Computational Study of Elastic, Structural, Electronic, and Optical Properties of GaMF₃ (M = Be and Ge) Fluoroperovskites, Based on Density Functional Theory

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Abstract: This paper explains our first-principle computational investigation regarding the structural, optical, elastic, and electrical characteristics of gallium-based GaMF₃ (M = Be and Ge) perovskite-type (halide-perovskite) compounds. Our current computation is based on density functional theory (DFT) and is achieved with the help of the WIEN2k code. We used the Birch–Murnaghan equation for optimization; in both compounds, we found that both GaBeF₃ and GaGeF₃ compounds are structurally stable. For the computation of elastic characteristics, the IRelast package for calculating elastic constants (ECs) is utilized. These compounds are mechanically ductile, scratch-resistant, anisotropic, and mechanically stable, showing huge opposition to plastic strain. The modified Becke–Johnson (TB-mBJ) potential approximation method is used to calculate different physical characteristics and shows that GaGeF₃ behaves as a metal, whereas the GaBeF₃ compound is insulating in nature. The involvement of various electronic states in band structures is calculated using the theory of the density of states. The different optical properties of these compounds can be studied easily using their band gap energy. At high energy ranges, these substances demonstrate strong absorption. At low energies, the GaGeF₃ compound is transparent, while the GaBeF₃ compound is opaque to incoming photons. Investigation of the optical characteristics has led us to the conclusion that both GaGeF₃ and GaBeF₃ compounds can be used for high-frequency ultraviolet device applications. This computational work is considered to be the first time that we can study these compounds, which to our knowledge have not previously been experimentally validated.

Keywords: density functional theory; fluoroperovskite; optical properties; structural properties; electronic properties

1. Introduction

New perovskite compounds with improved characteristics are constantly being developed by materials scientists. Those compounds that have the chemical formula ABF₃ generally have a fluoroperovskite structure. The atomic arrangement of this material was...
initially identified in the perovskite CaTiO$_3$. The A cation has twelve halide atoms linked to it in the perovskite structure, whereas the B cation has six atoms of fluorine bonded to it. Fluoroperovskite compounds are a unique family of materials, with a stable crystalline structure and outstanding electrical characteristics that range from semiconductors to insulators. Because of their crucial relevance, radiation dosimeters, material scintillation techniques, and the semiconductor industry [1–3] can utilize them in lens materials for photonic lithography; for this reason, in recent years, these chemicals have received much attention. Many studies have examined the characteristics of perovskite compounds, with the majority concluding that they are mechanically stable and elastically anisotropic [4–6]. Photovoltaic features with large efficiency and good energy storage have widespread applications in cars, electronics, and lenses in the form of ABF$_3$ composites [7–9]. Fluorine is combined with organic or inorganic elements, as well as transition metals (TM) to form stable fluoroperovskites. Fluoroperovskites with a wide band gap are the most widely applicable structures. These can be combined to make complex lattice-matched materials with huge bandgaps, allowing lattice matching and band gap engineering [1]. One common feature of these compounds is their broad energy band gap. These compounds have tremendous potential and offer low absorption edges; hence, in vacuum ultraviolet (VUV) and ultraviolet (UV) wavelengths they can be used as glass [10,11]. Recent work on fluoroperovskites has been reported in previous studies [12–14]. Harmel et al. [15] used DFT to explore some of the features of barium-based BaCsF$_3$ fluoroperovskites, concluding that due to its broad direct band gap and its bands of the imaginary factor of the insulating features in the ultraviolet range, BaCsF$_3$ will be suitable for optoelectronic devices. Daniel et al. [16] discussed a few of the characteristics of LiBaF$_3$ and found that these chemical compounds are suitable for storing energy.

GaBeF$_3$ is a new and significant class of ternary compounds; in terms of modern electrical technologies, these compounds have the potential to be used as a lens material. In the ultraviolet (UV) spectrum, compounds with band gaps that are bigger than 3.1 eV will perform better. The GaGeF$_3$ compound demonstrates a metallic nature; it is a good candidate for electrical applications because it is an electrical conductor with high transparency over a narrow band of energies. The purpose of this study is to use DFT and the FP-LAPW technique to study the basic electronic, elastic, optical, and structural characteristics of GaMF$_3$ (M = Ge and Be) fluoroperovskites, providing researchers with core data for future laboratory work on the above mentioned compounds.

2. Computational Methodology

The calculations for the compounds were carried out using the FP-LAPW technique [17–21], which is included in the WIEN2k Fortran simulation engine [22]. The electronic and other properties of the material, such as its optical properties and density of state, etc., were computed using the TB-mBJ method [23]. The exchange-correlation potential for structural and elastic features is managed using the generalized gradient approximation (GGA) [24]. To obtain a considerable degree of convergence, this study explores certain FP-LAPW base functions up to RMT (in the muffin-tin spheres, where RMT is the minimum radius) and is equal to 8, represented by $K_{\text{max}}$ in our example, where $K_{\text{max}}$ in the plane wave expansion shows the magnitude of the maximum, k. For GaMF$_3$ (M = Ge and Be) compounds and F, the RMT radii in the muffin-tin sphere are 2.50, 1.50, and 1.70 atomic units (a.u). Within the muffin-tin spheres, the spherical harmonics were extended to $l_{\text{max}} = 11$, but the Fourier-expanded charge density was reduced to $G_{\text{max}} = 13$ (a.u.). Within the energy range of 0.001 Ry, when the total energy is falling, the internally consistent field calculations are said to have converged. We obtained the physical parameters by placing the energy vs. volume curve using the state equation developed by Birch–Murnaghan [25]. The elastic constant for the cubic crystal symmetries was obtained using IRelast [26]; these were then utilized to examine the elastic properties. The dielectric function $\varepsilon(\omega)$ was also utilized to identify the optical characteristics [27,28].
3. Results and Discussion

This part of the paper contains a detailed scientific discussion of the outcomes produced using our proposed TB-MBJ methods. In this section, we shall explain the compounds’ structural and optical properties.

3.1. Structural Properties

GaMF₃ (M = Ge and Be) crystallizes as a Pm₃m (#221) cubic perovskite structure, with one molecule as the unit cell. Ga atoms appear at (0,0,0), M atoms (M = Ge and Be) appear at (0.5,0.5,0.5), and F atoms appear at (0,0.5,0.5), (0.5,0,0.5), and (0.5,0.5,0), respectively. The Ga-based fluoroperovskite compound possesses a cubic structure, as shown in Figure 1. Around V₀, we calculate the overall energy in terms of unit-cell volume (the cell volume in equilibrium conditions). The volume optimization approach can be used to forecast the structural features using the Birch–Murnaghan equation of state [25]. The Birch–Murnaghan equation is used to fit and establish ground state characteristics such as the lattice constant aₒ at equilibrium and the bulk modulus B, as well as the derivative of pressure B′; thus, we performed analytical estimations of our obtained locations. Figure 2 shows the optimization curves, with the unit cell’s lowest-energy value versus the appropriate volume. The ideal or ground state E₀ is the entire minimum energy value, versus volume. The volume is represented by V₀, the optimum or ground state minimum volume. It is assumed that the structure of the compound with the highest optimum energy will be the most stable. Table 1 lists the ideal structural parameters that were determined, including aₒ (optimized lattice constants), E₀ (optimized ground state energy), B₀ (bulk modulus), V₀ (optimized volume), and B’₀ (bulk modulus pressure derivative). Because the bulk modulus decreases as the lattice constant increases, these results are in line with the overall trend of this approximation, suggesting that the calculated outcomes are more accurate and realistic. GaGeF₃ has a steeper optimization fit curve than GaBeF₃, indicating that GaBeF₃ is structurally more stable. The above-mentioned Table 1 can also be used to compare structural stability.

Figure 1. The prototypical crystal structure of the ternary compound, GaMF₃ (M = Ge and Be).
Figure 2. The optimized curve of GaMF$_3$ (M = Ga and Be) compounds, fitted by Birch-Murnaghan’s equation of state.

Table 1. Optimized crystal unit cell characteristics of the GaMF$_3$ compound (M = Ge and Be).

| Structural Specification | GaBeF$_3$    | GaGeF$_3$    |
|--------------------------|--------------|--------------|
| $a_0$ (Å)                | 5.113        | 5.1035       |
| $V_0$ (a.u.$^3$)         | 891.00       | 897.01       |
| $B_0$ (Gpa)              | 33.20        | 33.79        |
| $B_0/(Gpa)$              | 4.7814       | 4.9494       |
| $E_0$ (Ry)               | 20,766.82    | 28,645.22    |

3.2. Electronic Properties (Density of States and Energy Band Structures)

To investigate the electronic characteristics of GaMF$_3$ (M = Ge and Be) compounds, we must determine the actual diagrams of band structures, their density of state (DOS), and the distribution of charges in this section. The LDA and GGA computations are well known for establishing the basic gaps of the bands of semiconductors and insulators [29,30]. The majority of this utility is due to their fundamental geometries failing to dependably reproduce both the exchange-correlation energy and its derivative of charge. To address this underestimating of band gaps, the modified Becke–Johnson potential (TB-Mbj) was adopted, and has been used successfully in a number of recent papers [14,31,32]. Figure 3 depicts the observed energy-band structures in the Brillouin zone for the geometry at the equilibrium of GaMF$_3$ (M = Ge and Be) along high-symmetry directions. At the valence band top, the Fermi energy, $E_F$, is chosen to be the zero-energy level. GaGeF$_3$ is identified as metal because the valence band (VB) maxima and conduction band minima overlap. The valence band’s maxima occur at symmetry point M, while the conduction band’s minima occur at symmetry point X, yielding an indirect (X-M) energy gap of 3.89 eV for GaBeF$_3$. To acquire a better understanding of the electronic structure, we have shown the TDOS and PDOS (total and partial atomic density of states) for GaMF$_3$ (M = Ge and Be) compounds in Figure 4. DOS displays the contribution of several electronic states to the valence and conduction bands. The Fermi energy, $E_F$, is shown by the vertical dashed lines at 0 eV, while the DOS spans –8 to 8 eV. The conduction band part of the DOS is to the right of $E_F$, whereas the valence band is to the left.
Figure 3. Energy band structures of compounds GaMF$_3$ (M = Ge and Be), using TB-mBJ approximation.

Figure 4. The TB-mBJ approximation approach was used to calculate the TDOS and PDOS of the GaMF$_3$ (M = Ge and Be) compounds.

The largest contributors to the DOS are F-tot and Ge-p; these represent states in the valence band with energies ranging from $-6$ to $-11$ eV and $-2$ eV to 0 eV, respectively, for GaGeF$_3$. The largest contribution in the conduction band is from the Ga-p state for GaBeF$_3$ in an energy range from 4 to 7 eV, whereas in GaBeF$_3$, the largest contribution is from Ga-p and F-tot in the valance band, in an energy range from $-4.2$ to $-8.3$ eV. The conduction band of F-p and Ga-p has the largest contribution, as shown in Figure 4.

3.3. Elastic Properties

The elastic properties of the crystal can be calculated from the elastic constants in response to the external forces exerted on the compound. These constants’ measured values provide useful information about a compound’s toughness and stability. The elastic constants of the compounds were calculated at zero pressure by computing the stress tensor components for tiny deformation and applying energy, in line with a lattice deformation that maintained volume [33]. The IRelast package, which is integrated into WIEN2k and is specifically designed for cubic systems, was utilized to determine the elastic constants.
(Ecs). Because of the cubic crystal lattice symmetry, the three different elastic constants are $C_{11}$, $C_{12}$, and $C_{44}$. These independent constants are summarized in Table 2. In order to have a mechanically stable cubic crystal structure, the following conditions of the elastic constants must be satisfied: $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, and also $B > 0$ [34]. Here, the measured elastic constant $C_{ij}$ values reveal the elastic stability of our compounds. The $C_{11}$ value for GaBeF$_3$ is 93.4057 GPa, which is smaller than that of GaGeF$_3$ at 98.525 GPa. Thus, GaGeF$_3$ is somewhat harder than GaBeF$_3$. The ability to form small cracks in materials is strongly linked to crystal A (elastic anisotropy), which can be implemented for specific purposes, especially in engineering research. From the supplied values of these elastic constants, we derived the A (anisotropy feature) to measure the elastic anisotropy of these materials, using the following equation:

$$A = \frac{2C_{44}}{(C_{11} \times C_{12})}$$ (1)

Table 2. For ternary GaMF$_3$ (M = Ge and Be) compounds, the calculated elastic constants, bulk modulus, anisotropy factor, Young’s modulus, Poisson’s ratio, Pugh ratio ($B/G$), and Cauchy’s pressure are shown.

| Elastic Parameters | GaGeF$_3$ | GaBeF$_3$ |
|--------------------|-----------|-----------|
| $C_{11}$ (GPa)     | 98.525    | 93.4057   |
| $C_{12}$ (GPa)     | 62.046    | 102.992   |
| $C_{44}$ (GPa)     | −7.316    | 68.648    |
| B (GPa)            | 172.03    | 172.03    |
| A                  | −0.40     | −14.322   |
| E (in GPa)         | 8.745     | 109.485   |
| $\nu$              | 0.492     | 0.394     |
| B/G                | −25.127   | 13.29     |
| G (GPa)            | −6.846    | 12.94     |

For an isotropic material, $A$ equals 1, whereas any quantity less than 1 indicates anisotropy. Since the value of $A$ fluctuates from 1, both of these materials are anisotropic, while the extent of the variant indicates the grade of anisotropy. From the computed data, as shown in Table 2, we know that this is $−14.322$ for GaBeF$_3$, whereas those for GaGeF$_3$ show that it is $−0.40$, indicating that GaGeF$_3$ has a significant degree of anisotropy. The shear modulus, $G$, Young’s modulus, $E$, and Poisson ratio, $\nu$, must be obtained using elastic constants by the application of the following formulae [35–37]:

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

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

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

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

$$A = \frac{2C_{44}}{C_{11} - C_{12}}$$ (6)

The values of $E$, $A$, $\nu$, and $G$ are computed from these equations and are shown in Table 2. To evaluate the level of ductility or brittleness of the material, a number of criteria can be used. The presence of ductility is shown as $(C_{11} - C_{44})$, which is a Cauchy’s pressure that shows the change between $C_{11}$ and $C_{44}$ [38]. If the change between $C_{11}$ and $C_{44}$ is positive, the material exhibits ductility; if it has a negative value, the material exhibits brittleness. Here, Cauchy’s pressure for both materials is positive; that is, 24.75 GPa for GaBeF$_3$ and 105.841 GPa for GaGeF$_3$, indicating that both materials show ductility. The
Pugh ratio, i.e., the B/G ratio, is another way to identify if a material is brittle or ductile. The limited value of the B/G ratio is 1.75 if a compound with a large Pugh ratio is supposed to be highly ductile [39]. Both compounds have different values from the critical point in this example, 13.29 for GaBeF₃, and −25.127 for GaGeF₃. As a result, GaGeF₃ has somewhat higher ductility than GaBeF₃. T. Frantsevich et al. [40] employed \( v \) (Poisson’s ratio) and reported a crucial value of 0.26 for discriminating between the ductility and brittleness of materials. Brittle materials have a value of less than 0.26, whereas ductile materials have a value greater than 0.26. As can be seen in Table 2, both ternary GaMF₃ \((M = \text{Ge and Be})\) compounds have a higher value than 0.26, namely, 0.394 for GaBeF₃ and 0.492 for GaGeF₃, confirming their ductile character. In conclusion, we found that the compounds of GaMF₃ \((M = \text{Ge and Be})\) are mechanically ductile, anisotropic, robust, and crack-resistant. We can certainly see multiple uses for these elastic characteristics in the future, in a variety of modern electronic technologies, based on these findings.

3.4. Optical Properties

We have exposed our material to light photons of energy starting at 14 eV; all the optical characteristics of both compounds are calculated using the expected lattice constant in equilibrium conditions. All optical characteristics may be found using the dielectric function \( \varepsilon(\omega) \).

3.4.1. The Dielectric Function

The dielectric function is represented mathematically by the symbol \( \varepsilon(\omega) \), which includes the real component and imaginary component, which can be interpreted as \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \). The measured real component is represented by \( \varepsilon_1(\omega) \) of the total dielectric function \( \varepsilon(\omega) \), which disperses the incident light emitted by the material and electronically polarizes it, as shown in Figure 5. At zero electron volt energy, the value of the dielectric function for the compound GaGeF₃ was found to be 2.5 and the highest peak value for the \( \varepsilon(\omega) \) was 5 at 4.3 eV, while for the other compound, GaBeF₃, the value was 2.6 at 0 eV and the greatest value was approximately 22 at 2.2 eV. At 1.2 eV, the value of \( \varepsilon_1(\omega) \) for GaBeF₃ was also 20. According to the Penn model [41], the higher the dielectric function at zero energy \( \varepsilon_1(0) \), the smaller the band gap energy, and vice versa.

![Figure 5. The calculated dielectric function \( \varepsilon(\omega) \) for the GaMF₃ compound \((M = \text{Ge and Be})\).](image)

The Penn model predicts that GaGeF₃ has a \( \varepsilon_1(0) \) value of 2.52, resulting in a large band gap of 5.131 eV, whereas GaBeF₃ has a band gap of 5 eV. Within the energy range of 14.0 eV, the calculated \( \varepsilon_2(\omega) \) (the second component) of \( \varepsilon(\omega) \) is shown in Figure 5.
According to our inspection of the \( \varepsilon_2(\omega) \) spectrum, the first essential peak (critical energy) of the \( \varepsilon(\omega) \) (dielectric permittivity) for the GaBeF\(_3\) and GaBeF\(_3\) takes place at around 6 eV. At the X-symmetry point, the absorption edge is responsible for a direct optical move from the valence to the conduction band. The curve begins to rise and fall over the threshold energy. GaGeF\(_3\) has a maximum peak of 5 at around 5.5 eV, while GaBeF\(_3\) has a maximum of 37.0 at 0.0 eV. Due to the direct broad band gap of the compound’s results, it is ideal for application in devices using ultraviolet light.

### 3.4.2. The Refractive Index

To calculate different physical parameters, the refractive index is represented by \( \eta(\omega) \), optical conductivity by \( \sigma(\omega) \), the absorption coefficient by \( I(\omega) \), and reflectivity, \( R(\omega) \), using \( \varepsilon_1(\omega) \) and \( \varepsilon_2(\omega) \). Figure 6 depicts the calculated refractive index, \( \eta(\omega) \). The static refractive index \( \eta(0) \) represents the refractive index at zero eV and it has a value of 0.5 and 6.2 for GaBeF\(_3\) and GaGeF\(_3\), respectively, as it is presented in the refractive index spectrum. It is obvious from Figure 6 that the curves of \( \eta(\omega) \) for the compounds do not match and show little change. GaGeF\(_3\) has a maximum peak refractive index of 6.2 at 0 eV photon energy, while GaBeF\(_3\) has the highest peak refractive index of 3.81 at a photon energy of 2.21 eV, as shown in Figure 5. From the value of the refractive index, we are able to establish how much light is refracted from the material compound, which is especially useful in photoelectric applications. From Figure 6, it is clear that the photons are facing the obstacle as they enter the compound, due to the interaction of the photons with the electrons; this is why the refractive index is greater than one (\( \eta(\omega) > 1 \)). The larger a material’s refractive index, the more photons are deflected as they pass through it. Every procedure that increases a material’s density of electrons likewise enhances its refractive index.

![Figure 6. The calculated refractive index of the GaMF\(_3\) compound (M = Ge and Be).](image)

### 3.4.3. Absorption Coefficient

The absorption coefficient \( I(\omega) \) can be obtained by the application of the dielectric function, \( \varepsilon(\omega) \). The selected compounds have major absorption factors at energy levels ranging from 0 eV to 14.0 eV for GaGeF\(_3\), while GaBeF\(_3\) has energy levels ranging from 4.0 eV to 14.0 eV, as shown in Figure 7. This is the point at which a compound starts to efficiently absorb electromagnetic radiation. Both of these compounds have different threshold points, which are 0.0 eV and 3.80 eV for GaGeF\(_3\) and GaBeF\(_3\), respectively. Different absorption peaks of 81, 130, 138, and 122 occur for GaGeF\(_3\) at 2.20, 7.50, 10.30, and 13.70 eV of energy, respectively, whereas the absorption peaks of 72, 70, 118, 75, and 100 occur for GaBeF\(_3\) at 5.3, 6, 7, 10, 12, and 12.2 eV of energy, respectively.
photon energy increases, the reflectivity increases. The values are 0.05, 0.25, 0.35, and 0.34 at 7.5, 10.5, and 13.5 eV, respectively. This is also the case for GaGeF₃; as the photon energy increases, the reflectivity increases. The values are 0.05, 0.25, 0.35, and 0.34 at 0, 54, 7.8, and 13.5 eV, respectively. The reflectivity of GaBeF₃ is very low compared to GaGeF₃; hence, GeBeF₃ is more transparent in the energy range from 0 to 4.4 eV than GaGeF₃. The material’s transparency indicates that these compounds could be used to make lenses.

3.4.5. Optical Conductivity

The mathematical representation of photon conduction is \( \sigma(\omega) \), which tells us the movement of electrons in a material, as caused by the application of an electromagnetic field. From the dielectric function, we can investigate the conductivity \( \sigma(\omega) \), as depicted in Figure 9. The photon conductivity starts from 0 at 0 eV for the compound GaGeF₃ and...
reaches a value of 5500 at 2.3 eV, then decreases to 100 in a range of energy of about 4.0 to 6.0 eV, reaching its maximum value of 6500 at 7.9 eV. Another peak of 4000 is observed at 10.3 eV, while for GeBeF₃, the optical conductivity is nil at an energy range from 0 to 4 eV. Its value then increases, and peaks of 3500, 4500, and 3000 are observed at 5.1, 7.2, and 10 eV, respectively. As a result, we found that the compound of GaGeF₃ was optically more conductive at low energy levels, compared to GeBeF₃.

3.5. The Energy Loss Function (ELF)

To find or characterize the intra-band, inter-band, and Plasmon interdependencies’ energy loss function (ELF), the energy-loss function can be employed. When a fast-moving electron enters the material and passes through it, the electron decelerates and loses energy. Figure 10 shows the calculated optical energy loss function (ELF) for both compounds. Initially, there was minimum energy loss in the range of photon energies from zero eV and 2.4 eV, then a significant loss occurred from 5.0 eV to 14.0 eV. The highest energy loss, of 1.55 for GaBeF₃ and 3.53 for GaGeF₃, occurred with the energies of the incident photon at 8.8 eV and 12 eV, respectively.

Figure 9. The computed conduction of incident light, represented by the $\sigma(\omega)$ of the GaMF₃ (M = Ge and Be) compound.

Figure 10. The computed optical energy loss function $L(\omega)$ of the GaMF₃ (M = Ge and Be) compound.
4. Conclusions

In the current research, we successfully examined the structural, optical, electrical, and elastic properties of ternary fluoroperovskite GaMF$_3$ (M = Ge and Be) compounds. These represent the most precise and creative results available. Based on optimal structural parameters, we came to the conclusion that GaMF$_3$ (M = Ge and Be) compounds are cubic and structurally stable. To predict the elastic parameters, such as the fundamental elastic constant, Poisson’s ratio, ductility, Cauchy’s pressure, shear modulus, Pugh ratio, and Young’s modulus, the IRelast package was used. These results give us confidence that these materials can be used in numerous contemporary electrical technologies. We investigated the fundamental electrical properties of the compounds of interest, using the TB-MBJ potential approximation method. GaGeF$_3$ is a metal, while GaBeF$_3$ is an insulator with an indirect (X-M) energy gap of 3.89 eV, as we have shown. The largest contributors to the DOS are F-tot and Ga-s, with states in the valence band for GaBeF$_3$, and the largest contribution to the conduction band is from the Ga-p state for GaGeF$_3$, whereas in GaGeF$_3$, the largest contribution is from Ga-p and F-tot in the valance band, while in the conduction band, Ge-tot and Ge-s show the largest contribution.

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