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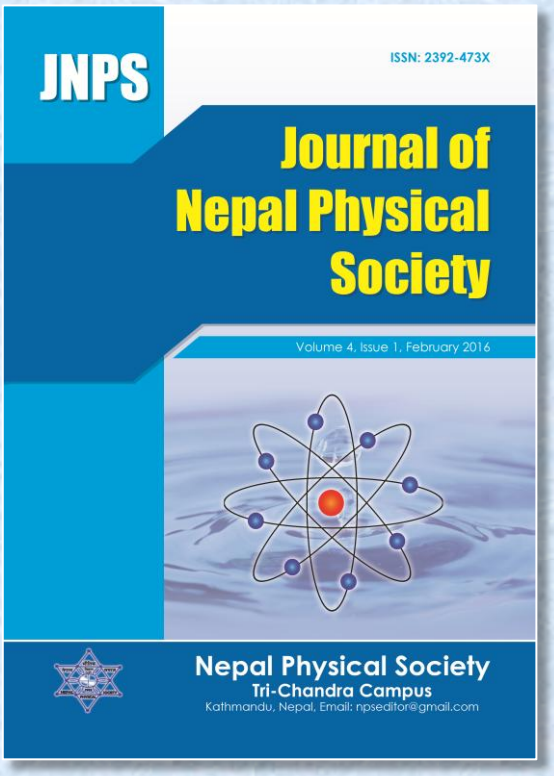
Journal of Nepal Physical Society

Volume 4, Issue 1, February 2017

ISSN: 2392-473X



JNPS, **4** (1), 23-26 (2017)

Published by:

Nepal Physical Society

P.O. Box : 2934

Tri-Chandra Campus

Kathmandu, Nepal

Email: npseditor@gmail.com

JNPS ***4*** *(1), 23-26 (2017)*
ISSN: 2392-473X

Research Article

Study of DOS and Band Structures of Fluoride Perovskite $RbMgF_3$ using FP-LAPW Method

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ABSTRACT

Materials with perovskite crystal structure represent an interesting class of materials which, due to their simple structures and unique electronic and dielectric properties, has a great potential for applications in various technological fields, such as mechanical, electro-optic and semiconducting. We perform calculation of density of states (DOS) and band structures for fluoride perovskite like $RbMgF_3$ using the full potential linearized augmented plane wave (FP-LAPW) method. To calculate the electronic properties, the exchange-correlation potential has been applied by using the generalized gradient approximation (GGA). From the calculation the lattice parameter of $RbMgF_3$ found to be 4.139 Å. The band gap of $RbMgF_3$ through the electron energy bands by GGA is obtained as 7.6 eV showing insulating behavior which is in good agreement with the available experimental data as well as previously calculated results.

Keywords: DFT, GGA, FP-LAPW, DOS, Band Structure.

INTRODUCTION

The ternary fluoroperovskite like $RbMgF_3$ has great potential for a variety of device applications in optical, ferroelectric, antiferromagnetic systems due to their wide band gaps (Riadh *et al.*, 2004; Zhang *et al.*, 2008). 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. $RbCaF_3$ is a technologically important fluoroperovskite, which finds application as a vacuum ultraviolet transparent material for lenses in optical lithography steppers in electro optical applications (Nishimatsu *et al.*, 2003; Horsch and Paus, 1986; Fukuda *et al.*, 2001). Neupane and Thapa (2016) have found the band gap of $RbCaF_3$ as 6.8 eV and 7.2 eV for $KMgF_3$ from the theoretical study which shows the insulating behavior. In the last decade, experimental and theoretical investigations have been done to the study of perovskite-type fluorides and perovskite-type hydride (Lamichhane *et al.*, 2015). In this communication, we will present a theoretical study of the electronic properties of $RbMgF_3$ using density functional theory (DFT) in which GGA is applied. The calculations of DOS and energy band have been done by using the full potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT) as implemented in the WIEN2K code (Blaha *et al.*, 2012). The generalized gradient approximation (GGA) types of exchange-correlation potential are used (Perdew *et al.*, 1996) throughout the calculation. The main purpose of the present study is to calculate the DOS and energy bands of the fluoride system.

CRYSTAL STRUCTURE AND COMPUTATIONAL DETAILS

The unit cell of fluoroperovskite $RbMgF_3$ with space group (Pm-3m) each contains three atoms that form the cubical structure. The atoms of $RbMgF_3$ are located at the Wyckoff positions Rb(0.0,0.0,0.0), Mg(0.5,0.5,0.5), F1(0.0,0.5,0.5), F2(0.5,0.0,0.5) and F3(0.5,0.5,0.0) (Gregory, 2004) to form the crystal structure as shown in figure 1.

For volume optimization of $KMgF_3$, we have used the calculated lattice constant a =3.992 Å (Syrotyuk and Shved, 2015) and the optimized volume vs energy curve is shown in figure 2.

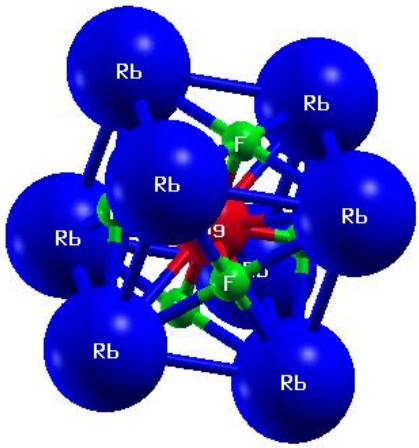

Fig.1. Crystal structure of $RbMgF_3$.

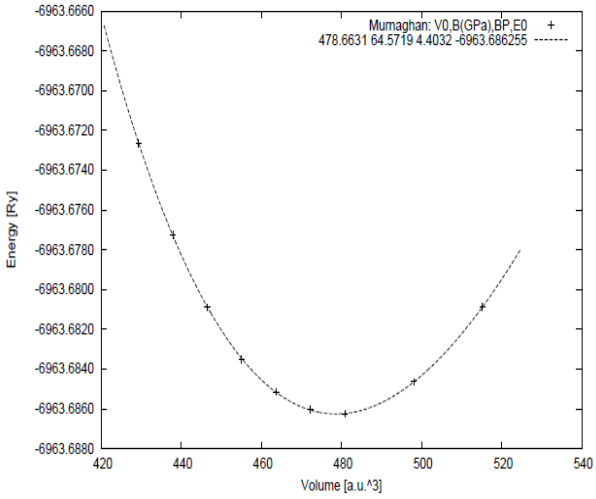

Fig.2. Volume optimization curve.

The optimized lattice constant, pressure, pressure derivative and total energy are found as 4.1395 Å, 64.5719GPa, 4.4032 and -6963.69 Ry respectively. This optimized lattice constant is used to study the density of state (DOS) and band energy of $RbMgF_3$ by using the full potential linearized augmented plane wave (FP-LAPW) method of KS-DFT (Kohn and Sham, 1965) as implemented in the WIEN2K code. We used here GGA to describe the electron exchange and correlation potential. Non spherical contributions to the charge density and potential within the muffin tin (MT) spheres are considered and the 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 $a.u^{-1}$. The number of k-points used in the irreducible part of the Brillouin zone is 1000. The criterion for the convergence of the self-consistent 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 spin-orbit (SO) coupling.

RESULTS AND DISCUSSION

Crystal structure

The variation in the total energy as a function of volume is shown in figure 2. The calculated value of the equilibrium lattice constant 'a' is found as 4.139 Å. The energy versus volume data was fitted to a Murnaghan equation of state (Kohn and Sham, 1965) to obtain the bulk modulus (B) and its first pressure derivative (B'). Our calculated values of lattice constant, B, and B' are compared with previous experimental and theoretical results which are shown in table 1. We note that the result of the lattice constant obtained is slightly higher than the calculated values (Syrotyuk and Shved, 2015).

Table 1: Comparison of Lattice Constant and Bulk Modulus

	Lattice Constant a (in Å)	Bulk Modulus B (in GPa)	Pressure Derivative B'
Present study	4.139	64.572	4.403
Other, GGA	3.992 (Syrotyuk and Shved, 2015)	62.485 (Syrotyuk and Shved, 2015)	4.716 (Syrotyuk and Shved, 2015)

Density of states (DOS)

Fig.3 shows the total DOS of RbMgF3 and individual atoms Rb, Mg and F respectively. We find the maximum peak at 0.98 eV and another peak at 6.22 eV below the Fermi level in the valence band due to the contribution of F and Rb atoms respectively. We have observed the maximum peak at 17.68 eV and other small peaks from 10.49 eV to 18.68 eV in the conduction band which are due to the contribution of atoms Rb, F and Mg.

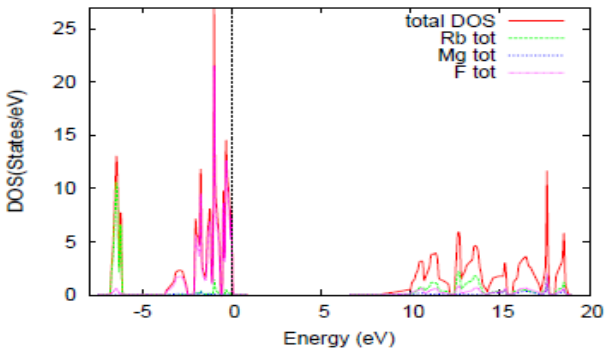

Fig.3. Plot of total DOS for $RbMgF_3$, Rb, Mg and F(Fermi energy is set at zero)

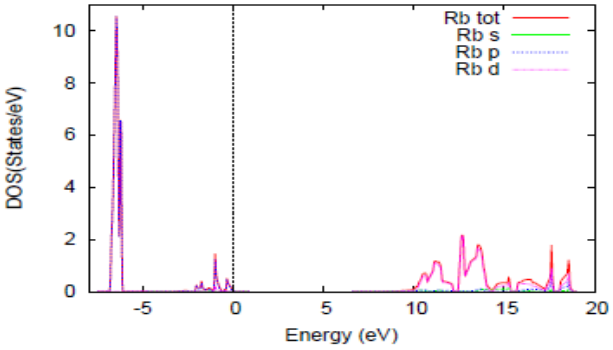

Fig.4. Plot of total and partial DOS of Rb (Fermi energy is set at zero).

From the partial DOS plots of Rb atom as shown in figure 4, we find the maximum peak at 6.22 eV due to the contribution *p* state electrons in the valence band and small peaks are occuring from 10.49 eV to 18.66 eV in the conduction band due to the main contribution of *d* state electrons.

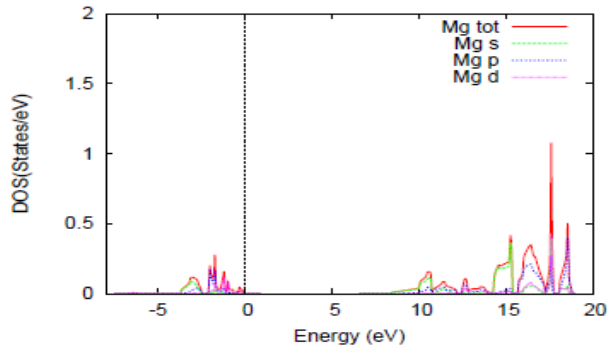

Fig. 5. Plot of total and partial DOS of Mg (Fermi energy is set at zero)

From the partial DOS of plots of Mg atom as shown in figure 5, we find small peaks from 0.43 eV to 2.93 eV due to the contribution of *s*, *p* and *d* state electrons below the Fermi level in the valence band. However, in the conduction band, *p* state electron contributes to the occurrence of peak at 18.66 eV and small peaks are observed from10.49eV to 18.66 eV due to the contribution of *s*, *p* and *d* state electrons above the Fermi level which is the evident from figure 5.

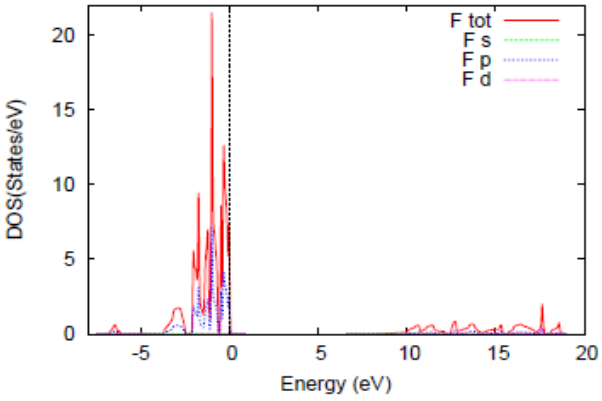

Fig.6. Plot of total and partial DOS of F(Fermi energy is set at zero)

Figure 6 shows the plot of total and partial DOS of F. In the valence band, there is a sharp peak occurring at 0.98 eV and small peaks are observed from 0.49 eV and 3.0 eV below the Fermi level due to the *p* state electrons and virtually with no contribution by *s* and *d* state electrons. However, in the conduction band, there are very small peaks occur from 10.49 eV to 18.66 eV due to the *s*, *p* and *d* state electrons.

Band structures

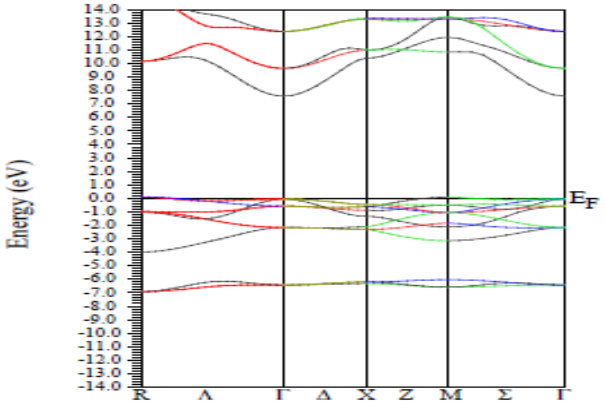

Fig.7. Electronic band structure of $RbMgF_3$ along the high-symmetry directions of the first Brillouin zone.

In the valence band, the lowest lying band has been found to occur at 6.9 eV below the Fermi level due

to the core state electrons of Rb, Mg and F atoms and we also observe from figure 7 that the maximum band energy occurs at the Fermi level at the point R. In the conduction band, minimum in energy occurs at 7.6 eV above the Fermi level at the point symmetry Γ and from this plot in figure7, we find that it is an indirect type of transition which takes place along R - Γ symmetry directions. The calculated value of indirect band gap is 7.6 eV which is 0.15 eV higher than that obtained by Syrotyuk and Shved (2015) for $RbMgF_3$.

CONCLUSIONS

From the volume optimization in Figure 2, we have found the optimized lattice constant; pressure, pressure derivative and total energy are as 4.1395 Å, 64.5719GPa, 4.4032 and -6963.69 Ry respectively. From the total DOS plots of $RbMgF_3$ as given in figure 3, we find that maxima in peaks in the valence region are due to F and Rb atoms. This is also evident from the partial DOS plots of Rb and F atoms as given in figure 4 and figure 6 respectively. We find here also that the maxima in peak are due to *p*-state electrons of Rb and F atoms. The peak heights in partial DOS due to electrons from Mg atom in the valence region are negligible. Similarly in the conduction region, it is only *d*-state electrons of Rb (figure 6) which is contributing to the maxima in the total DOS of $RbMgF_3$.We have found from our study (figure 7) that the band gap of $RbMgF_3$ is 7.6 eV which is large and hence $RbMgF_3$ is an insulator.

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