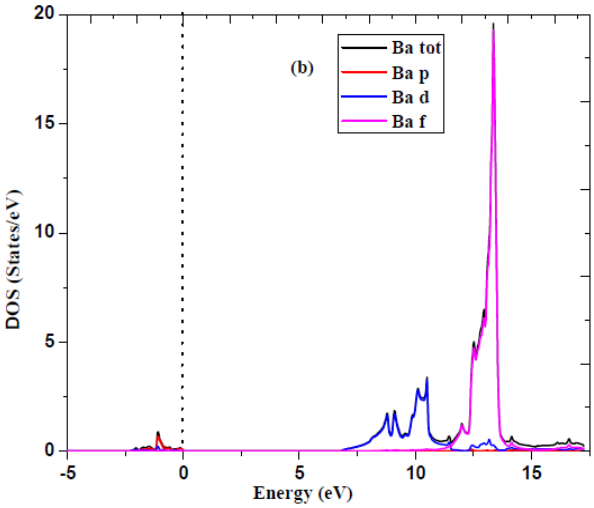

Fig. 2 Total and partial DOS of Ba.

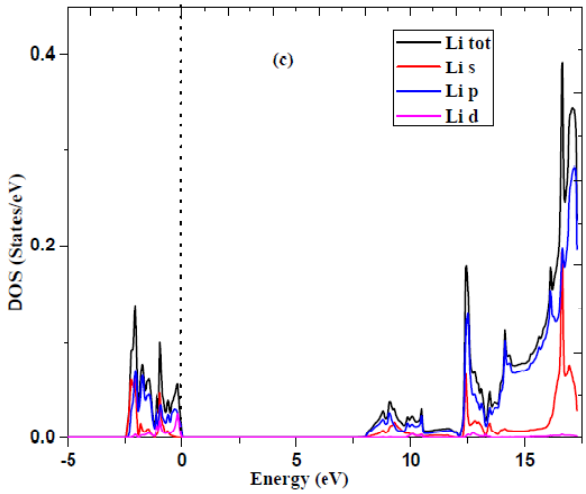

Fig. 3 Total and partial DOS of Li.

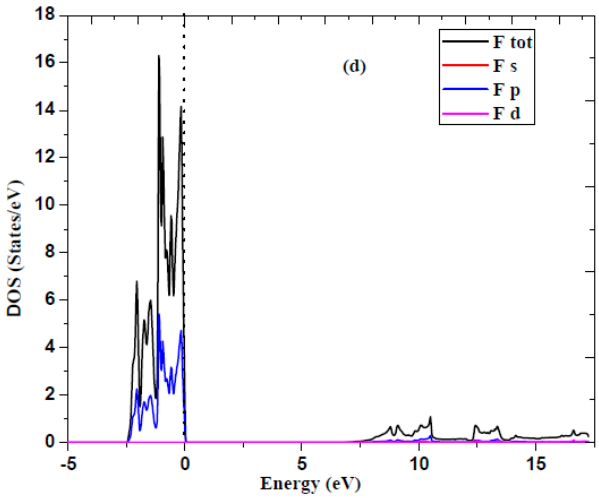

Fig. 4 Total and partial DOS of F.

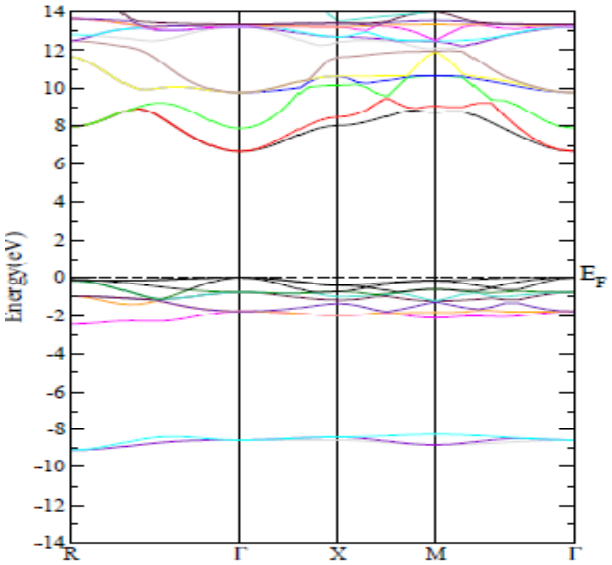

Fig. 5 Electronic band structure of $BaLiF_3$.

4. Conclusions

From the total DOS plots of $BaLiF_3$ as given in Fig. 1, we find that maxima in peaks in the valence region are due to only F atom. This is also evident from the partial DOS plots of Ba, Li and F atoms as given in Figs. 2-4 respectively. From Fig. 4, we find that the maxima in peaks are due to *p* state electrons of F atom in the valence region. We have found a maximum peak at 13.36 eV due to the main contribution of Ba atom in the conduction region that is shown in Fig. 1. From the plot of partial DOS of Ba, Li and F in Figs. 2-4 respectively, we have found that the maxima peaks are observed due to the main contribution of *p* and *f* state electrons of Ba atom. In Fig. 5, we have found from our study that the band gap of $BaLiF_3$ is 6.8 eV which is large and hence $BaLiF_3$ is an insulator.

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