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Investigation of the structural, electronic and optical properties of the cubic $RbMF_3$ perovskites (M = Be, Mg, Ca, Sr and Ba) using modified Becke-Johnson exchange potential

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HIGHLIGHTS

- Closer estimate of the band-gaps of $RbMF_3$ with experimental results using GGA and mBJ results predicting them to be absorption devices and substrates for thin film growth.
- The $RbMF_3$ were also found to be potential candidate for in absorption devices in UV-region which were correlated to their calculated optical properties.
- The materials are transparent, so may be used as substrates for thin film growth, for the optoelectric applications.

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ABSTRACT

The structural, electronic and optical properties of the cubic $RbMF_3$ perovskites (M = Be, Mg, Ca, Sr, Ba) have been investigated using the full-potential linearized augmented plane wave (FP-LAPW) method. The exchange and correlation potential was applied using the generalized gradient approximation for calculating the structural properties In addition, the modified Becke-Johnson (TB-mBJ) potential was used for calculating the electronic and optical properties. It was found that the lattice constant increases while the bulk modulus decreases with the change of cation (M) in going from Be to Ba in the $RbMF_3$ perovskites (M = Be, Mg, Ca, Sr, Ba). The reflectivity and absorption properties were also studied using the mBJ method to understand the inter-band transitions and their possible applications in absorption devices in the UV-region.

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1. Introduction

Cubic fluoro-perovskites (AMF_3) have attracted attention in recent time due to their simple crystal structure with important physical properties. Nishimatsu *et al.* [1] have carried out first-principles band structure studies on various AMF_3 using the local density approximation (LDA) with the pseudopotential method [2]. The authors established that these materials may be used in the making of lenses in the optical lithography steppers where the studies were carried out on the use of the solid solution $LiBaCaSrF_3$ on $LiSrF_3$ for the manufacture of light emitting diode [3]. San-Dong Guo and Bang-Gui Liu have studied the electronic and optical properties of $SrTiO_3$ and $BaTiO_3$ at room temperature using Tran and Blaha's modified Becke and Johnson exchange potential to report a comparatively better than previous first-principles results with respect to experimental values [4]. Bonding nature as well as structural, electronic, chemical bonding and optical properties of

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$KCaF_3$, $RbCaF_3$, and $CsCaF_3$ were studied using FP-LAPW based method within the generalized gradient approximations to report wide direct band-gap and optical properties to predict their usefulness in the optoelectronic and optics technology [5]. Several rare earth based system have been studied using FP-LAPW GGA as well as GGA + U approximations in the past to explain the optical properties [6–9]. But system which do not have correlated electrons mainly semiconductors and insulators were found more suited for the recent modified Becke–Johnson potential (TB-mBJ) approximation. It was not only preferable in terms of results but also from the point of view of computational cost. Murtaza *et al.* [10] have used the modified Becke–Johnson potential (TB-mBJ) to calculate the electronic and optical properties to report a decrease in bulk modulus increase in lattice parameter. Solid solutions LiKBaMgF_3 on LiBaF_3 had been done for the purpose of their application in the deep-ultraviolet region [11]. Structural phase transition in $RbCdF_3$ was carried out by Studzinski [12] experimentally. The cubic fluoro perovskites $ACaF_3$ (A = K, Rb, Cs) have been investigated as the potentially active materials for core-valence luminescence (CVL) [13]. The important parameters for CVL are: (1) the electron energy gap between the core *p*-states of K, Rb, and Cs, and the p-states of F forming the top of the valence band; (2) the width of the upper part of the valence band; (3) the band gap E_g studies further renewed the interest in these systems using first-principles studies in the recent past. Babu *et al.* [14], Mousa *et al.* [15] and Zhen-Li *et al.* [16] have carried out studies on cubic perovskites with emphasis on their optical properties using the full-potential linearized augmented plane wave (FP-LAPW) method, with the generalized gradient approximation (GGA) and LDA approaches. The temperature dependence of the structural parameters and structural phase transition of $RbCaF_3$ were studied to suggest an order-disorder character of the 193 K and 50 K phase transitions [17]. However, the electronic properties of the cubic perovskites $RbMF_3$ have not been obtained using the TB-mBJ [18] based approximation and the optical properties are also not investigated previously. It thus motivated us to perform these studies using the FP-LAPW method, based on the density functional theory (DFT), as mBJ based results were expected to generate important optical properties addressing the band-gaps and transitions more precisely. Thus, we have investigated the optical properties and supplement the band-structure results to explain the inter-band transitions along with the comparisons with the previous results.

2. Crystal structures and computational details

The inter-metallic compound $RbMF_3$ (where M = Be, Mg, Ca, Sr and Ba) with space group, Pm3 m crystallizes in a cubic structure as shown in Fig. 1. The Rb, M and F atoms are positioned at the 1a (0, 0, 0), 1b (0.5, 0.5, 0.5) and 3c (0, 0.5, 0.5) sites of the Wyckoff coordinates, respectively [19]. DFT is a renowned quantum mechanical approach for the many-body problems [20]. In this work, the DFT-based FP-LAPW method as implemented in the Wien2k code [21] has been applied to perform the first-principles total energy calculations, which is one of the most efficient methods for the calculation of the ground state properties of materials [22,23]. The unit cell was divided into (I) non-overlapping atomic spheres (which are centered at the atomic sites) and (II) an interstitial region. In these two types of regions, different basis sets are used. To take into account of the exchange and correlation effects, GGA as parametrized by Perdew *et al.* [24] has been used. We have chosen the muffin tin (MT) radii for the Rb, Be, and F atoms to be 2.43 a.u., 1.59 a.u. and 1.94 a. u, respectively, in the $RbBeF_3$ compound. In addition, for the following compounds, the MT radii used for the Rb, Mg and F atoms are at 2.50 a.u., 1.77 a.u. and 1.86 a.u, respectively, in the $RbMgF_3$ compound, for the Rb, Ca and F atoms, the MT radii are at 2.50 a.u., 1.98 a.u. and 2.08 a.u, respectively, in the $RbCaF_3$ compound, for the Rb, Sr and F atoms, the MT radii are at 2.50 a.u., 2.13 a.u. and 2.23 a.u., respectively, in the $RbSrF_3$ compound and for the Rb, Ba and F atoms, the MT radii are at 2.50 a.u., 2.20 a.u. and 2.31a.u., respectively, in the $RbBaF_3$ compound. Integrations in the reciprocal space were performed using 1000 spatial *k*-points in the irreducible wedge of the Brillouin zone (BZ). The value for the convergence parameters is taken to be $R_{MT}\times K_{MAX} = 7$ which controls the size of the basis sets consisting of the plane waves. G_{MAX} is chosen to be $12(a.u.)^{-1}$ for consistency and convergence is achieved

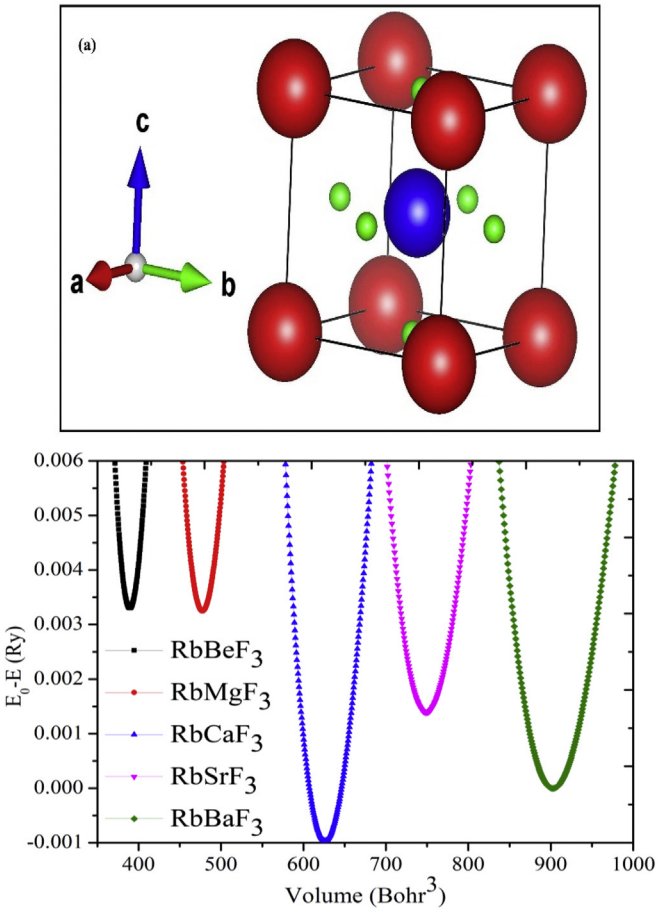

Fig. 1. (a) Crystal structure for the $RbMF_3$ (M = Be, Mg, Ca, Sr, Ba) compounds where the red sphere represents the Rb atom; the blue sphere represents the Be, Mg, Ca, Sr and Ba atoms; while the green sphere represents the F atom. The volume optimization curves for the (b) $RbBeF_3$ $RbMgF_3$ $RbCaF_3$, $RbSrF_3$ and $RbBaF_3$ compounds. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Calculated results of the optimized parameters a_0, as compared to the lattice parameters a, bulk moduli (B) and Pressure derivatives (B_0') of the $RbMF_3$ (M = Be, Mg, Ca, Sr, Ba) compounds.

$RbMF_3$	a_0 (a.u)	a (a.u)	B_0 (G Pa)	B_0'
$RbBeF_3$	7.302	7.307 [31]	86.021	4.879
$RbMgF_3$	7.816	7.544 [31]	62.485	4.716
$RbCaF_3$	8.555	8.413 [31]	47.244	4.828
		8.413 [18]	50.400 [15] Expt.	5.100 [15] -GGA-WC
		8.419 [19]	46.600 [15] GGA-WC	4.400 [15] -GGA-PBE
			51.300 [15] GGA-PBE	0.300 [15] –LDA
			59.300 [15] LDA	
$RbSrF_3$	9.082	9.044 [31]	39.172	4.970
$RbBaF_3$	9.664	9.367 [31]	32.276	4.704

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