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

A presented theoretical comprehensive study predicts and examine the outcomes of Structural, elastic, electronic and optical properties of Beryllium-Based Flouoroperovskites $BeMF_3$ (M = Ti and V) compounds which is performed based on DFT (Density Functional Theory). The theoretical computation is done through the simulation package of WIEN2K, in which the implemented method of Full-Potential Linearized Augmented Plane Wave (FP-LAPW) is used. For the treatment of exchange correlation potential, the Generalized Gradient Approximation (GGA) is used for structural and elastic properties while the Modified Becke–Johnson (mBJ) exchange potential is used for the better understanding of elctronic and optical properties. Structural optimization is done with Birch–Murnaghan equation of state, for the outcomes of fundamental optimized lattice parameters. The optimized 4.0833 Å and 4.0112 Å lattice constants are founded for the $BeTiF_3$ and $BeVF_3$ respectively and we found that both these compounds are structuraly stable. For the computation of elastic constants (ECs) of these crystals, the IRelast package is used. Elastically these compounds are founded to be mechanically stable because it satisfy the stability criteria, anisotropic and ductile in nature. Both the compounds of interest are metallic in nature having an overlapping valence and conduction bands. The TDOS and PDOS (total and partial density of state) plots are used to infer the relevance of states contributed by each constituent element to the valence and conduction bands. Important optical properties namely Dielectric function $\varepsilon(\omega)$, optical conductivity $\sigma(\omega)$, reflectivity $R(\omega)$, refractive index $n(\omega)$ and extinction coefficient $k(\omega)$ are examined and evaluated in a wide energy range (0–40 eV). Both the compounds posseses high optical conductivity in the low energy range, due to which the properties of both the materials can be

deemed in many modern electronic devices. To our deep knowledge, this is the first precise theoretical insight to the some of the physical properties of $BeMF_3$ (M = Ti and V) compounds, which is yet to be verified experimentally.

Keywords: WIEN2K, FP-LAPW, GGA, mBj, Fluoroperovskites, Structural Properties, Elastic Properties, Optical Properties and Electronic Properties.

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Introduction

The ternary group of crystalline structures includes the perovskites structure with ABX_3 stoichiometry, in which A, B is metallic cations and X is an anion. A subclass of perovskites is ABF_3 (the Fluoroperovskites), in which X in ABX_3 is replaced by F. Depending on the A and B constituent atoms in combination with F, these Fluoroperovskites family has a wide range of applications in many fields because of its simple crystalline structure. The applications of Fluoroperovskites class have founded in radiation dosimeter [1] optical properties [2][3][4] tunable laser [5] ferroelectricity [6] high-temperature super-ionic behavior [7] semiconductivity [8][9][10] antiferromagnetism [11] catalytic activity [12] piezoelectricity [13][14] and superconducting properties [15][16]. Fluoroperovskites mixtures in combination with transition elements form a stable crystal structure [17][18]. Recently Fluoroperovskites compounds gained a remarkable interest for the material scientists due to its astonishing desirable properties. Mudasser Husain *et al.* reported some physical properties of $ZnXF_3$, X = Y, Bi using GGA within FP-LAPW method incorporated in 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 as can be seen in [20]. Due to the complex composition of A and B elements in these $BeMF_3$ (M = Ti and V) compounds, there applications can be deemed in many modern electronic devices. To the best of 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 get understanding the some basic physical properties we have chosen and computed $BeMF_3$ (M = Ti and V) compounds through WIEN2K package

based on DFT scheme of study. As these compounds are new and this is the first precise presented attempt for the outcomes of some physical properties, which will provide and facilitate material scientists to confirm experimentally. 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 is the Wien2k [21] simulation code based on the scheme of DFT. For solving the Kohn–Sham equations the incorporated FP-LAPW [22] scheme in wien2k is used. This methodology is a fundamental quantum mechanical procedure for many body problems and it has 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 is used for the predicting outcome of physical properties. We employ a parameter RMT×Kmax = 8 to define matrix size (convergence) in the computations shown here, where Kmax is the plane wave cut-off and RMT is the smallest of all 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 is used. Optimized lattice parameters are gained from the Birch-Murnaghan equation of states [24]. The complex dielectric function $\mathscr{E}(\omega) = \mathscr{E}_1(\omega) + i\mathscr{E}_2(\omega)$ is commonly used to delineate the optical properties characteristics of a solid. All other optical parameters are measured from the $\mathscr{E}(\omega)$. For the computation of cubic elastic constants (ECs) and other mechanical properties the IRelast package developed by Jamal Murtaza *et al.* [25] is used effectively.

Structural Properties

The major goal of this research is to use the FP-LAPW methods to compute 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 Flouoroperovskites $BeMF_3$ (M = Ti and V) compounds exits in an ideal cubic Perovskites crystal structure having Pm-3m (#221) space group. Flouoroperovskites

$BeMF_3$ (M = Ti and V) crystal structure is depicted in figure.01 in which Be atom lies at (0,0,0), M atoms (M = Ti and V) positioned at (0.5, 0.5, 0.5) and 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.01.

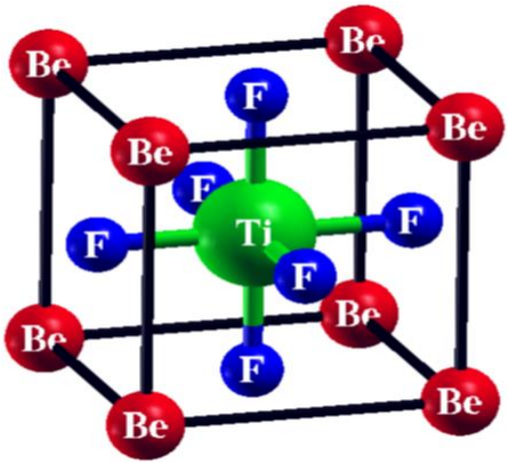

Figure 01 Unit cell crystal structure of $BeMF_3$ (M = Ti and V).

A volume optimization technique founded by Murnaghan's equation of states is used to conduct structural relaxation. From the optimized fit curve, the basic structural parameters are measured. The minimize total energy is gained through when the lattice constants is considered the equilibrium lattice constant of a crystal. The Murnaghan's fitted curve presented in term of unit cell volume versus unit cell energy is displayed in figure.02. From the figure it can be obviously seen that first for both the compounds the unit cell energy is maximum at certain volume and by varying the unit cell volume the corresponding energy of the cell decreases. A point reached where the system gain stability and all the parameters can be taken into consideration from the optimized state.

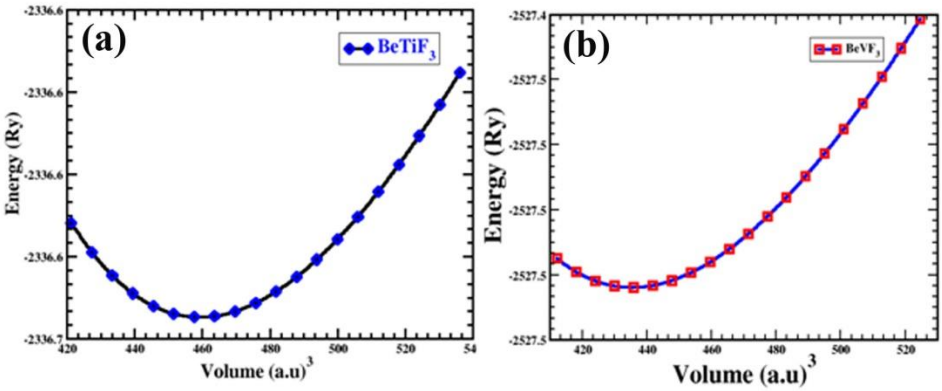

Figure 02 Unit cell Structural optimization of BeMF3 (M = Ti and V) compounds.

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

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

Where, H represent enthalpy, *Eo* corresponds to minimum energy, *P* shows bulk pressure, V_0 is 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.01 and it is found that these compounds are structurally stable and have negatives values of enthalpy, which point out the confirmation for the stability.

Table.01: 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, the distortion produced in cubic unit cell when an appropriate strain tensor is applied, yielding in an energy strain correlation. For this task the IRelast package developed by Jamal Murtaza is used very effectively. Table.03 summarizes the C_{ij} and other mechanical characteristics measured. 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 be prompt a standard: $C_{12} < B < C_{11}$, which meets the mechanical stability requirements for cubic crystals system [28]. As 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, 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 anisotropy factor, υ is the poison 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 the table.03, 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.03) the magnitude of the anisotropy factor is 0.29 for $BeTiF_3$ and 0.34 for $BeVF_3$, thus depicts an anisotropic nature. The material having a greater E value is stiffer, accordingly a fine indicator of the material's stiffness. Bonding force information is provided by υ. The rate of the Poisson's ratio (υ) is small ($\upsilon < 0.1$) for covalent

materials; however, it is 0.25 for ionic compounds [30]. $BeTiF_3$ has a value of 0.48100 for υ, while $BeVF_3$ has a value of 0.57157 in these studies. As a result, 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 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 the table.03 it is clearly depicted that for both the material 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 and mechanically stable and ductile.

Table.03: Computed elastic parameters of $BeMF_3$ (M = Ti and V) Flouoroperovskites 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**
υ	**0.49**	**0.53**
B/G	**4.65**	**3.48**
B (GPa)	**88.932**	**95.576**

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) Flouoroperovskites 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, are calculated, as shown in Figure. 03. From the figure.03 of bands structures for $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds, it can be seen that for both the materials the valence band (VB) and conduction band (CB) overlaps, resulting a metallic nature. This strong metallic nature is due to the presence of transition elements i-e M = Ti and V. It's worth noting that, to our knowledge, there haven't been any theoretical predictions or experimental data about the band gap of these perovskites compounds to match these findings. We're confident in the precision of reported results, because it is 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 future research prospective.

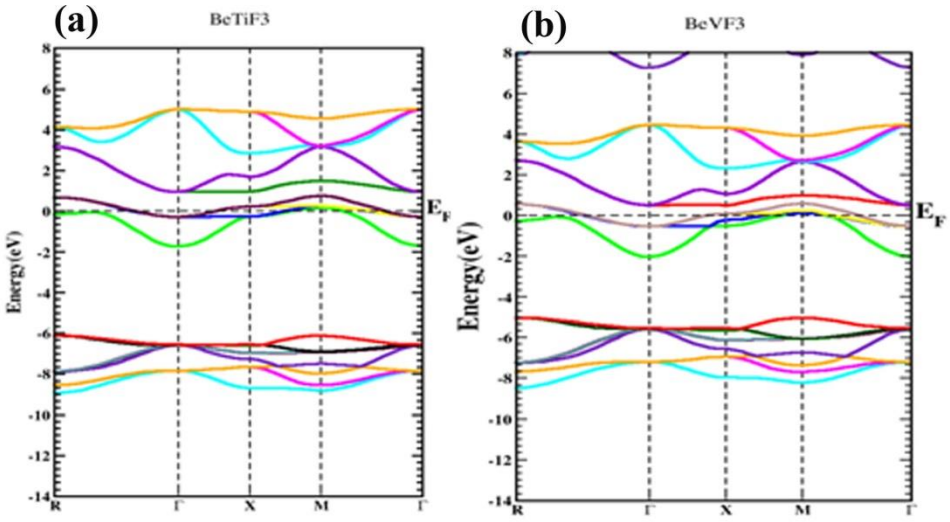

Figure 03 Electronic band structures of $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

Density of States (DOS)

To understand the contribution of various states to 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 is presented in figure.04.

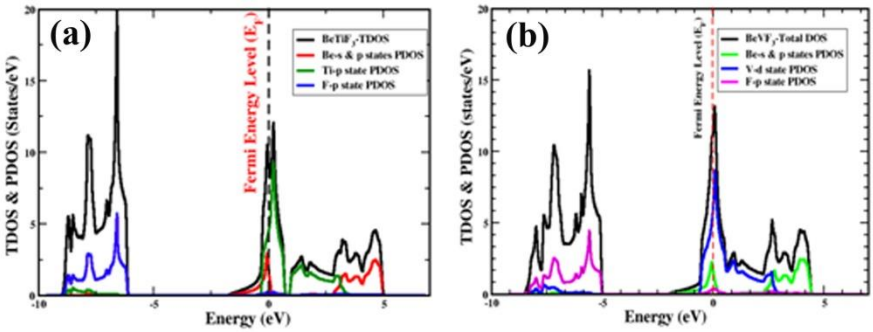

Figure 04 Computed TDOS and PDOS for $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

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 are completely overlaps, which confirms the metallic nature. TDOS and PDOS shows the participation of sates to the valence and conduction bands. Figure.04 depicts that the overlapping nature is majorly 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 $\mathscr{E}(\omega) = \mathscr{E}_1(\omega) + i\mathscr{E}_2(\omega)$, which describes the medium's optical response completely at photon energies in the extent from 0 eV to 40 eV.

The Dielectric Function ($\mathcal{E}(\omega)$)

The expression for the complex dielectric function is: $\mathscr{E}(\omega) = \mathscr{E}_1(\omega) + i\mathscr{E}_2(\omega)$, from which the completely optical response at photon energies in the extent from 0 eV to 40 eV can be explained. The $\mathscr{E}_1(\omega)$ is the real component and $\mathscr{E}_2(\omega)$ 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 $\mathscr{E}_1(\omega)$ dielectric functions [32] for $BeTiF_3$ and $BeVF_3$ compounds and is depicted in figure.05.

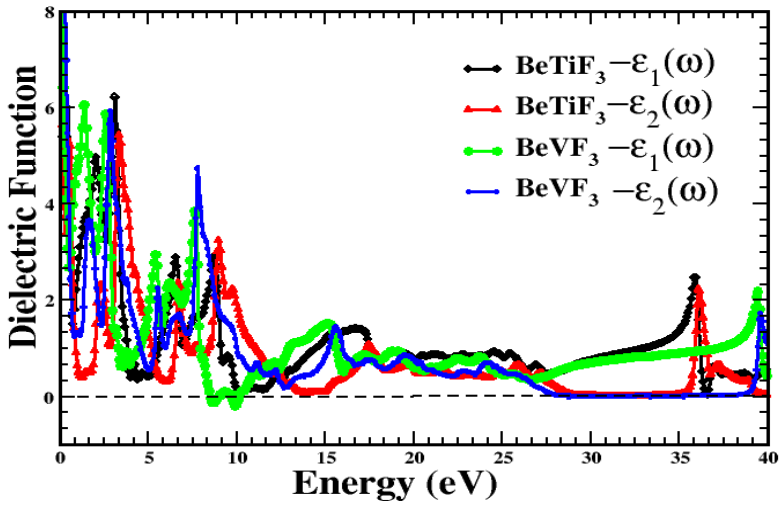

Figure.05: Simulated optical Dielectric function $\mathscr{E}(\omega)$, of $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

The figure.05 depict both the real and imaginary part of dielectric function i-e $\mathscr{E}_1(\omega)$ and $\mathscr{E}_2(\omega)$. The function "$\mathscr{E}_1(\omega)$" returns information about a material's electronic polarizability. The zero frequency limit $\mathscr{E}_1(0)$ 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 the same figure.05.The curves of real part of $\mathscr{E}(\omega)$ varies and reaching a maximum of 6.13 and 6.19 for $BeTiF_3$ and $BeVF_3$ respectively at low energy range.

The imaginary part $\mathscr{E}_2(\omega)$ which is closely tied to a material's electronic band structure and explains the material's absorptive behaviour. The spectrum of $\mathscr{E}_2(\omega)$ is shown in the same figure.05 for both the $BeMF_3$ (M = Ti and V) compounds. Figure.05 display that both the materials possesses considerable optical absorption at about 3.5 eV energy, thus these materials are found to be good optical conductors.

Optical Conductivity

The optical conductivity $\sigma(\omega)$ which is calculated from the complex dielectric function $\mathscr{E}(\omega)$, describes the conduction of electrons caused by an applied electromagnetic field and the computed spectrum is shown in figure.06.

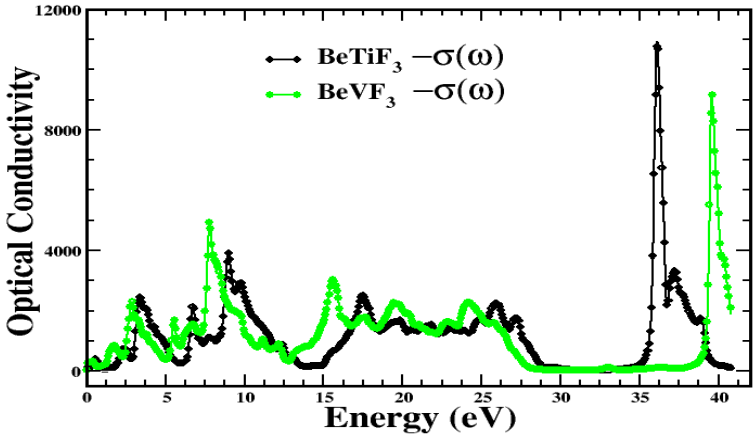

Figure.06: Simulated Optical conductivity σ(*ω*), of $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

The optical conductivity figure display that both the material are optically more conductive at high incident photon energy.

Optical Reflectivity (R(*ω*))

As demonstrated and shown in Fig. 1, the spectrum of reflectivity R(*ω*) is formed out of 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.

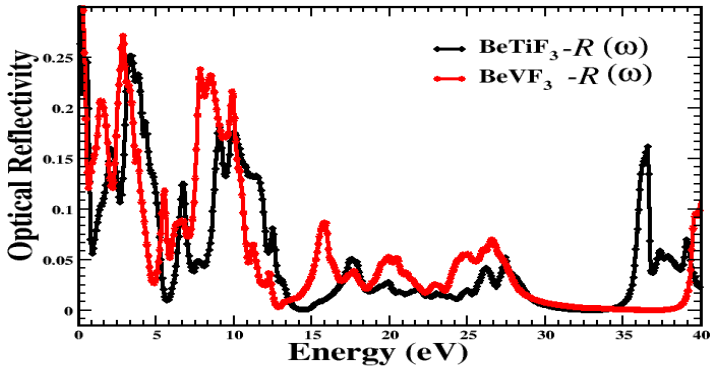

Figure.07: Simulated optical reflectivity R(*ω*) of $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

The reflectivity exists high at 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.

Refractive Index and Extinction Coefficient

The refractive index is a vital parameter to understand about 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.08. The figure.08 represents two parts: the refractive index and extinction coefficient.

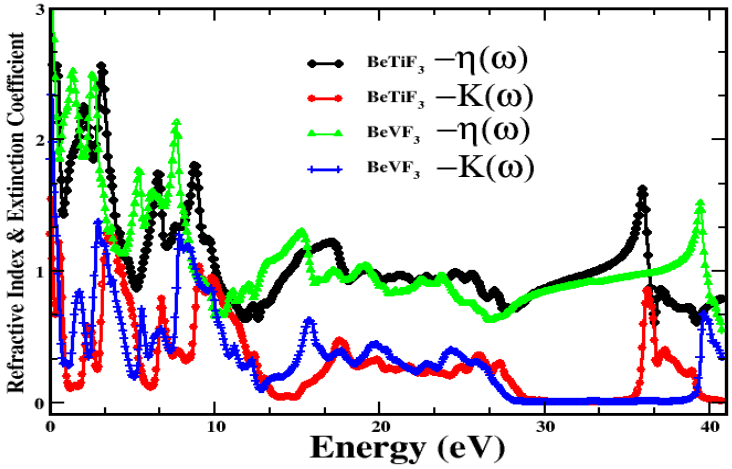

Figure.08: Simulated refractive index η(ω) and extinction coefficient K(ω) of $BeMF_3$ (M = Ti and V) Flouoroperovskites compounds.

The static η(0) refractive index is observed to be 2.57 for $BeTiF_3$ and 3 for $BeVF_3$ at zero energy. This static refractive index is also the maximum peaks 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 to the same figure.08 for imaginary part which is extinction coefficient K(ω). It is very clear from the figure that both the material 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 $BeVF_3$ has positive and high value of extinction coefficient in the energy range of 0 eV to 40 eV. In summary these material possesses a good optical properties, in which it is concluded that both the materials are metallic, transparent to incident light, optically more conductive and absorptive and has a high value of refractive index. The reported outcomes are very precise and provide a ground basis for experimental verification.

Conclusion

DFT based work on structural, elastic, electronic and optical properties of $BeMF_3$ (M = Ti and V) Flouoroperovskites 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 having 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 material are mechanically stable, brittle and anisotropic. It is concluded in optical properties for these compounds that these material are transparent to incident light, optically more conductive and absorptive and has a high value of refractive index. Such materials can be applicable to develop lenses and anti-reflection coatings.

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