



Modeling structural, elastic, electronic and optical properties of ternary cubic barium based fluoroperovskites MBaF_3 ($\text{M} = \text{Ga}$ and In) compounds based on DFT

Jaffer Saddique^{a,***}, Mudasser Husain^{b,*}, Nasir Rahman^{c,**}, Rajwali Khan^c, Zulfiqar^d, Anwar Iqbal^e, Mohammad Sohail^c, Shaukat Ali Khattak^d, Saima Naz Khan^d, Abid Ali Khan^e, Ali H. Reshak^{f,g,h}, Aurangzeb Khan^{d,i}

^a College of Materials Science and Technology, Jiangsu Key Laboratory of Materials and Technology for Energy Conversion, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China

^b Department of Physics, Kohat University of Science & Technology, Kohat, 26000, Pakistan

^c Department of Physics, University of Lakki Marwat, Lakki Marwat, 28420, Khyber Pakhtunkhwa, Pakistan

^d Department of Physics, Abdul Wali Khan University, 23200, Mardan, Pakistan

^e Department of Chemical Sciences, University of Lakki Marwat, Lakki Marwat, 28420, Khyber Pakhtunkhwa, Pakistan

^f Physics Department, College of Science, University of Basrah, Basrah, Iraq

^g Department of Instrumentation and Control Engineering, Faculty of Mechanical Engineering, CTU in Prague, Technicka 4, Prague, 6 166 07, Czech Republic

^h Center of Excellence Geopolymer and Green Technology, University Malaysia Perlis, 01007, Kangar, Perlis, Malaysia

ⁱ University of Lakki Marwat, Lakki Marwat, 28420, Khyber Pakhtunkhwa, Pakistan

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ABSTRACT

This work presents in detail the Ab-initio computational research work on the structural, elastic, electronic, and optical properties of Perovskite-type (Halide-Perovskites) barium-based MBaF_3 ($\text{M} = \text{Ga}$ and In) compounds. The work is based on density functional theory (DFT) within WIEN2K. Structurally both GaBaF_3 and InBaF_3 based on optimization of Birch Murnaghan fit are found to be stable. The IRelast package for the calculations of elastic constants (ECs) is employed for the computation of elastic properties. Mechanically these compounds are identified to be ductile, hard to scratch, anisotropic, mechanically stable, and demonstrate strong resistance to plastic deformation. The precise modified Becke–Johnson (mBJ) potential is employed for electronic properties. Band structures of these compounds possess an insulating nature of direct wide energy band gap of 5 eV for GaBaF_3 and 5.1 eV for InBaF_3 from X-X symmetries points. To know the contribution of different electronic states to the band structures, the TDOS and PDOS i-e (total and partial density of states) are exploited. The insulating direct wide band gap energy nature presented a straightforward direction to study the optical properties of these compounds. The optical properties, of both the compounds, were studied deeply in the energy range from 0 eV to 40 eV. These compounds possess high absorption and optical conduction at high energy ranges. Both materials are transparent to incident photons at low energy ranges. We have concluded from the optical properties investigations that these compounds are suited for high-frequency UV device applications. To our deep knowledge, this is the first systematic theoretical computation of MBaF_3 ($\text{M} = \text{Ga}$ and In) with structural, elastic, electronic and optical, properties that have yet to be verified experimentally.

1. Introduction

Materials scientists are working hard to develop new Perovskites

compounds with improved properties. The fluoroperovskite structure is found in the majority of compounds with the general formula ABF_3 . The atomic arrangement in this structure was first discovered in the mineral

* Corresponding author.

** Corresponding author.

*** Corresponding author.

E-mail addresses: jaffer@nuaa.edu.cn (J. Saddique), mudasserhusain01@gmail.com (M. Husain), nasir@ulm.edu.pk (N. Rahman).

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CaTiO_3 , which is a perovskites. The A cation is coordinated with twelve Fluorine atoms in the perovskites structure, while the B cation is coordinated with six atoms of Fluorine. As a result, the A cation is usually slightly greater than the B cation. Fluoroperovskite compounds form a fascinating class of materials that have a mechanically stable crystal structure and exhibit good electronic behavior, ranging from semiconductors to insulators. Owing to their fundamental significance as a lens material in optical lithography, radiation dosimeters, scintillation materials, and the semiconductor industry, these compounds have gained a lot of attention in recent years [1–3]. Numerous researchers investigated different properties of cubic Perovskites compounds and the majority of cubic Perovskites compounds have been reported to be elastically anisotropic and mechanically stable [4–6]. ABF_3 compositions have applications in high-efficiency photovoltaic properties, energy storage for automobiles, devices, and lenses [7,8]. The mixture of fluorine with organic or inorganic and transition metals (TM) produces stable fluoroperovskites. One of the most useful candidates is wide band-gap fluoroperovskites. They can be amalgamated to create complex lattice-matched materials crystal structures and large band gaps, enabling band gap engineering and lattice matching [1]. Furthermore, fluoroperovskites compound can be utilized in medical fields to determine dose throughout radiation therapy, as well as in the production of radiation imaging plates for X-rays, thermal neutrons, and gamma-rays for medical and non-destructive testing purposes [9]. The wide energy bandgap of these compounds is a common characteristic. Because of their short absorption edges, they have significant potential as glass materials in the vacuum ultraviolet (VUV) and ultraviolet (UV) wavelength regions [10,11]. Some of the recent work regarding fluoroperovskites is reported as can be seen in Refs. [12–14]. Harmel et al. [15] investigated some of the properties of barium-based CsBaF_3 fluoroperovskite based on DFT and reported the CsBaF_3 based on the wide direct band gap and the spectra of the imaginary component of the dielectric functions in the UV field, will be appropriate for optoelectronic applications. Daniel et al. reported in Ref. [16] some of the properties of LiBaF_3 and concluded that the compound is favorable for energy storage applications. MBaF_3 ($M = \text{Ga}$ and In) is a significant class of ternary materials since it possibly is deemed to apply as a material for lenses and modern electronic technologies. It is common knowledge that material having band gaps greater than 3.1 eV perform better in the ultraviolet (UV) range [17–19]. The objective of this work is to use DFT and the full potential linearized augmented plane wave (FP-LAPW) framework to explore the fundamental structural, elastic, electronic, and optical properties of fluoroperovskite MBaF_3 ($M = \text{Ga}$ and In), to supply baseline data for researchers to perform experimental work on these compounds that has yet to be confirmed.

1.1. Computational methodology

This research work is done, with the use of the FP-LAPW method [20, 21], which was integrated within the Wien2K simulation code [22]. For the structural and elastic properties, the exchange-correlation potential is handled applying the generalized gradient approximation (GGA) [23] while the recently most used and precise modified Becke Johnson potential (TB-mBJ) [24] is used for the electronic and optical properties. This study considers some FP-LAPW basis functions up to $\text{RMT} \times K_{\text{max}}$ (where RMT is the minimum radius of the muffin-tin spheres) equal to 8 to achieve a satisfactory degree of convergence and K_{max} gives the magnitude of the largest k-vector in the plane wave expansions. For M where ($M = \text{Ga}$ and In), Ba, and F, the muffin-tin sphere radii RMT are 2.5, 1.5, and 1.7 atomic units (a.u.) respectively. The spherical harmonics within the muffin-tin spheres have been extended up to $l_{\text{max}} = 10$, but the Fourier expanded charge density has been reduced at $G_{\text{max}} = 12$ (a.u.)⁻¹. When the total energy is secure within 0.001 Ry, the self-consistent calculations are assumed converged. The structural parameters are determined by fitting the energy versus volume curve with the Birch-Murnaghan equation of state [25]. The IRelast package [26]

determines the elastic constants (ECs) of crystal symmetries such as Cubic, which are then used to investigate elastic properties. The $\epsilon(\omega)$ i.e. dielectric function can be used to define the optical properties [27,28].

2. Results and discussion

This section presents the results obtained through our methodology and a deep scientific discussion of the said results.

2.1. Structural properties

The ternary MBaF_3 ($M = \text{Ga}$ and In) compounds crystallize as a cubic perovskites structure with the space group $\text{Pm}\bar{3}\text{m}$ (# 221) and a single molecule as its unit cell. M atoms where $M = \text{Ga}$ and In are at (0,0,0), Ba atoms seem to be at (1/2,1/2,1/2), and F atoms are at (0,1/2,1/2), (1/2,0,1/2), and (1/2,1/2,0) accordingly. Fig. 1 shows the Ba-based fluoroperovskite compounds investigated here that have an ideal cubic structure.

In this portion, we'll measure overall energy accordant with unit-cell volume around V_0 (the equilibrium cell volume). Structural properties are predicted from the process of volume optimization, which can be achieved by fitting the Birch Murnaghan equation of state [25]. We evaluate the ground state properties namely the equilibrium lattice constant a_0 , the bulk modulus B, and its pressure derivative B' by performing an analytical interpolation of our computed points from Birch Murnaghan fit which express the variation of volume versus total energy. Unit cell minimum energy can be gained by minimizing the unit cell total energy with the corresponding volume, as depicted in optimization curves of Fig. 2.

The total minimum energy versus volume is known to be optimum or ground state energy E_0 and the volume is the optimum or ground state volume V_0 . The compound having more optimized energy is predicted to be structurally more stable. The computed optimized structural parameters comprising a_0 (optimized lattice constants), E_0 (the optimized ground state energy), the bulk modulus B_0 , the optimized volume V_0 , and bulk modulus pressure derivative B_0' are depicted in Table .1. A smaller bulk modulus is often observed when the lattice constant is higher, so these results are persistent on the general fashion of this approximation confirming that the computed results are more precise and realistic.

The optimization fit curve for InBaF_3 is sharper than for GaBaF_3 , thus InBaF_3 is encountered to be structurally more stable. Structural stability can also be compared from the above listed Table .1.

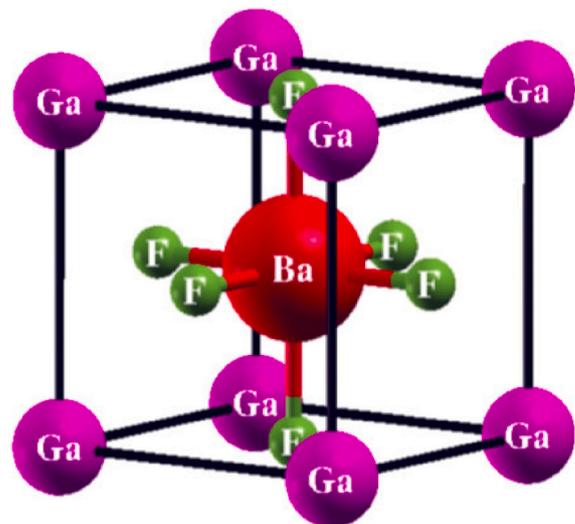


Fig. 1. Prototype crystal structure of ternary MBaF_3 ($M = \text{Ga}$ and In) compounds.

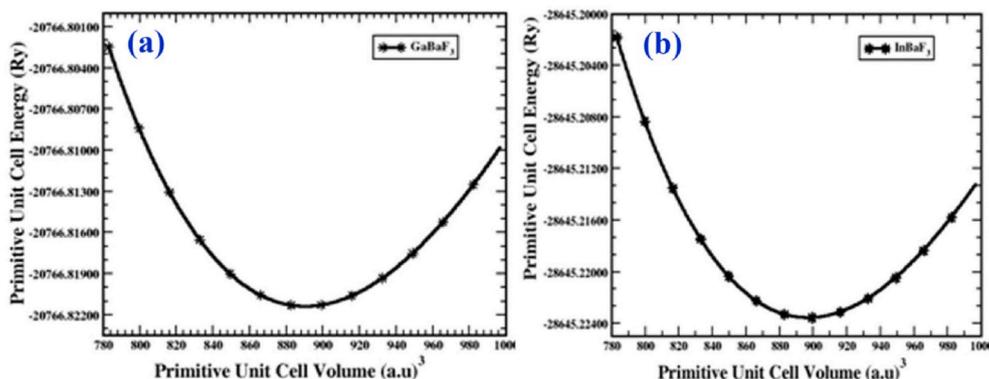


Fig. 2. Birch Murnaghan equation of state fitted optimization curve of MBaF₃ (M = Ga and In) compounds.

Table 1

Optimized crystal unit cell parameters of ternary MBaF₃ (M = Ga and In) compounds.

Structural Specifications	GaBaF ₃	InBaF ₃
a ₀ (in Å)	5.0913	5.1035
V ₀ (in a.u. ³)	890.62	897.01
B ₀ (in GPa)	33.23	33.79
B ₀ '	4.7814	4.9494
E ₀ (in Ry)	-20766.82	-28645.22

2.2. Electronic properties (bands structures and density of states DOS)

In this segment, we calculate the actual energy band structures, DOS, and charge distribution to examine the electronic properties of MBaF₃ (M = Ga and In) compounds. It is well understood that the fundamental band-gap of semiconductors and insulators is underestimated by LDA and GGA calculations [29,30]. Most of this is due to their basic shapes, which are not functional enough to reliably replicate both the exchange-correlation energy and its charge derivative. We used the modified Becke Johnson potential (mBJ) to resolve the underestimation of the band gaps, which has been used successfully in multiple recent papers [14,31,32]. In the Brillouin zone, the measured energy-band structures for the equilibrium geometry of MBaF₃ (M = Ga and In) along higher symmetry directions are shown in Fig. 3. The top of the valence band is chosen as the zero-energy level known as the Fermi

energy E_F. Fig. 3, shows that for both compounds the valence band (VB) maximum is at the X-symmetry points, while the conduction band (CB) minima are also at the same X-symmetry points, resulting in a direct (X-X) energy band gap of 5 eV for the GaBaF₃ and 5.13 eV for InBaF₃ compound.

The high band gap energy for both the compounds reveals an insulating nature. For both, the compounds there exist energy bands in the energy range of -14 eV-8 eV, in which the horizontal dotted line at 0 (zero) eV represents the Fermi energy level. The bands that coincide below the Fermi level are referred to as the valence band and the band above the reference Fermi line is the conduction band.

We have shown the TDOS and PDOS (total and partial atomic density of states) for MBaF₃ (M = Ga and In) compounds in Fig. 4 to gain a deeper insight into the electronic structure. DOS shows the contribution of the different electronic states to valence and conduction bands.

The DOS ranges from -2 eV to 8 eV, within which the vertical dotted line at the 0 eV represents the Fermi level energy E_F. The part of DOS to the left of E_F depicts valence while to the right is the conduction band. It can be seen that the energy range is divided into two classes i-e from -2 eV to 0 eV (the valence band) and from 5 eV to 6 eV (conduction band) based on the distribution of PDOS. It can be depicted that the major contribution to the DOS is from Ga-s, Ba-s, and In-s with addition to F-p states in the valence band having energy ranges from -2 eV to 0 eV. In the conduction band of energy range from 5 to 6 eV the total dominant part is from Ga-p and In-p states.

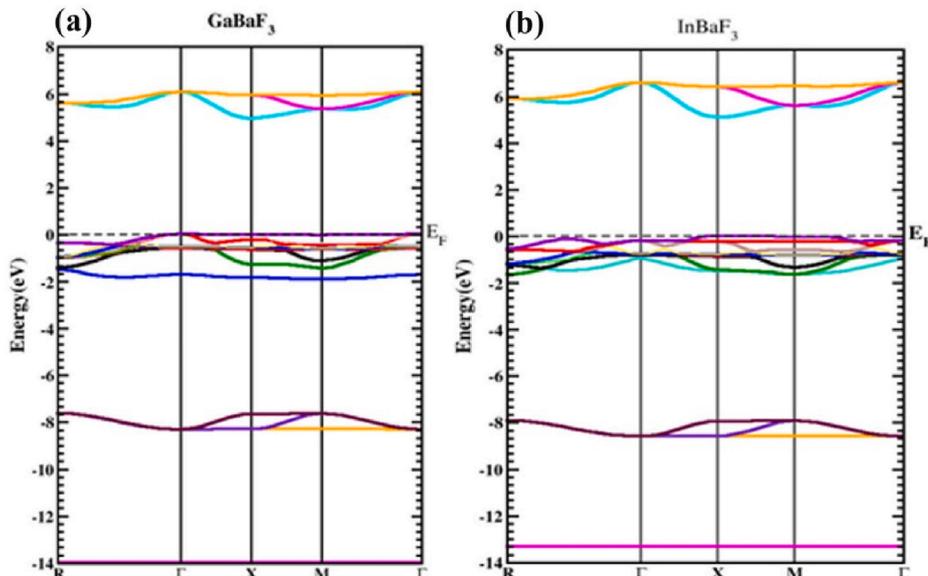


Fig. 3. Electronic energy band structures of ternary MBaF₃ (M = Ga and In) compounds using TB-mBJ approximation.

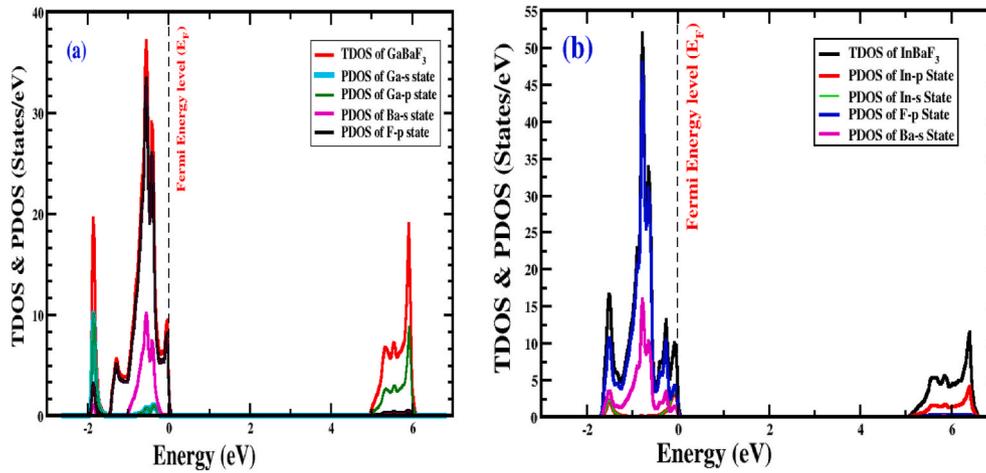


Fig. 4. Computed TDOS and PDOS of ternary MBaF₃ (M = Ga and In) compound using TB-mBJ.

2.3. Elastic properties

The elastic constants govern the crystal's response to external forces and are crucial in explaining the elastic property of materials. The measured value of these constants provides useful knowledge about a material's stability and toughness. The elastic constants of the interest, material were measured at zero pressure by calculating the components of the stress tensor for small strains and applying the energy in accordant with lattice strain that sustained volume [33]. The IRelast package interfaced within Wien2k, specially developed for cubic systems has been used to calculate elastic constants (ECs). The cubic crystal lattice symmetry reduces the total number of independent elastic constants C_{ij} to just three: C_{11} , C_{12} , and C_{44} . The estimated elastic constants and other elastic parameters measured from the theoretical elastic constants are summarized in Table 2. The constraints on the elastic constants are imposed by the criterion of mechanical stability in a cubic crystal are $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, and also $B > 0$ [34]. These stability conditions are obeyed by our measured C_{ij} values, suggesting that these compounds are elastically stable.

The value of C_{11} for GaBaF₃ is 76.758 GPa, which is less great than 75.584 GPa for InBaF₃, thus depicting that GaBaF₃ is a little harder than InBaF₃. The ability to create micro-cracks in materials is highly associated with the A (elastic anisotropy) of crystals, which has crucial implications in engineering research. We calculated the A (anisotropy factor) to quantify the elastic anisotropy of these materials from the presented values of elastic constants as:

$$A = 2C_{44} / (C_{11} - C_{12}) \quad (1)$$

A is equal to 1 for an isotropic material, whereas any number lesser

Table 2

Computed elastic constants with other elastic parameters comprising bulk modulus, anisotropy factor, Young modulus, Poison ratio, Pugh ratio (B/G), and Cauchy's pressure for ternary MBaF₃ (M = Ga and In) compounds.

Elastic Parameters	GaBaF ₃	InBaF ₃
C_{11} (in GPa)	76.758	75.584
C_{12} (in GPa)	12.152	14.580
C_{44} (in GPa)	3.628	8.419
B (in GPa)	33.700	35.009
A	0.112	0.277
E (in GPa)	28.186	38.260
ν	0.517	0.449
B/G	3.254	2.412
B/ C_{44}	9.289	4.158
$C_{11}-C_{12}$ (in GPa)	64.569	60.719
G (in GPa)	10.358	14.516
$C_{11}-C_{44}$ (in GPa)	72.372	67.165

or bigger than 1 implies anisotropy. Both these materials are anisotropic, as the value of A varies from 1 and the extent of variation shows the degree of anisotropy. It can be seen from Table 2 that the measured values of A for GaBaF₃ are 0.112 and that for InBaF₃ is 0.277, which depicts that InBaF₃ possesses a high degree of anisotropy. It is important to find out other elastic parameters like G (shear modulus), E (Young's modulus), and ν (Poisson ratio) from the presented elastic constants by utilizing the following expressions [35–37]:

$$E = \frac{9BG}{3B + G} \quad (2)$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (3)$$

$$G_V = \frac{1}{5} (C_{11} - C_{12} + 3C_{44}) \quad (4)$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \quad (5)$$

The A, G, E, and ν are calculated from the above-presented relations and its values are presented in Table 2. Several characteristics can be used to determine whether a material is ductile or brittle. The $(C_{11} - C_{44})$, which is a Cauchy's pressure is the difference between C_{11} and C_{44} is considered the identity of ductility [38]. If the difference of C_{11} and C_{44} is positive, the material is known to be ductile and if found negative it predicts a brittle nature. In this case for both the materials the Cauchy's pressure is positive i.e. 72.372 GPa for GaBaF₃ and 67.165 GPa for InBaF₃ which confirm that both the materials are ductile. The B/G (Pugh ratio) is another identification for the brittle or ductility classification. The critical value of the B/G ratio is 1.75, the materials having a high Pugh ratio are considered to be more ductile [39]. In this reported case both the compounds possess varied values from the critical point, i. e. 3.254 for GaBaF₃ and 2.412 for InBaF₃. Thus GaBaF₃ is a little more ductile than InBaF₃. Frantsevich et al. [40] use ν (Poisson's ratio) to discern between ductility and brittleness of materials and reported the critical value of 0.26. For brittle materials, the value is less than 0.26, while for ductile it will have a high value. For ternary MBaF₃ (M = Ga and In) compounds, both possess a higher value from 0.26, i.e. 0.517 for GaBaF₃ and 0.449 for InBaF₃ as can be seen from the same Table 2, which again confirms the ductile nature. In summary, we concluded that the compounds of interest are mechanically ductile, anisotropic, tough, and possess high resistance to cracks. From these findings of elastic properties, we surely deemed its applications in many modern electronic technologies.

2.4. Optical properties

For the photon energies up to 40 eV, all-optical properties are determined using the theoretical equilibrium lattice constant. All the optical properties can be determined from the dielectric function $\epsilon(\omega)$.

2.5. The dielectric function

The dielectric function $\epsilon(\omega)$ comprises of two parts i.e the real and imaginary part, which can be expressed as $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. The measured real part $\epsilon_1(\omega)$ of $\epsilon(\omega)$, which shows the materials photon dispersion and electronic polarizability is shown in Fig. 5.

At low energy, the curve displays increases, drops, and then reduces to achieve a negative value of $\epsilon_1(\omega)$, followed by a steady rise towards zero. The maximum peak of 4.2 for GaBaF₃ and 4.9 for InBaF₃ occurs at about 5 eV photon energy. Approximately 2.16 for GaBaF₃ and 2.23 for InBaF₃ is the computed static dielectric constant $\epsilon_1(0)$. Based on the Penn model [41], the materials having a greater value of static dielectric function $\epsilon_1(0)$ will have smaller band gap energy, and for which $\epsilon_1(0)$ posses' smaller value will have a larger band gap. These compounds do not obey the Penn model, in which InBaF₃ has a $\epsilon_1(0)$ value of 2.23, thus having a greater value of 5.13 eV energy band gap while $\epsilon_1(0)$ is 2.16 for GaBaF₃ which possesses a band gap of 5 eV. The computed $\epsilon_2(\omega)$ (imaginary part) of $\epsilon(\omega)$ is displayed in the same Fig. 5 within the energy range of 40 eV. The first critical peaks (threshold energy) of the ϵ (dielectric function) for both GaBaF₃ and InGaF₃ occurred at roughly 6 eV, according to our investigation of the $\epsilon_2(\omega)$ spectrum. At the X-symmetries point, this point known as the basic absorption edge is the direct optical transition within the highest VB (valence band) and the lowest CB (conduction band). Beyond the threshold energy, the increase and drops occur in the curve. The maximum peak of 5 occurs for InBaF₃ at about 6 eV, while for GaBaF₃ it is noticed to be 4.5 at about 18.17 eV. As a result, the compound's wide direct band-gap nature builds it suited for high-frequency UV device application.

2.6. The refractive index

The refractive index $\eta(\omega)$, optical conductivity $\sigma(\omega)$, absorption coefficient $I(\omega)$, and reflectivity $R(\omega)$ can all be calculated using $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$. Fig. 6 displays the computed refractive index $\eta(\omega)$. The $\eta(0)$ i.e. static refractive index has a value of 1.49, and 1.5 for GaBaF₃ and InBaF₃ respectively, according to the refractive index spectrum. It can be explicitly seen from Fig. 6 that curve of $\eta(\omega)$ for both the compounds coincide with a slight change. The maximum peak value of the refractive index is 2.3 for InBaF₃ at about 5 eV photon energy while that for GaBaF₃ is 2.15 at the same photon energy of 5 eV for GaBaF₃. The refractive index is a crucial parameter for determining the degree of refraction of light, as it is particularly useful in photoelectric

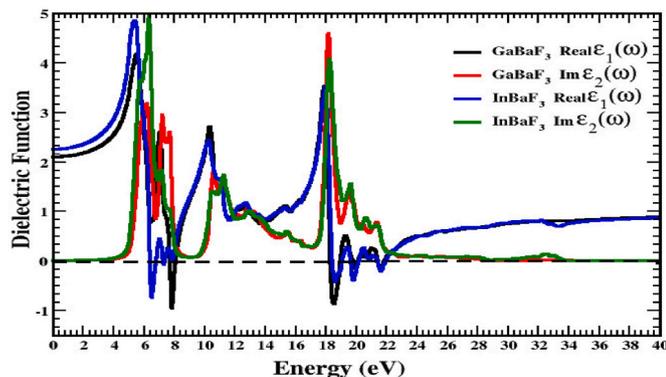


Fig. 5. Computed Dielectric function $\epsilon(\omega)$ for MBaF₃ (M = Ga and In) compounds.

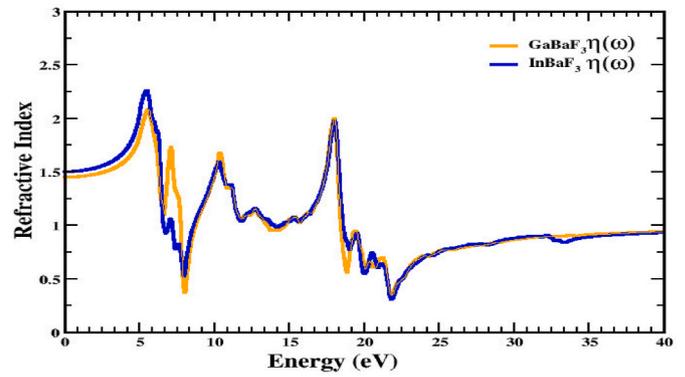


Fig. 6. Computed refractive index of MBaF₃ (M = Ga and In) compounds.

applications. $\eta(\omega) > 1$ (refractive index is greater than one), because photons are slowed as they enter a substance due to interactions with electrons. The greater the refractive index of a material, the more photons is retarded while traveling through it. In general, every mechanism that raises the electron density in a material raises the refractive index as well.

2.7. The absorption coefficient

The $I(\omega)$ (absorption coefficient) curves computed from the dielectric function $\epsilon(\omega)$ are manifested in Fig. 7.

It is very obvious from Fig. 7 that the compounds of interest have considerable absorption coefficients at high energy ranges from 5 eV to 35 eV. The threshold point at which a substance begins to absorb electromagnetic radiation effectively. The threshold point for both these compounds exists uniquely i.e. 5 eV. The maximum absorption of 265 cm^{-1} for GaBaF₃ and 250 cm^{-1} for InBaF₃ at the same photon energy of 18 eV.

2.8. The reflectivity R(ω)

The $R(\omega)$, computed from the dielectric function is plotted within energy range from 0 eV to 40 eV and is shown in Fig. 8.

The zero-frequency reflectivity $R(0)$ is observed at 0.03 for both GaBaF₃ and InBaF₃ and on increasing photon energy the reflectivity increases gaining a maximum of 0.4 at 8 eV for GaBaF₃ and 0.36 at about 23 eV. The reflectivity is very low at the energy range equal to the band's gap, so for incident photon the materials are transparent; thus, the transparency of the material in this low energy, indicating that these

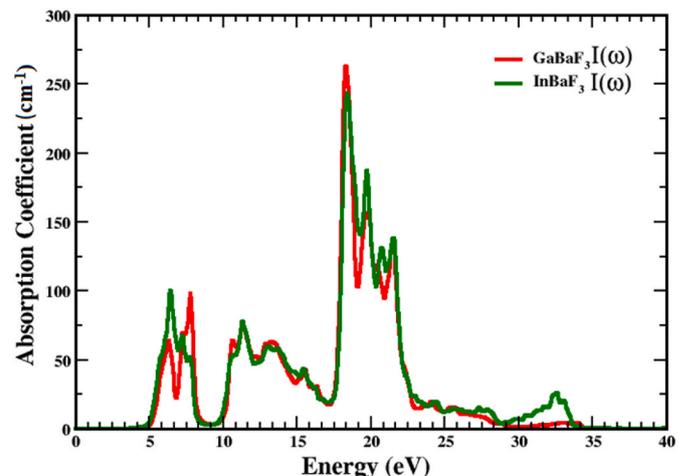


Fig. 7. Computed absorption coefficient of MBaF₃ (M = Ga and In) compounds.

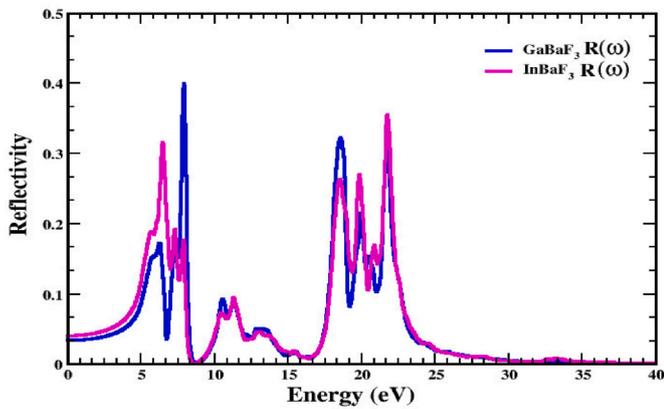


Fig. 8. Computed optical reflectivity $R(\omega)$ of MBaF_3 ($M = \text{Ga}$ and In) compounds.

compounds are a potential choice for fabricating lenses.

2.9. The optical conductivity

The optical conductivity $\sigma(\omega)$, describes the conduction of electrons caused by an applied electromagnetic field. The $\sigma(\omega)$ investigated from the dielectric function is plotted and depicted in Fig. 9.

It is very clear from Fig. 9 that optical conductivity starts for both the compounds at the rate of the energy band gap, i.e. at about 5 and 5.1 eV. This threshold optical conductivity confirms our predicted band gap energy. It can also be depicted clearly from the figure that both GaBaF_3 and InBaF_3 optical conductivity curves have the same pattern. The maximum optical conductivity of $11,550 \Omega^{-1}\text{cm}^{-1}$ for GaBaF_3 and $10,000 \Omega^{-1}\text{cm}^{-1}$ for InBaF_3 at the unique photon energy of 19 eV. Thus we concluded that both the compounds are optically conductive at a high photon energy range.

2.10. The Energy Loss Function (ELF)

The intra-band, inter-band, and Plasmon interdependencies are described from electron energy-loss function (ELF). ELF is the energy lost by a fast-moving electron as it travels through a substance. The computed optical ELF for both materials is presented in Fig. 10.

It is very clear from Fig. 10 that there is no energy loss at a photon energy of 0 eV–5 eV and after that, a sharp loss in energy starts from 5 eV to 35 eV. For both the materials the maximum energy loss of 4.5 for GaBaF_3 and 5.3 for InBaF_3 occurs at photon energy of 23 eV.

3. Conclusion

In the presented research work, we have successfully done the structural, elastic, electronic, and optical properties of ternary fluoroperovskites MBaF_3 ($M = \text{Ga}$ and In) compounds. The most precise and novel results are outlined as:

- ❖ From optimized structural parameters, we have concluded that MBaF_3 ($M = \text{Ga}$ and In) are cubic and structurally stable.
- ❖ Using the IRelast package, the elastic properties i.e fundamental elastic constant, anisotropy factor, Poisson ratio, ductility, Cauchy's pressure, shear modulus, Pugh ratio, Young modulus are predicted. From these basic elastic parameters, we found that both the compounds are elastically stable, anisotropic, hard to scratch, and ductile. Due to these findings, we confidently deem the application of these materials in many modern electronic technologies.
- ❖ The basic electronic properties of the compounds of interest were investigated using TB-mbj approximation. From the electronic properties (Band structures and DOS) we found that these materials

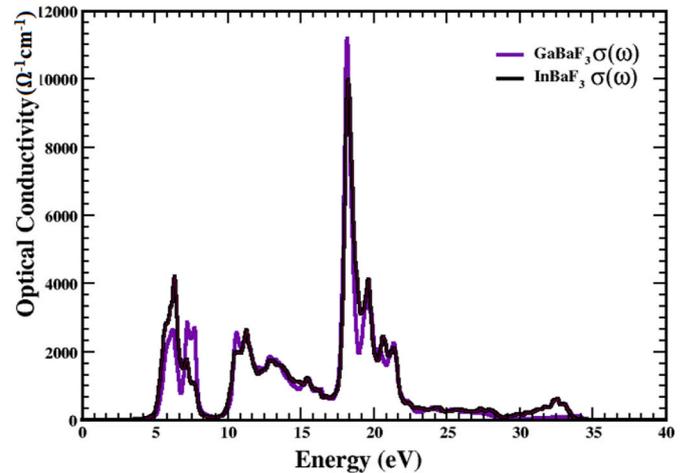


Fig. 9. Computed optical conductivity $\sigma(\omega)$ of MBaF_3 ($M = \text{Ga}$ and In) compounds.

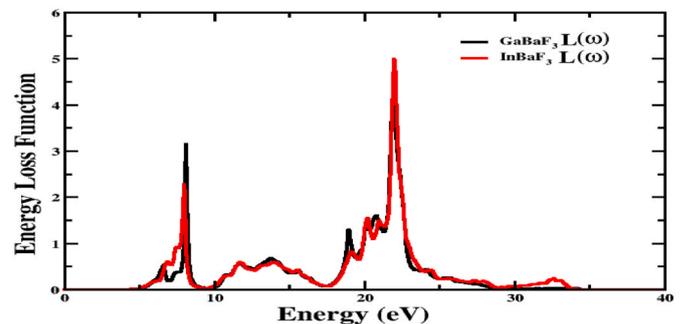


Fig. 10. Computed optical Energy Loss Function $L(\omega)$ of MBaF_3 ($M = \text{Ga}$ and In) compounds.

are wide direct band gap insulators from X-X symmetry points with band gap energy of 5 eV for GaBaF_3 and 5.1 eV for InBaF_3 . We have concluded from the DOS that the dominant contribution in the valence band of both the compounds is due to the F-p state, while Ga-p and In-p contribute largely in the conduction band.

- ❖ From the electronic properties, we found that both materials are wide direct band gap insulators. This sort of study directed focus on studying optical properties. Optical properties of ternary MBaF_3 ($M = \text{Ga}$ and In) fluoroperovskites compounds were studied and presented very deeply. We have concluded from the optical properties investigations that these compounds are suited for high-frequency UV device applications. These compounds possess high absorption and optical conduction at high energy ranges. Both the materials are transparent for incident photons at a low energy range.

Declaration of competing interest

The authors have no conflict of interest.

Acknowledgments

The first two authors Jaffer Saddique and Mudasser Husain have equal contributions to this research work.

References

- [1] T. Nishimatsu, N. Terakubo, H. Mizuseki, Y. Kawazoe, D.A. Pawlak, K. Shimamura, et al., Band structures of perovskite-like fluorides for vacuum-ultraviolet-transparent lens materials, *Jpn. J. Appl. Phys.* 41 (2002) L365.

- [2] C. Dotzler, G. Williams, A. Edgar, Rb Cd F 3: Mn 2+: a potential ultraviolet dosimeter material, *Appl. Phys. Lett.* 91 (2007), 181909.
- [3] G. Vaitheeswaran, V. Kanchana, R.S. Kumar, A. Cornelius, M. Nicol, A. Svane, et al., High-pressure structural, elastic, and electronic properties of the scintillator host material K Mg F 3, *Phys. Rev. B* 76 (2007) 14107.
- [4] S. Naeem, G. Murtaza, R. Khenata, M. Khalid, First principle study of CsSrM3 (M= F, Cl), *Phys. B Condens. Matter* 414 (2013) 91–96.
- [5] A. Mubarak, Ab initio study of the structural, electronic and optical properties of the fluoropervskite SrXF3 (X= Li, Na, K and Rb) compounds, *Comput. Mater. Sci.* 81 (2014) 478–482.
- [6] A. Mubarak, S. Al-Omari, First-principles calculations of two cubic fluoropervskite compounds: RbFeF3 and RbNiF3, *J. Magn. Magn Mater.* 382 (2015) 211–218.
- [7] N.-G. Park, Organometal perovskite light absorbers toward a 20% efficiency low-cost solid-state mesoscopic solar cell, *J. Phys. Chem. Lett.* 4 (2013) 2423–2429.
- [8] N. Dimov, A. Nishimura, K. Chihara, A. Kitajou, I.D. Gocheva, S. Okada, Transition metal NaMF3 compounds as model systems for studying the feasibility of ternary Li-MF and Na-MF single phases as cathodes for lithium-ion and sodium-ion batteries, *Electrochim. Acta* 110 (2013) 214–220.
- [9] J. Donaldson, G. Williams, S. Raymond, Characterization of a Fluoropervskite Based Fibre Coupled Optical Dosimeter for Radiotherapy, 2014.
- [10] K. Shimamura, T. Fujita, H. Sato, A. Bensalah, N. Sarukura, T. Fukuda, Growth and characterization of KMgF3 single crystals by the Czochralski technique under CF4 atmosphere, *Jpn. J. Appl. Phys.* 39 (2000) 6807.
- [11] A. Bensalah, K. Shimamura, K. Nakano, T. Fujita, T. Fukuda, Growth and characterization of LiSrGaF6 single crystal, *J. Cryst. Growth* 231 (2001) 143–147.
- [12] M. Husain, M.S. Ahmad, N. Rahman, M. Sajjad, A. Rauf, A. Habib, et al., First principle study of the structural, electronic, and Mechanical properties of cubic fluoropervskites:(ZnXF 3, X= Y, Bi), *Fluoride* 53 (2020).
- [13] M.S. Ahmad, A. Habib, A. Rauf, M.U. Haq, J. Saddique, M. Nisar, et al., Theoretical investigation of the structural, electronic, and mechanical properties of the magnesium-based fluoropervskite compounds XMgF3 (X= Ga, Al, In), *Theoretical Invest.* 1 (2020) 1.
- [14] N. Rahman, M. Husain, J. Yang, M. Sajjad, G. Murtaza, M.U. Haq, et al., First principle study of structural, electronic, optical and mechanical properties of cubic fluoro-perovskites:(CdXF 3, X= Y, Bi), *European Physic. J. Plus* 136 (2021) 1–11.
- [15] M. Harmel, H. Khachai, A. Haddou, R. Khenata, G. Murtaza, B. Abbar, et al., Ab initio study of the mechanical, thermal and optoelectronic properties of the cubic CsBaF3, *Acta Phys. Pol.* 128 (2015) 34–42.
- [16] D.J. Daniel, U. Madhusoodanan, R. Nithya, P. Ramasamy, Irradiation effect on luminescence properties of fluoropervskite single crystal (LiBaF3: Eu2+), *Radiat. Phys. Chem.* 96 (2014) 135–139.
- [17] M. Maqbool, I. Ahmad, H. Richardson, M. Kordesch, Direct ultraviolet excitation of an amorphous AlN: praseodymium phosphor by codoped Gd 3+ cathodoluminescence, *Appl. Phys. Lett.* 91 (2007), 193511.
- [18] G. Murtaza, I. Ahmad, Shift of indirect to direct bandgap and optical response of LaAlO3 under pressure, *J. Appl. Phys.* 111 (2012), 123116.
- [19] G. Murtaza, I. Ahmad, B. Amin, A. Afaq, M. Maqbool, J. Maqssod, et al., Investigation of structural and optoelectronic properties of BaThO3, *Opt. Mater.* 33 (2011) 553–557.
- [20] G.K. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, L. Nordström, Efficient linearization of the augmented plane-wave method, *Phys. Rev. B* 64 (2001), 195134.
- [21] K. Schwarz, P. Blaha, G.K. Madsen, Electronic structure calculations of solids using the WIEN2k package for material sciences, *Comput. Phys. Commun.* 147 (2002) 71–76.
- [22] P. Blaha, K. Schwarz, G.K. Madsen, D. Kvasnicka, J. Luitz, WIEN2k: An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties, Vienna University of Technology, 2001.
- [23] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* 77 (1996) 3865.
- [24] F. Tran, P. Blaha, Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential, *Phys. Rev. Lett.* 102 (2009), 226401.
- [25] F. Murnaghan, The compressibility of media under extreme pressures, *Proc. Natl. Acad. Sci. U.S.A.* 30 (1944) 244.
- [26] M. Jamal, M. Bilal, I. Ahmad, S. Jalali-Asadabadi, IRelast package, *J. Alloys Compd.* 735 (2018) 569–579.
- [27] J. Bechhoefer, Kramers–kronig, bode, and the meaning of zero, *Am. J. Phys.* 79 (2011) 1053–1059.
- [28] C.C. Kim, J. Garland, P. Raccah, Modeling the optical dielectric function of the alloy system Al x Ga 1– x as, *Phys. Rev. B* 47 (1993) 1876.
- [29] P. Dufek, P. Blaha, K. Schwarz, Applications of Engel and Vosko's generalized gradient approximation in solids, *Phys. Rev. B* 50 (1994) 7279.
- [30] Z. Charifi, H. Baaziz, F.E.H. Hassan, N. Bouarissa, High pressure study of structural and electronic properties of calcium chalcogenides, *J. Phys. Condens. Matter* 17 (2005) 4083.
- [31] M.A. Ali, N. Alam, Meena, S. Ali, S.A. Dar, A. Khan, et al., A theoretical study of the structural, thermoelectric, and spin-orbit coupling influenced optoelectronic properties of CsTmCl3 halide perovskite, *Int. J. Quant. Chem.* 120 (2020) e26141.
- [32] A. Mohamed, A. El Houssine, F. Nejmaa, B. Ibrahim, Ab-initio study of electronic, optical and thermoelectric properties of TiO2 phases using mBJ approximation, in: 2020 IEEE 6th International Conference on Optimization and Applications, ICOA, 2020, pp. 1–5.
- [33] M.J. Mehl, Pressure dependence of the elastic moduli in aluminum-rich Al-Li compounds, *Phys. Rev. B* 47 (1993) 2493.
- [34] J. Wang, S. Yip, S. Phillpot, D. Wolf, Crystal instabilities at finite strain, *Phys. Rev. Lett.* 71 (1993) 4182.
- [35] R. Hill, The elastic behaviour of a crystalline aggregate, *Proc. Phys. Soc.* 65 (1952) 349.
- [36] W. Voigt, *Lehrbuch der Kristallphysik (Textbook of crystal physics)*, BG Teubner, Leipzig und Berlin, 1928.
- [37] A. Russ, *Mater. Phys* 9 (1929) 49.
- [38] D. Pettifor, Theoretical predictions of structure and related properties of intermetallics, *Mater. Sci. Technol.* 8 (1992) 345–349.
- [39] S. Pugh, XCII. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals, *The London, Edinburgh, Dublin Philosophical Magazine J. Sci.* 45 (1954) 823–843.
- [40] I. Frantsevich, *Elastic Constants and Elastic Moduli of Metals and Insulators*, Reference book, 1982.
- [41] D.R. Penn, Electron mean-free-path calculations using a model dielectric function, *Phys. Rev. B* 35 (1987) 482.