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DFT BASED FIRST-PRINCIPLE STUDY OF THE STRUCTURAL, ELASTIC, ELECTRONIC, AND OPTICAL PROPERTIES OF BERYLLIUM-BASED FLUOROPEROVSKITES $BeMF_3$ (M = TI AND V)

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Abstract: We present a theoretical comprehensive study which predicts and examines the outcomes of the structural, elastic, electronic, and optical properties of beryllium-based fluoroperovskite $BeMF_3$ (M = Ti and V) compounds which was performed based on DFT (Density Functional Theory). The theoretical computation was done through the simulation package of WIEN2k, in which the implemented method of Full-Potential Linearized Augmented Plane Wave (FP-LAPW) was used. For the treatment of exchange correlation potential, the Generalized Gradient Approximation (GGA) was used for structural and elastic properties while the Modified Becke-Johnson (mBJ) exchange potential was used for a better understanding of the electronic and optical properties. Structural optimization was done with the Birch-Murnaghan equation of state, for the outcomes of fundamental optimized lattice parameters. The optimized 4.0833 Å and 4.0112 Å lattice constants were found for the $BeTiF_3$ and $BeVF_3$, respectively, and we found that both these compounds were structurally stable. For the computation of the elastic constants (ECs) of these crystals the lRelast package was used. Elastically these compounds were found to be mechanically stable because they satisfy the stability criteria, and are anisotropic and ductile in nature. Both the compounds of interest are metallic in nature and have overlapping valence and conduction bands. The TDOS and PDOS (total and partial density of state) plots were used to infer the relevance of the states contributed by each constituent element to the valence and conduction bands. Important optical properties, namely the dielectric function $\mathcal{E}(\omega)$, optical conductivity $\sigma(\omega)$, reflectivity R(ω), refractive index $\eta(\omega)$, and extinction coefficient k(ω) were examined and evaluated in a wide energy range (0–40 eV). Both the compounds were found to possess high optical conductivity in the low energy range, and because of these properties both the materials can be deemed to be likely to be of value in many modern electronic devices. To the best of our knowledge, this is the first precise theoretical insight into the some of the physical properties of $BeMF_3$ (M = Ti and V) compounds. These properties are still to be verified experimentally.

Keywords: Elastic properties; Electronic properties; Fluoroperovskites; FP-LAPW; GGA; mBj; Optical properties; Structural properties; WIEN2k.

INTRODUCTION

The ternary group of crystalline structures includes the perovskites with the structure of ABX_3 stoichiometry, in which A and B are metallic cations and X is an anion. A subclass of perovskites is ABF_3 (the fluoroperovskites), in which X in

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ABX_3 is replaced by F. Depending on the A and B constituent atoms in combination with F, this fluoroperovskite family has a wide range of applications in many fields because of its simple crystalline structure. The applications of the fluoroperovskites class have found in radiation dosimeter,[1] optical properties,[2-4] tunable laser,[5] ferroelectricity,[6] high-temperature super-ionic behavior,[7] semiconductivity,[8-10] antiferromagnetism,[11] catalytic activity,[12] piezoelectricity,[13,14] and superconducting properties.[15,16] Fluoroperovskite mixtures in combination with transition elements form a stable crystal structure.[17,18] Recently fluoroperovskite compounds gained a remarkable interest for the material scientists due to their astonishing desirable properties. Mudasser Husain et al. reported some physical properties of $ZnXF_3$, X = Y, Bi using GGA within the FP-LAPW method incorporated in the WIEN2k simulation code.[19] Sajid Khan et al. investigated some of the physical properties of Tl-based fluoroperovskite compounds $TlXF_3$ (X = Ca, Cd, Hg, and Mg), based on *ab-initio* DFT calculations.[20] Due to the complex composition of A and B elements in these $BeMF_3$ (M = Ti and V) compounds, their applications can be deemed to be relevant in many modern electronic devices. To the best of the authors' knowledge, there have been insufficient experimental and theoretical research focused to the fundamental structural, elastic, electronic, and optical properties of $BeMF_3$ (M = Ti and V) compounds. For the purpose of getting a better understanding of some of the basic physical properties we have chosen and computed $BeMF_3$ (M = Ti and V) compounds through the WIEN2k package based on the Density Functional Theory (DFT) scheme of study. These compounds are new and this is the first attempt to present precisely some of their physical properties, which will be available for material scientists to confirm experimentally. A theoretical exploration of the structural, elastic, electronic, and optical properties of these compounds is required in order to fully exploit their properties for future technological applications.

COMPUTATIONAL METHODOLOGY

The computational approach used for this study was the WIEN2k[21] simulation code based on the scheme of density functional theory (DFT). For solving the Kohn–Sham equations the incorporated FP-LAPW[22] scheme in WIEN2k was used. This methodology is a fundamental quantum mechanical procedure for many body problems and it has been confirmed to be among the most reliable approaches for identifying physical properties. To tickle with the exchange correlation potential, the GGA and mBj[23] potential approximations are used for the predicting the outcome of physical properties. We employ a parameter RMT×Kmax = 8 to define the matrix size (convergence) in the computations shown here, where Kmax is the plane wave cut-off and RMT is the smallest of all the atomic sphere radii. The radii of the muffin tins (MT) are selected to be roughly proportionate to the ionic radii. The overall system energy is stable within 10^{-3} Ry, at which the self-consistent computations are called converged. The charge density within Fourier expanded up to Gmax = 14, whereas the wave functions inside the valence spheres were enlarged up to lmax = 10. For precise and confident computation the Monkorst-Pack 3000 special k-points were carried out and taken in the Brillouin zone. For precise bands and optical properties predictions the mBj approximations were used. Optimized lattice parameters are

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gained from the Birch-Murnaghan equation of states.[24] The complex dielectric function

$$\mathcal{E}(\omega) = \mathcal{E}_1(\omega) + i\mathcal{E}_2(\omega)$$

is commonly used to delineate the optical properties characteristics of a solid. All other optical parameters are measured from the $\mathcal{E}(\omega)$. For the computation of cubic elastic constants (ECs) and other mechanical properties, the IRelast package developed by Jamal Murtaza et al.[25] was used effectively.

STRUCTURAL PROPERTIES

The major goal of this research is to use the FP-LAPW methods to compute the total energy as a versus unit-cell volume almost at the equilibrium cell volume V_0 in $BeMF_3$ (M = Ti and V) compounds. Beryllium-based fluoroperovskites $BeMF_3$ (M = Ti and V) compounds exit in an ideal cubic perovskites crystal structure having the Pm-3m (#221) space group. The fluoroperovskite $BeMF_3$ (M = Ti and V) crystal structure is depicted in Figure 1 in which the Be atom lies at (0,0,0),the M atoms (M = Ti and V) are positioned at (0.5, 0.5, 0.5), and the F atom is at the Wyckoff positions of (0, 0.5, 0.5) or (0.5, 0, 0.5) or (0.5, 0.5, 0) as can be seen from Figure 1.

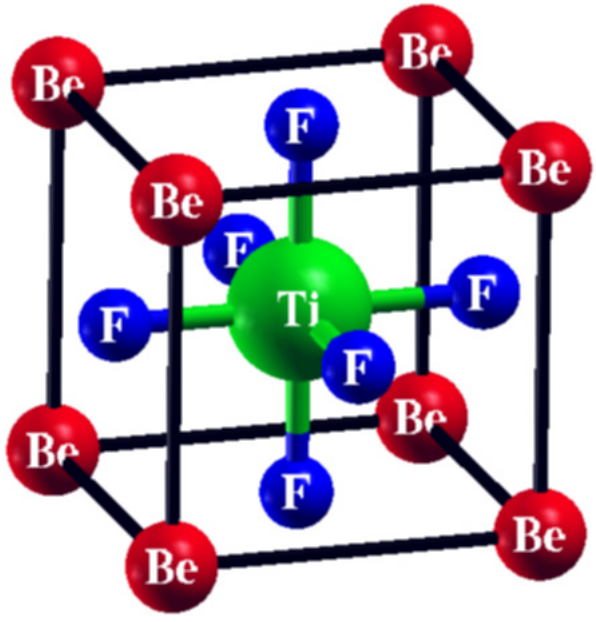

Figure 1. Unit cell crystal structure of $BeMF_3$ (M = Ti and V)

A volume optimization technique found by using Murnaghan's equation of states was used to conduct structural relaxation. From the optimized fit curve, the basic structural parameters were measured. The minimal total energy was gained when the lattice constants were considered as the equilibrium lattice constant of a crystal. The Murnaghan's fitted curve, presented in terms of the unit cell volume versus unit cell energy, is displayed in Figures 2A and 2B. From these Figures it can obviously be seen that for both the compounds the unit cell energy is maximum at a certain volume and by varying the unit cell volume the corresponding energy of the cell decreases. A

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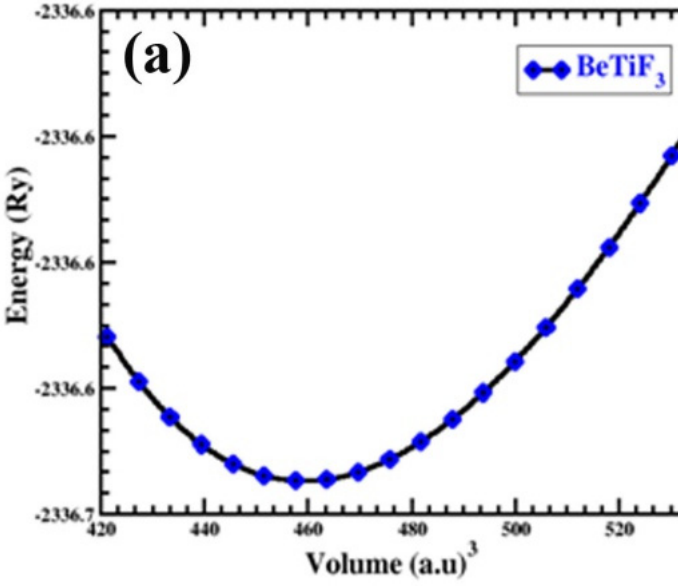
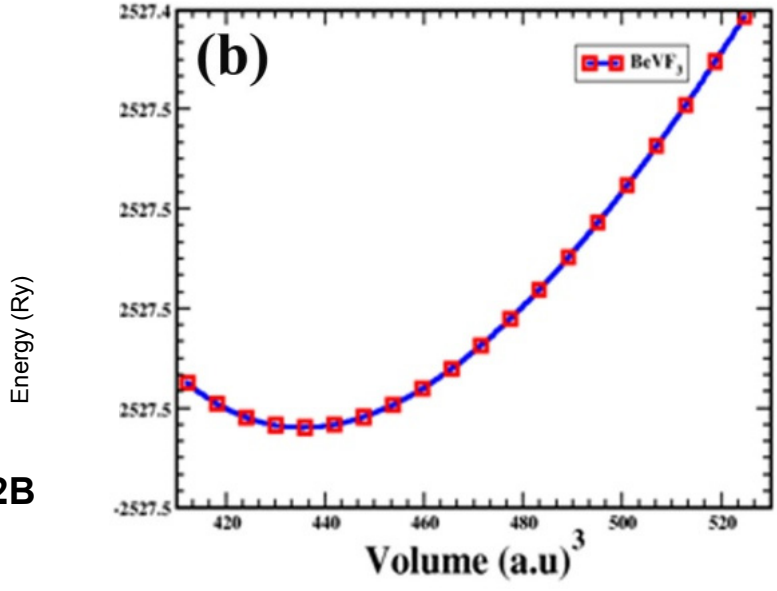
point reached where the system gains stability and all the parameters can be taken into consideration from the optimized state.



2A



2B

Figures 2A and 2B. Unit cell structural optimization of $BeMF_3$ (M = Ti and V) compounds. 2A = $BeTiF_3$; 2B = $BeVF_3$.

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The enthalpy (H) can be determined using the following relation to study the synthesizability of the presented compounds

$$H = E_0 + PV_0 \quad \text{(i)}$$

Where, H represents enthalpy, *Eo* corresponds to minimum energy, *P* shows bulk pressure, and V_0 is the bulk volume of the system.

The stability of the compounds beside disintegration into stable solid structures is shown by negative enthalpy values.[26] The computed fundamental structure parameters for $BeMF_3$ (M = Ti and V) compounds are listed in Table 1 and it is found that these compounds are structurally stable and have negative values of enthalpy, which point out the confirmation for the stability.

Table 1. Computed optimized structural parameters comprising lattice constant a_o (Å), Bulk Modulus B (Gpa), Bulk Modulus pressure derivative $B^/$ (Gpa), optimized energy E_0 (Ry), optimized volume V_0 ((a.u)^3) and Enthalpy H (J) for $BeMF_3$ (M = Ti and V) compounds.

Optimized Structural parameters	$BeTiF_3$	$BeVF_3$
Lattice Constant (a_0)	4.0833	4.0112
Bulk Modulus (B)	90.9087	96.7167
Derivative of Bulk Modulus ($B^/$)	4.8294	5.2337
Ground state energy (E_0)	-2336.6574	-2527.492
Ground State Volume (V_0)	459.3713	435.5521
Enthalpy (H)	-137.187	-105.383

ELASTIC PROPERTIES

The elastic constants C_{ij} can be used to investigate the mechanical behavior of materials. The criterion of elastic constant parameters explains the reaction to an applied macroscopic stress. Constants of elasticity C_{ij} of solids establishes a physical link between mechanical and active functioning, as well as defining in what way a deformation can be created by stress applied and subsequently restored to its initial stage after the applied stress has passed.[27] C_{ij} provides critical features of a material that provide valuable insights for its structure stability, anisotropy, and bonding character between adjacent atomic planes. C_{11}, C_{12}, and C_{44} are three self-reliant elastic constants found in cubic compounds. To obtain these parameters, a measurement is made of the distortion produced in cubic unit cell when an appropriate strain tensor is applied, thus yielding in an energy strain correlation. For

this task the IRelast package developed by Jamal Murtaza is used very effectively. Table 2 summarizes the C_{ij} and other mechanical characteristics measured.

Table 2. Computed elastic parameters of $BeMF_3$ (M = Ti and V) fluoroperovskites compounds, using the IRelast package

Computed Elastic Parameters	$BeTiF_3$	$BeVF_3$
C_{11} (GPa)	**164.8000**	**154.676**
C_{12} (GPa)	**32.0806**	**47.6173**
C_{44} (GPa)	**12.765**	**27.245**
E (GPa)	**47.563**	**51.464**
G (GPa)	**22.78**	**19.34**
A	**0.29**	**0.34**
v	**0.49**	**0.53**
B/G	**4.65**	**3.48**
B (GPa)	**88.932**	**95.576**

Because the elastic constant C_{ij} and bulk modulus "B" examined are positive, the criterion: $(C_{11}–C_{12}) > 0$; $(C_{11} + 2C_{12}) > 0$; $C_{44} > 0$; and the B should prompt a standard: $C_{12} < B < C_{11}$, which meets the mechanical stability requirements for a cubic crystals system.[28] To our best of knowledge, no experimental findings or theoretical results for the elastic constants of the presented compounds have been provided, so these elastic property calculations might be utilized as a citation for future research. The following relationships are used to calculate the other elastic parameters A, G, and E.[29]

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad \text{(ii)}$$

$$\upsilon = \frac{3B-2G}{2(2B+G)} \quad \text{(iii)}$$

$$E = \frac{9GB}{3B+G} \quad \text{(iv)}$$

$$G = \frac{1}{2}(G_\upsilon + G_R) \quad \text{(v)}$$

$$G_\upsilon = \frac{1}{5}(C_{11} - C_{12} + 3C_{44} \quad \text{(vi)}$$

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

Where A, in equation-ii is the anisotropy factor, v is the Poisson ratio (equation-iii), E in equation-iv shows Young's modulus, G is in equation-v is the shear modulus, G_V is Voigt's shear modulus in equation-vi, subsequent to the G upper limit values and and G_R is Reuss's shear modulus in equation-vii, subsequent to the lower bound of G values. From Table 2, it is very clear that the elastic constants and bulk moduli of both the compounds are positive and thus are mechanically stable. A is equal to one for an isotropic compound; nevertheless, a greater or lesser number indicates anisotropy. The extent of the variation from 1 determines the elastic anisotropy of crystals. As in this reported work (Table 2) the magnitude of the anisotropy factor is 0.29 for $BeTiF_3$ and 0.34 for $BeVF_3$, and it thus depicts an anisotropic nature. A material having a greater E value is stiffer, and accordingly E is a fine indicator of the material's stiffness. Bonding force information is provided by v. The value of the Poisson's ratio (v) is small (< 0.1) for covalent materials; however, it is 0.25 for ionic compounds.[30] $BeTiF_3$ has a value of 0.48100 for v, while $BeVF_3$ has a value of 0.57157 in these studies. As a result, an excessively ionic contribution in intra-bonding ought to be expected for these two materials. Mechanical characteristics of materials such as ductility and brittleness are described by the proposed B/G relationship. The standard criteria for the B/G relationship is 1.75, known as Pugh's criteria.[31] If the B/G ratio is more than 1.75, the material appears to be ductile. From Table 3 it is clearly depicted that for both the materials the Pugh's ratio appears to be greater than 1.75, i.e., 2.36 for $BeTiF_3$ and 2.67 for $BeVF_3$ and thus $BeMF_3$ (M = Ti and V) compounds are mechanically ductile. This is the first reported theoretical study of elastic properties for $BeMF_3$ (M = Ti and V) compounds, which can be used as a reference data for future research perspectives. Thus in summary, both the materials are hard, anisotropic, mechanically stable, and ductile.

ELECTRONIC PROPERTIES

Bands structure

The energy band structures, as well as total and partial density of states, are employed to outline the electronic properties of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds. We employed the modified Becke–Johnson approximation to evaluate these features, since the GGA underestimates a material's energy band gap. The band structures of these compounds, at the equilibrium volume with high symmetry direction in the first Brillion zone, were calculated, as shown in Figure 3. From Figure 3 of the band structures for $BeMF_3$ (M = Ti and V) fluoroperovskite compounds, it can be seen that for both the materials the valence band (VB) and conduction band (CB) overlap, resulting a metallic nature. This strong metallic nature is due to the presence of transition elements, i.e., M = Ti and V. It is worth noting that, to our knowledge, there have not been any theoretical predictions or experimental data about the band gap of these perovskite compounds to match these findings. We are confident in the precision of reported results, because it was obtained utilizing 3000 massive K-points within the irreducible Brillion zones (IBZ) within the most accurate modified Becke–Johnson method. Thus the presented results provide a ground reference for a future research prospective.

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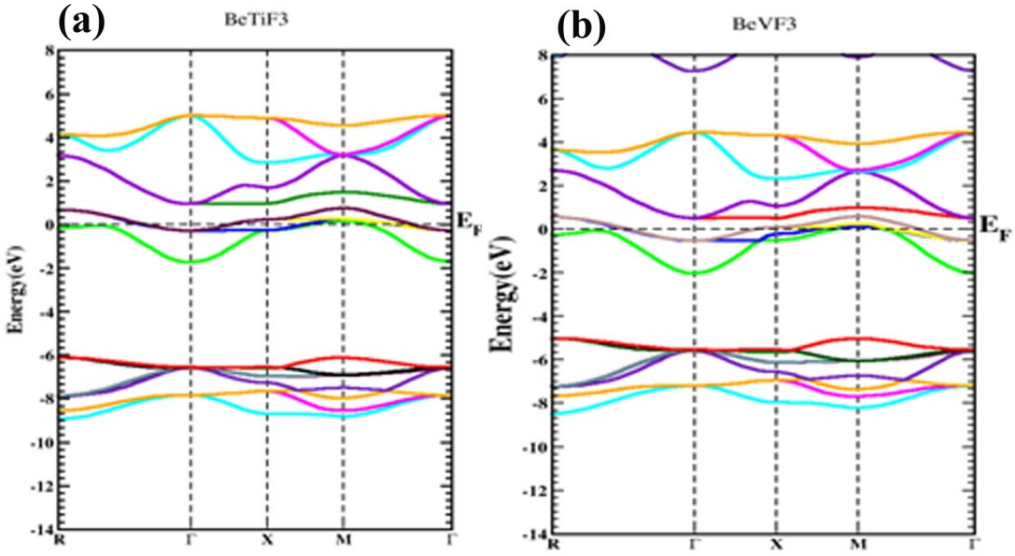
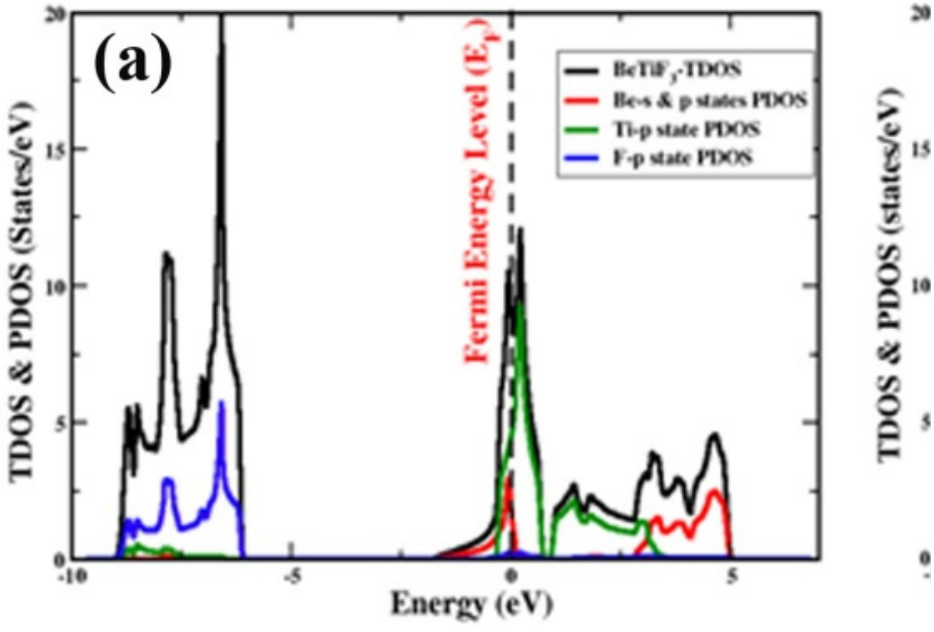


3A 3B

Figures 3A and 3B. Electronic band structures of BeMF3 (M = Ti and V) fluoroperovskites compounds. 3A: $BeTiF_3$, 3B: $BeVF_3$.

Density of states (DOS)

To understand the contribution of various states to the band structures, the electronic density of state (DOS) is crucial. For the said purpose, the total and partial density of states, i,e., TDOS and PDOS are presented in Figures 4A and 4B.



4A

Figure 4A. Computed TDOS and PDOS for the $BeMF_3$ (M = Ti) fluoroperovskite compound.

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4B

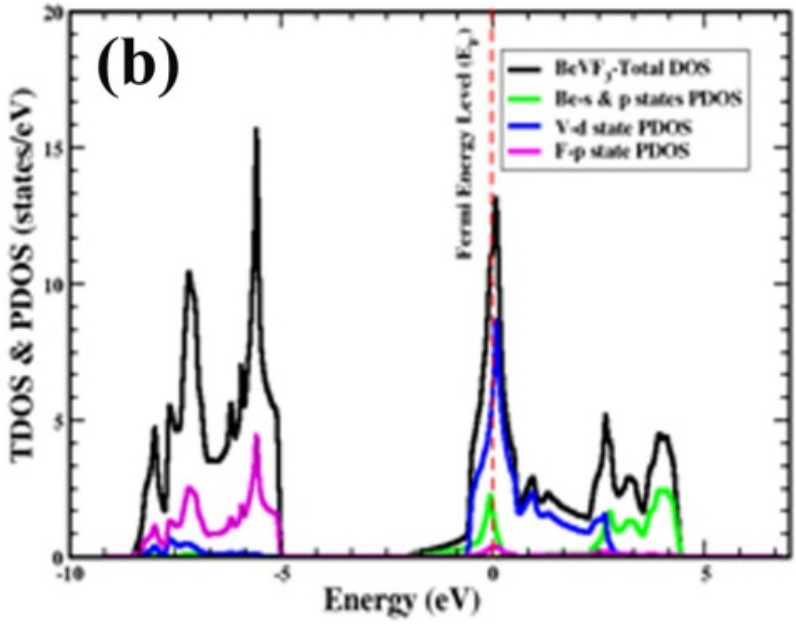

Figure 4B. Computed TDOS and PDOS for the $BeMF_3$ (M = V) fluoroperovskite compound.

The dotted line at 0 eV energy represents Fermi energy level E_F. It can be very neatly seen that in both $BeMF_3$ (M = Ti and V) compounds the valence and conduction band completely overlap, which confirms the metallic nature. TDOS and PDOS shows the participation of the states to the valence and conduction bands. Figures 4A and 4B depict that the overlapping nature is to a major extent due to the transition elements of Ti in $BeTiF_3$ and V in $BeVF_3$. For both the compounds the number of states within the conduction band is maximum, which shows strong electrical conduction.

OPTICAL PROPERTIES

The FP-LAPW is a useful theoretical scheme for calculating a compound's optical characteristics. The optical characteristics of $BeTiF_3$ and $BeVF_3$ compounds have been studied using a complex dielectric function of the type:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

which describes the medium's optical response completely at photon energies in the extent from 0 eV to 40 eV.

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The dielectric function:

The expression for the complex dielectric function is:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

from which the completely optical response at photon energies in the extent from 0 eV to 40 eV can be explained. The $\varepsilon_1(\omega)$ is the real component and $\varepsilon_2(\omega)$ is the imaginary part of the dielectric function, that is directly associated to a material's electronic bands structure and determines absorptive behavior. The Kramers-Kronig dispersion relation is used to calculate the spectrum of $\varepsilon_1(\omega)$ dielectric functions for $BeTiF_3$ and $BeVF_3$ compounds and is depicted in Figure 5.[32]

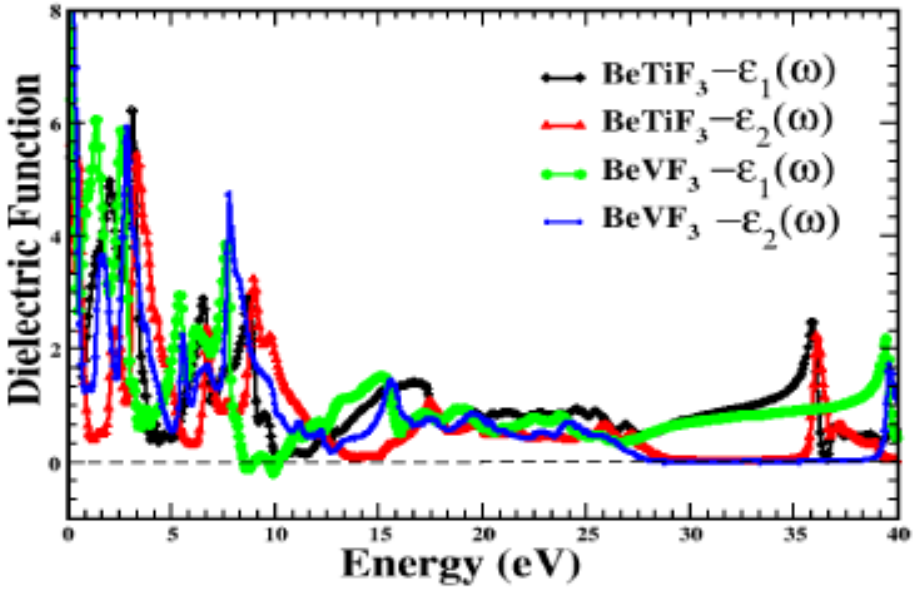

Figure 5. Simulated optical dielectric function $\varepsilon(\omega)$ of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds.

Figure 5 depicts both the real and imaginary part of dielectric function, i.e., $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ The function "$\varepsilon_1(\omega)$" returns information about a material's electronic polarizability. The zero frequency limit $\varepsilon_1(0)$ is used to calculate the static dielectric constant at zero, which lies at about 1.9 for $BeTiF_3$ and 3.26 for $BeVF_3$, as can be seen from Figure 5. The curves of the real part of $\varepsilon_1(\omega)$ vary and reaching a maximum of 6.13 and 6.19 for $BeTiF_3$ and $BeVF_3$, respectively, at a low energy range.

The imaginary part $\varepsilon_2(\omega)$ is closely tied to a material's electronic band structure and explains the material's absorptive behaviour. The spectrum of $\varepsilon_2(\omega)$ is shown in Figure 5 for both the $BeMF_3$ (M = Ti and V) compounds. Figure 5 also displays that both the materials possesses considerable optical absorption at about 3.5 eV energy and thus these materials are found to be good optical conductors.

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Optical conductivity σ(ω):

The optical conductivity σ(ω) which is calculated from the complex dielectric function, *Ɛ(ω)*, describes the conduction of electrons caused by an applied electromagnetic field and the computed spectrum is shown in Figure 6.

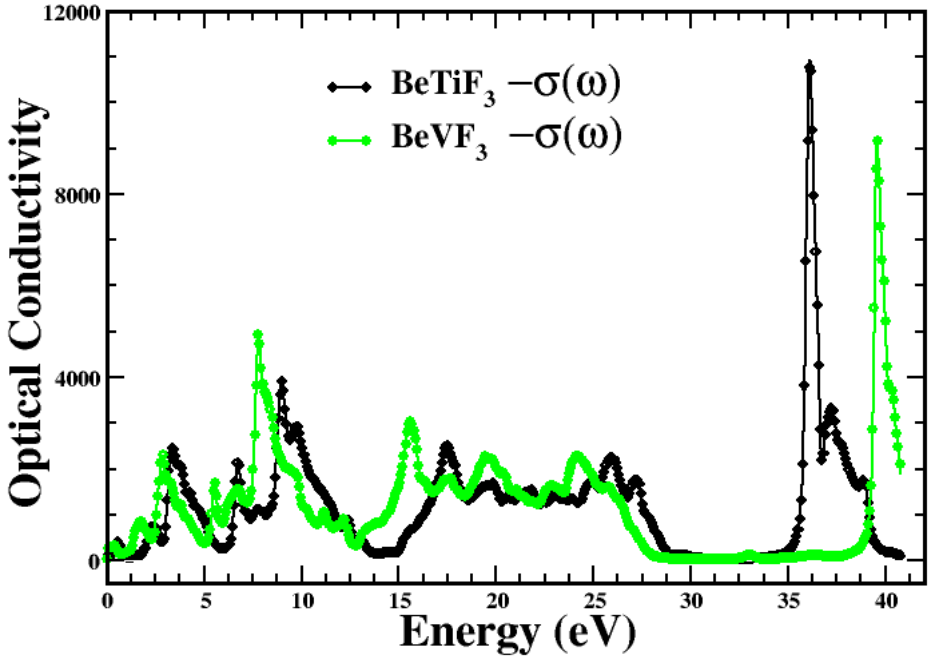

Figure 6. Simulated optical conductivity σ(ω) of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds.

The optical conductivity figure, Figure 6, displays that both the material are optically more conductive at high incident photon energy.

Optical reflectivity (R(ω)): As demonstrated and shown in Figure 7, the spectrum of reflectivity R(*ω*) is formed out of the contribution of Ti-p states at the Fermi level and V-d state, i.e., the reflectivity occurs from the overlapping nature of valence and conduction bands.

The reflectivity exists at a high level at a low incident photon energy for both the compounds. The reported compounds are transparent to incident photons in the aforementioned domains, implying that they can be used to make lenses and anti-reflection coatings.

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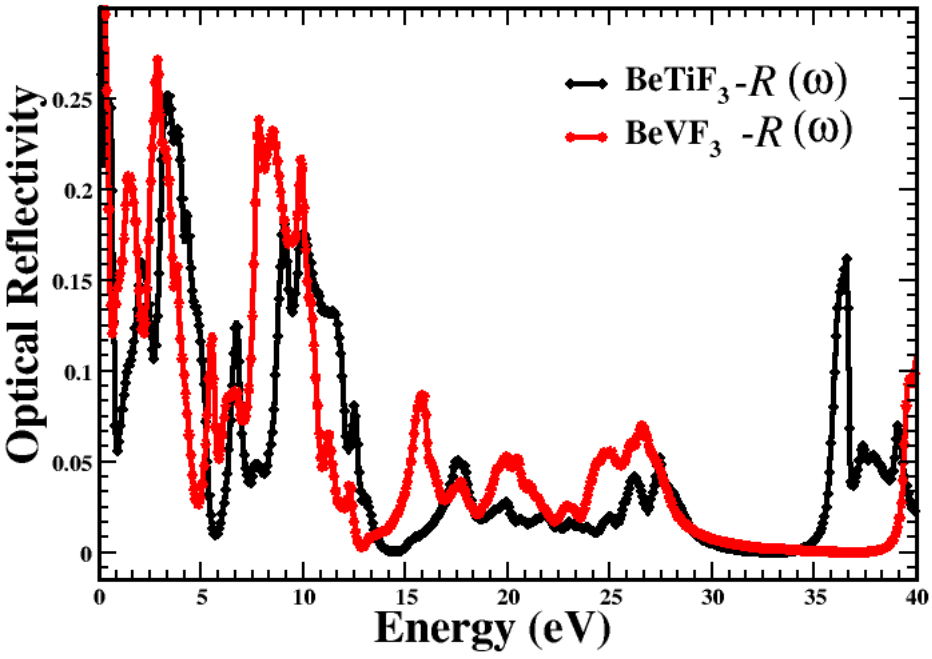

Figure 7. Simulated optical reflectivity R(ω) of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds.

Refractive index and extinction coefficient:

The refractive index is a vital parameter to understand when calculating the extent of refraction of light, as it is particularly valuable in photoelectric applications. We have observed an anisotropic nature of these compounds. The measured refractive index for the compounds of interest is presented in Figure 8 which represents the two parts: the refractive index and the extinction coefficient.

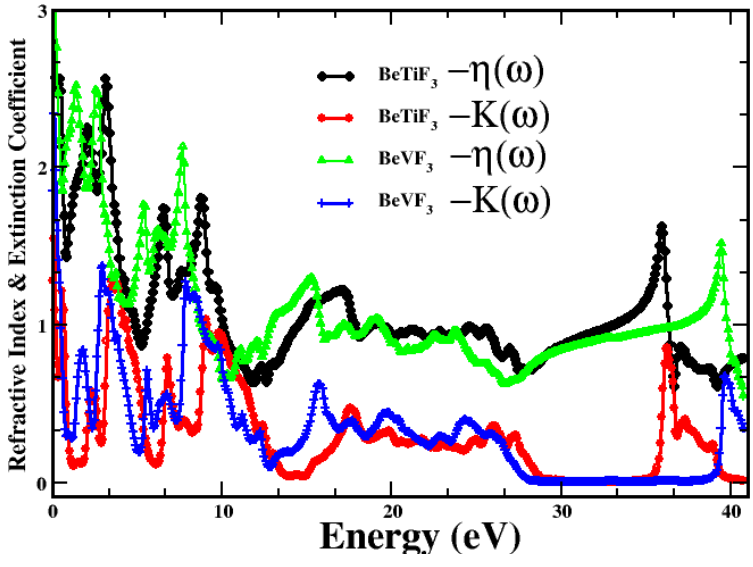

Figure 8. Simulated refractive index η(ω) and extinction coefficient K(ω) of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds.

The static $\eta(0)$ refractive index was observed to be 2.57 for $BeTiF_3$ and 3 for $BeVF_3$ at zero energy. This static refractive index is also the maximum peak value for both the compounds. Because photons are slowed as they enter a substance due to interactions with electrons, the refractive index is greater than one. The greater the refractive index of a material, the more photons is retarded while travelling through it. In general, every mechanism that raises the electron density in a material raises the refractive index as well. Looking at Figure 8 for the imaginary part, which is the extinction coefficient $K(\omega)$, it is very clear from the Figure that both the materials display the same pattern of curve, i.e., extinction coefficient. As the extinction coefficient represents different measures of the absorption of light in a medium, so it is found that both $BeTiF_3$ and $BeVF_3$ have a positive and high value of extinction coefficient in the energy range of 0 eV to 40 eV.

In summary, these materials possesses good optical properties, and it can be concluded that the materials are metallic, transparent to incident light, optically more conductive and absorptive, and have a high value of refractive index. The reported outcomes are very precise and provide a groundwork for experimental verification.

CONCLUSIONS

DFT based work on structural, elastic, electronic, and optical properties of $BeMF_3$ (M = Ti and V) fluoroperovskite compounds is computed precisely and is presented. Optimized structural parameters are computed and the calculation is based on the computed optimized parameters. Structurally both the materials are found to be stable with a negative value of enthalpy. The most precise mBj approximation is used for the prediction of band structure of these compounds. The electronic properties reveal that these compounds are metallic in nature with having overlapping valence and conduction bands at the Fermi level. With the use of IRelast package for elastic properties, it is found and concluded that both the materials are mechanically stable, brittle, and anisotropic. It is concluded in the optical properties for these compounds that these material are transparent to incident light, optically more conductive and absorptive, and that they have a high value of refractive index. Such materials can be applicable for the development of lenses and anti-reflection coatings.

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