Focusing on the Structural, Electronic, Optic and Elastic Behaviours of RhBiSe Compound by Ab-initio Calculations

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Abstract

Some physical features such as structural, electronic, optic and elastic of RhBiSe compound were investigated theoretically by Density Functional Theory within Generalized Gradient Approximation. The lattice parameter, total ground state energy, bond types and bond lengths were calculated in the structural features frame. The calculated lattice parameter is in good agreement with the literature. In order to investigate the electronic features of RhBiSe compound, the electronic band structure, density of states (DOS) and partial density of states (PDOS) graphs were plotted. Focusing on the electronic properties has shown that RhBiSe is a semiconductor with an indirect band gap. The density of states and partial density of states were also compatible with each other and electronic band structure of RhBiSe compound. In the optic features examination, the complex dielectric function, and the fundamental optic features obtained and it is noticed that RhBiSe is very convenient for the optical application areas such as optoelectronic devices. For the investigation of elastic features the elastic stiffness constants were computed, and afterwards the Bulk, Shear, Young Module, Poisson's ratio, flexibility coefficient, Debye temperature and Zener anisotropy factor were calculated. It was also exhibited that RhBiSe is a fragile material. The calculations on elastic features also revealed that RhBiSe is a mechanically stable, elastically anisotropic material with a high thermoelectric conductivity property.

Keywords: "RhBiSe, pyrite-marcasite family, electronic properties, elastic properties, optic properties."

1. Introduction

The global warming is the main problem of the earth. One of the most important causes of the global warming is the use of fossil fuels. The burning of fossil fuels releases carbon into the atmosphere, which threatens the global climate. In order to save the earth, it is very important to use alternative clean and renewable energy sources. The most important renewable energy source is solar energy, which is free, harmless and unlimited. For these kind of alternative methods photoactivity performance of the materials such as metal oxides, metal chalcogenides, carbides and transition metal dichalcogenides (TMDCs) are very important. Among these, the TMDCs have excellent catalytic activities, sizable bandgaps, distinct crystal structures, notable physical and chemical properties [1, 2]. The transition metal dichalcogenides have become useful materials for the development of photocatalyst because of their optical, electrical, thermal and mechanical properties [3]. The TMDCs have received significant consideration because they are low-cost and earth-abundant materials [1]. They have wide application areas such as energy storage, gas sensing and valley physics [4]. Additionally, transition metal dichalcogenides found in two crystal structures such as cubic pyrite-type and orthorhombic marcasite-type structures. Actually the chemical formula of pyrite and marcasite are the same, that is FeS_2. However, the cubic structure of FeS_2 is known as pyrite and the orthorhombic structure is known as marcasite.

Hulliger and Mooser [5] have studied on pyrites and marcasites and they showed that there are many binary and ternary compounds which have the same properties with pyrite and marcasite families. They revealed that this is a broad family of compounds with AX_2, AY_2 and AXY chemical formulas, where A is a transition element, X and Y are elements those belong to VI B and VB groups, respectively. Additionally, they crystallize in pyrite and marcasite type of structures that is why it is called pyrite-marcasite family [6]. In all of the family members, the cations have six anion neighbors occupying the corners of a octahedron whereas the anions have a tetrahedral neighborhood (generally chalcogen atoms) [5]. Furthermore, X and Y form covalently bonded pairs [7] in other words X_2, Y_2 or XY form anion molecules [8]. In the present study we focused on a material which belongs to pyrite-marcasite family, namely, RhBiSe.

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The compounds of the pyrite-marcasite family have high carrier mobility, high Young's modulus, functional electrical, mechanical, and thermal properties with a stable structure [9], high optical absorption coefficient in the visible region [1], they are semiconductors with a narrow band gap [10] and they have tunable electronic configurations [3, 11]. These compounds can be used in photocatalysts, photovoltaics [12, 13], optoelectronic devices, solar cells, electrolysis and energy storage devices [14].

Most of the pyrite-marcasite family members were synthesized in the laboratory, such as; RhXY, IrXY, NiXY, PdXY etc. where X: P, As, Sb, Bi and Y: S, Se, Te [5]. Among that synthesized group we investigated RhBiSe compound theoretically in the present study by using the Density Functional Theory (DFT). The DFT is very useful since it provides opportunity to make calculations in a very large scale, in a shorter time with high accuracy. There are many studies performed with DFT [15, 16]. By using the ABINIT programme, which depends on the DFT, we saw that, RhBiSe exhibits all features of pyrite-marcasite family which belongs to TMDCs, such as good electronic properties with a narrow band gap, convenient optic properties, and elastic properties. We could not compare our results with the literature except for the lattice parameters since there are not such studies on RhBiSe compound in the literature. However, we have shown that all the features of RhBiSe are consistent within this study and the features of TMDCs and pyrite-marcasite family. That is why we believe that this study will help to the future studies on RhBiSe compound. Also we have seen that this material is very convenient to the application areas such as solar cells, optoelectronic devices and energy storage devices.

2. Computational Method

All calculations of structural, electronic, optic and elastic features were done by Density Functional Theory within Generalized Gradient Approximation using ABINIT [17] computer programme. The self-consistent Fritz Haber Institute-type [18] norm-conserving pseudopotentials with the Troullier-Martins scheme [19] have been used. In order to figure out the Kohn-Sham equations [20] the conjugate gradient minimization method [21] was utilized. The exchange-correlation effects were taken into account by using the Perdew-Burke-Ernzerhof [22] functions. The plane waves were used as the basis set. The valance electrons for the RhBiSe are chosen as $4f^{14} 5d^{10} 6s^2 6p^3$ for Bi, $4p^6 5s^2 4d^7$ for Rh and $4s^2 3d^{10} 4p^4$ for Se. A kinetic cut off energy was chosen as 1088.45 eV was used. The number of k-points were 84 within the 12x12x12 Monkhorst-Pack mesh grid [23].

3. Results and Discussion

The investigation on features of RhBiSe compound started with the examination of the structural features. The RhBiSe is in cubic crystal structure with $P2_1 3$ space group (No:198). There are four molecules of RhBiSe in the unit cell, so the number of atoms in a unit cell of RhBiSe is 12. (The atomic positions of the atoms of RhBiSe crystal in its unit cell are given in Appendix A.) So far only lattice parameter of this compound is calculated in literature as 6.3823 Å [24]. First, the geometry optimization was performed in order to obtain the atomic coordinates. Afterwards volume optimization was performed to obtain the calculated lattice parameter. The calculated lattice parameter is 6.3421 Å which is very close to the literature. The minimum energy for the decisive crystal structure of RhBiSe is calculated as -6736.18 eV. The volume of RhBiSe is calculated as 255.09 (Å)^3 for its decisive state.
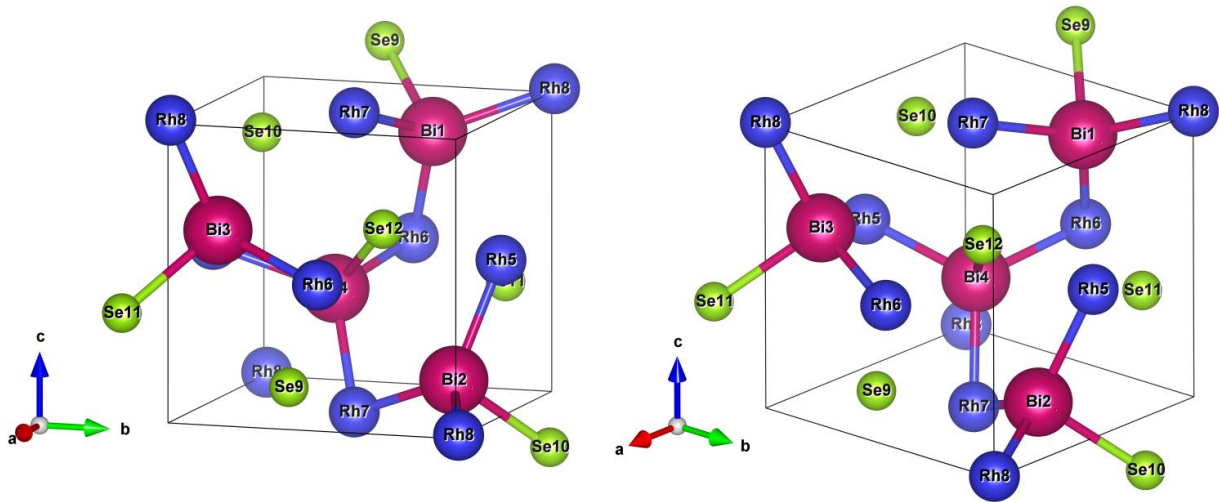

Figure 1. The crystal structure od RhBiSe in its unit cell.

Table 1. Bonds and bond lengths of RhBiSe crystal.

Bonds	Bond Lenghts (Å)
Bi-Rh	2.7228
Bi-Se	2.7679
Rh-Se	2.5748

The unit cell of RhBiSe was drawn by using Vesta [25] programme with two different point of views (Fig.1). It is noticed that there are bonds between Bi-Rh, Bi-Se and Rh-Se atoms, those bond lenghts are also computed by using the Vesta programme and are given in Table 1. In the RhBiSe compound, Bi (VB group) atoms and Se (VIB group) atoms have a covalent bond and they formed an anion molecule. In Fig. 1, the bonds which are not beyond the boundary of the unit cell are also shown.

As the next step of the present study, the electronic features of RhBiSe compound were examined. The electronic band structure (EBS), density of states (DOS) and partial density of states (PDOS) are calculated and their graphs are drawn. In Fig. 2, the EBS graph is given. The electronic band structure is obtained throughout the $\Gamma - X - M - \Gamma - R - X$ high symmetry points in the first Brilliouin zone. The Fermi level is represented with red dashed line. Below this level the valance bands and above conducting bands of RhBiSe compound are found. When Fig. 2 examined in detail, it is noticed that, there are core electron energy levels at around -15 eV and -10 eV energy values. There are forty valance bands with the core electron levels. We investigated ten energy levels from the conducting bands. It is clear from Fig.2 that, RhBiSe is a semiconductor in structure with a indirect band gap. The value band gap is 0.475 eV.
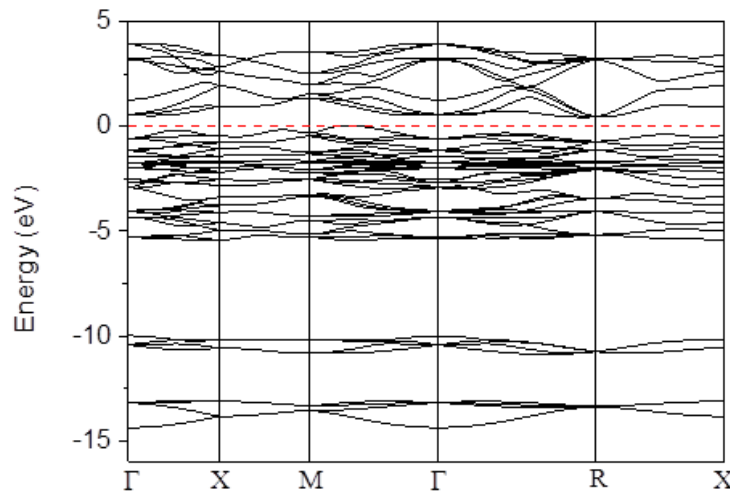

Figure 2. Electronic band structure of RhBiSe compound.
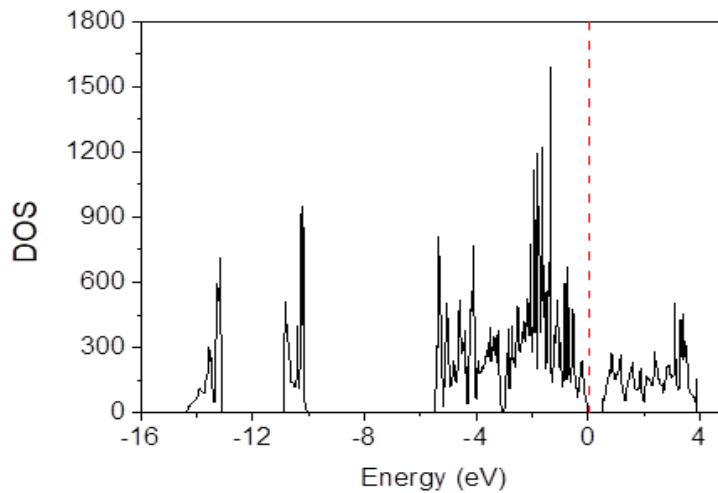
Figure 3. Density of states (DOS) graph of RhBiSe compound.

The DOS values are given in arbitrary units (Fig.3). The DOS and the EBS graphs of RhBiSe compound are compatible with each other. The energy values of core electrons, the boundary energy values of valance and conducting bands and the band gap are the same with the values obtained from the EBS graph. It is known that, the partial density of states (PDOS) are the contributions of the atoms to the density of states of a compound. The PDOS graphs are given in Fig. 4. In the PDOS graphs *l*

values are the quantum numbers which specifies the orbital angular momentum. The s, p, d and f states are designated by $l = 0$, 1, 2 and 3 values, respectively. Again the Fermi level is represented with dashed line in each graph. There are four Bi atoms in the unit cell and the contributions of Bi atoms are in the same character which is valid also for the Rh and Se atoms. It is seen from Fig. 4 that, the contribution of core electrons with -10 eV comes from the Bi atoms with s states. There is also slight contributions of Bi atoms to valance and conduction bands with f states. If one examines Rh atoms, it is seen that the main contribution comes from the valance bands and the slight contribution comes from the conduction bands, all contributions with d states. The contribution of Se atoms mainly comes from the core electrons which have -15 eV, with s states. There are also contributions of Se atoms from valance bands and slightly from conduction bands both with p states.

The optic features obtained by using the complex dielectric function of RhBiSe compound. Actually, complex dielectric functions are represented by rank one tensors, with three components along the 100, 010 and 001 crystal axes directions. Since cubic structures are optically isotropic, so just one component of complex dielectric function is adequate. The complex dielectric function has real (ε_1) and imaginary (ε_2) parts. In Fig. 5, these parts of dielectric constant are plotted as a function of phonon energy. The real and imaginary parts are related to each other by Kramers-Kronig equations. Imaginary part of the complex dielectric constant is related with the electronic band structure and interband transitions, especially absorptive behaviour of the material. The real part related with the physical properties, especially the dispersion behaviour.

As seen from Fig. 5, real part has negative values between the 2.89 and 11.96 eV photon energies interval. In this interval RhBiSe crystal reflects all coming light. At 2.89 and 11.96 eV the value of real part equals to zero. The zero value of the real part conforms to plasmon excitations. The static dielectric constant is the value of the real part at 0 eV energy, that is 25.78 for RhBiSe compound. The peaks in the imaginary part shows the interband transitions from valance to conduction bands. There is a major peak at 1.50 eV energy level for RhBiSe compound. This peak points out the transition from Rh-4d to Se-4p states, as shown in PDOS graphs (Fig.4).
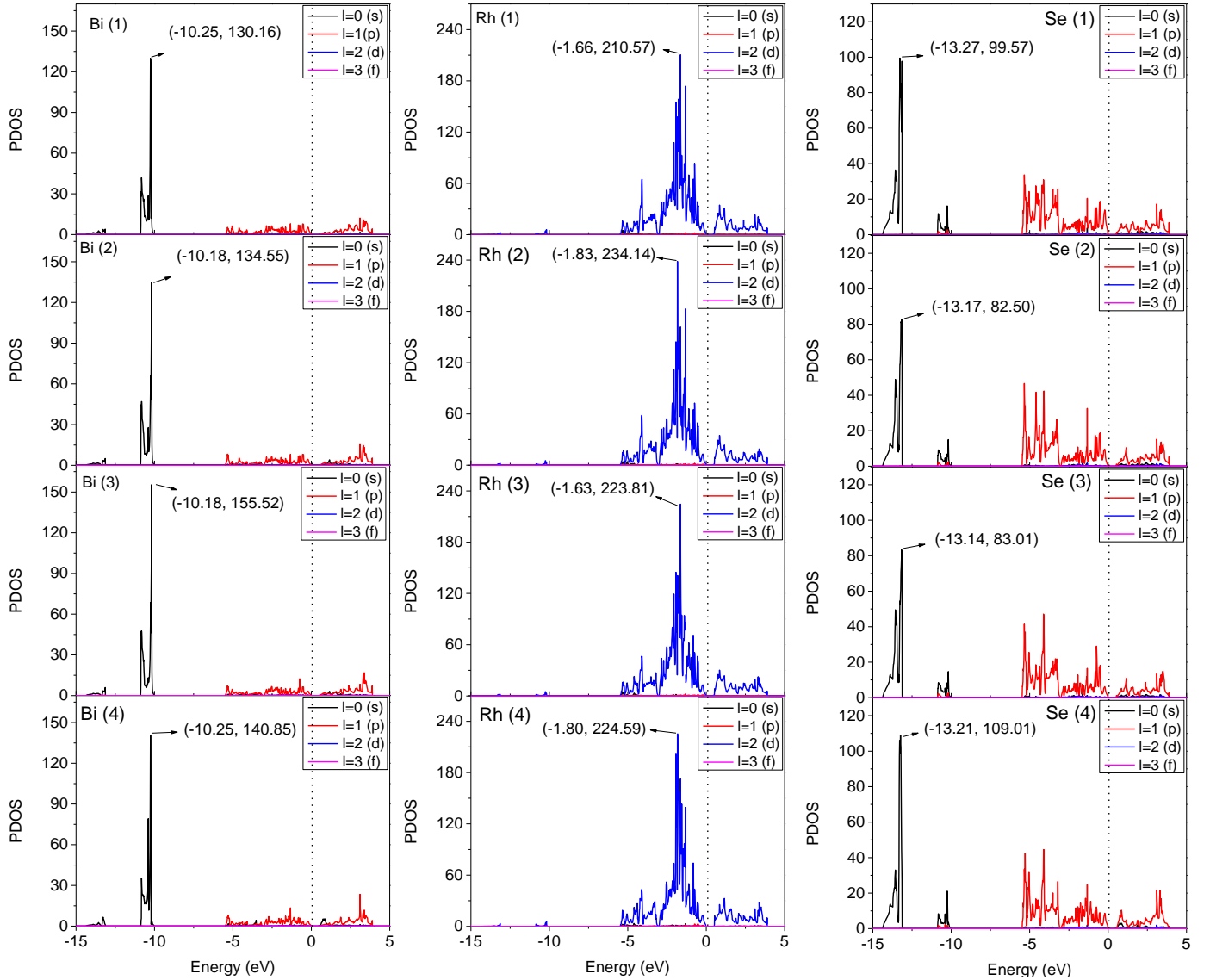
Figure 4. Partial density of states graphs of the atoms in RhBiSe compound.
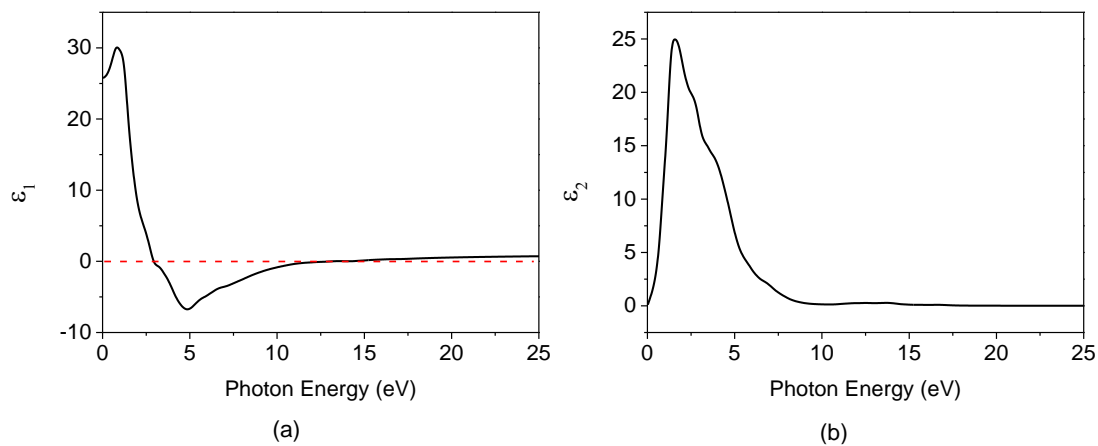
Figure 5. The (a) real and the (b) imaginary parts of the complex dielectric function of RhBiSe compound.
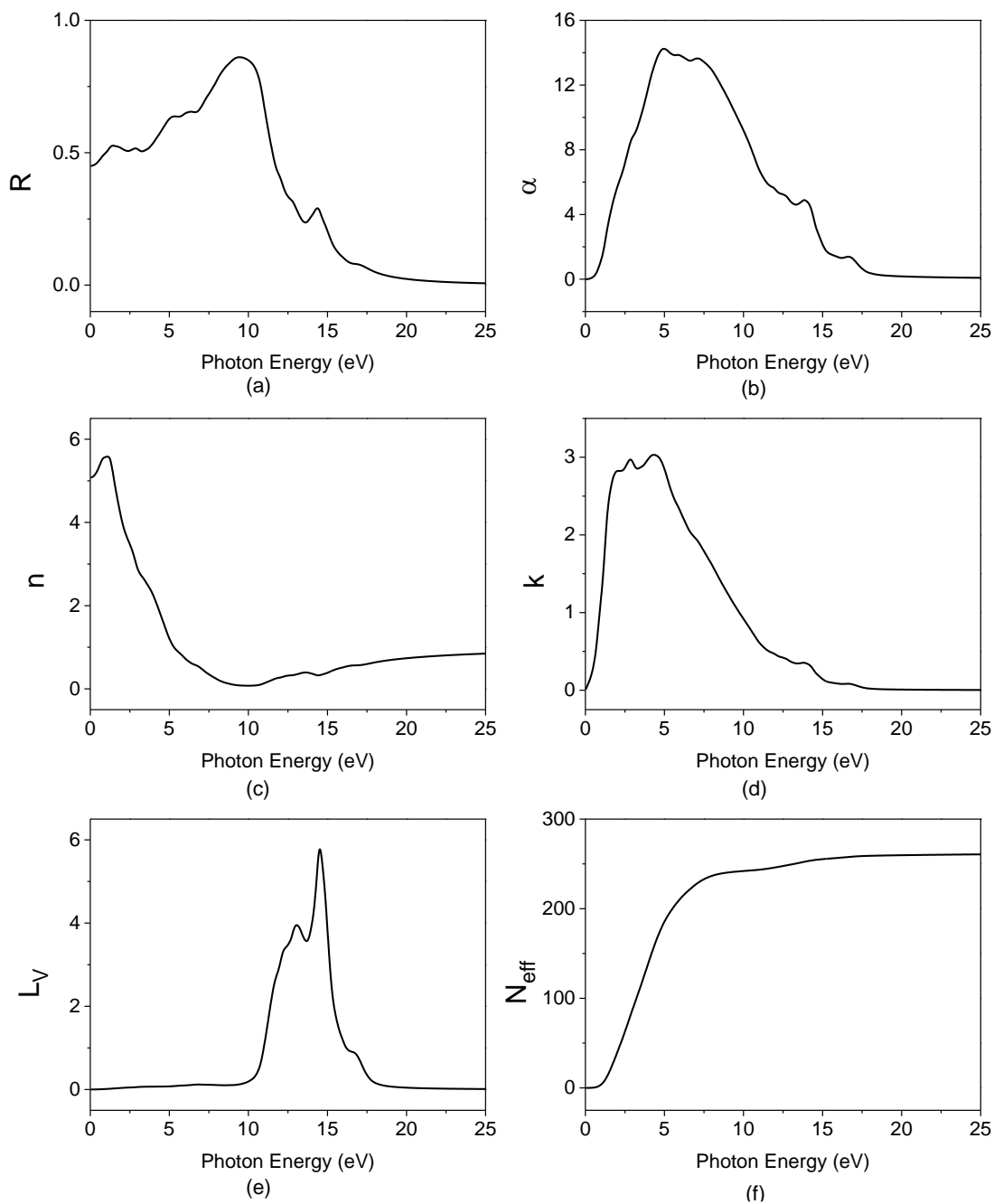
Figure 6. (a) Reflectivity, (b) absorption, (c) refractive index, (d) extinction coefficient, (e) energy loss function of volume and (f) effective number of valence electrons in the unit cell.

In extention, the main optic features such as reflectivity, absorption, refractive index, extinction coefficient, energy loss function and effective number of valence electrons were calculated and graphs of those were given in Fig.6. All these features including real and imaginary parts of complex dielectric function have been calculated in the 0-20 eV and plotted 0-25 eV energy range, since it is clear from the EBS graph, difference between the minimum energy value of the valance bands and the maximum energy value of the conduction bands occupy around 20 eV. The first slight peak of reflectivity graph (Fig.6(a)) is at around 2 eV and the highest peak is at around 10 eV energy values which are consistent with the negative parts of the real dielectric function. Between these energy values, reflection occurs dominantly. It is seen from absorption graph (Fig. 6(b)) that, absorption starts at 0.45eV (which is consistent with the band gap value) and finishes at around 17.80 eV. Between these energy values absorption occurs, in other words, the value of the absorption is different than zero. The static refractive index value of RhBiSe is 5.07 (Fig. 6(c)). The profile of extinction coefficient looks like the absorption feature of RhBiSe compound as seen from Fig. 6(d). Energy loss function (L_V) determines the energy loss of an electron which passes through a material. N_{eff} represents the contribution throughout the transition between the electronic bands. When N_{eff} reaches its saturated value, it means that there will not be any transitions between the electronic bands.

In the last part of the study, we focused on the elastic features on RhBiSe crystal. First, we calculated the elastic stiffness constants. When a force applied on a continuous material, the neighboring particles inside this material continue to transfer this force between each other which is called stress. Stress is actually a second rank tensor (σ_{ij}). The stress sometimes causes a deformation on a material which is called strain. The strain is also second rank tensor (ε_{ij}). Some materials may gain its original shape again, when the stress is removed. Those materials called as elastic materials. However, some of them may have permanent deformation. In order to understand the elastic features of a material, first thing to do is to calculate the elastic stiffness constants. According to Hooke's law with small amounts of stress and strain, the ratio of them gives elastic stiffness constants ($\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$). These are four rank tensors. They have 81 components but by using a matris notation they can be shown with just two indices, and 36 components that is 21 of them are independent components. This form of elastic stiffness constants are not tensors anymore [26].

Table 2. The elastic stiffness constants of RhBiSe compound.

	(C_{11} (GPa) $= C_{22} = C_{33}$)	(C_{12} (GPa) $= C_{13} = C_{21} = C_{23} = C_{31} = C_{32}$)	(C_{44} (GPa) $= C_{55} = C_{66}$)
RhBiSe	200.13	54.27	52.60

Table 3. The calculated values of Bulk, Shear, Yound modulus, Poisson's ratio, Flexibility coefficient, Debye temperature and Zener anisotropy factor of RhBiSe compound

Elastic Property of RhBiSe	Symbol (unit)	Calculated Values
Bulk Modulus	B_V (GPa)	102.89
Shear Modulus	G_V (GPa)	60.73
Young Modulus	E (GPa)	150.64
Poisson's Ratio	v (-)	0.256
Flexibility Coefficient	$K = B_{VRH}/G_{VRH}$ (-)	1.716
Debye Temperature (K)	Θ_D	134.35
Zener Anisotropy Factor	A	0.7

Additionally, the number of components changes according to the crystal structures because of the symmetry features. Cubic crystals have 12 elastic stiffness components and 3 of them are independent, which are C_{11} ($= C_{22} = C_{33}$), C_{12} ($= C_{13} = C_{21} = C_{23} = C_{31} = C_{32}$) and C_{44} ($= C_{55} = C_{66}$). The calculated values of those coefficients are given in Table 2. By using these C_{ij} values and Born stability criterias, one can examine the mechanical stability of a material. The Born stability conditions [27] can be summarized as follows;

$$C_{11} + 2C_{12} > 0, \; C_{44} > 0, \; C_{11} - C_{12} > 0, \; C_{11} > 0, \; and \; C_{12} < B < C_{11} \tag{1}$$

Here in the last criteria B is the bulk modulus. As seen from Table 2, RhBiSe compound satisfies all these criterias, so this material is mechanically stable.

After the elastic stiffness constants, we calculated some fundamental elastic features such as Bulk, Shear and Young modulus. Additionally, we calculated the Poisson's ratio, flexibility coefficient, Zener anisotropy factor and Debye temperature values as given in Table 3. There are some tests to decide the elastic structure of a material. The critical value of Poisson's ratio is 0.26 and of flexibility coefficient is 1.75. If the calculated values of these elastic features are smaller than their critical values, than it shows that the material is fragile, otherwise elastic material. As seen from Table 3, the calculated value of both Poisson's ratio and the flexibility coefficient are smaller than the critical values. It is noticed that RhBiSe is a fragile material. If the calculated value of the Zener anisotropy equals to 1, that material is elastically isotropic. Since the calculated value of RhBiSe (Table 3) equals to 0.7 this material is elastically anisotropic. In this section of the study, the Debye temperature is calculated.

The Debye temperature gives information about the energies of the high frequency modes and the thermal conductivity of a material. Our calculated Debye temperature value is 134.35 K. For the temperatures above Debye temperature, the high-frequency modes have the $k_B T$ energy value, under Debye temperature they are frozen. Additionally, from our previous studies and experiences, the materials with Debye temperature values higher than approximately 70 or 80 K have thermal conductivity property [28]. The calculated Debye temperature of RhBiSe compound is very high than that value, so the thermal conductivity of this compound is very high. Therefore, RhBiSe is a very good candidate for many application areas with thermal conductivity.

4. Conclusions

The calculations on physical properties of RhBiSe compound done by Density Functional Theory within the Generalized Gradient Approximation using the ABINIT computer programme. During the investigation of structural features of RhBiSe, the lattice parameter, bonds and bond lenghts, unit cell view, volume and total energy values are obtained. The calculated lattice parameter value is consistent with the literature. Focusing on the electronic properties, it is found that the RhBiSe compound is a semiconductor with an indirect transition. The DOS and all PDOS graphs are obtained. Main optic features are calculated and the graphs of them are plotted. It is seen that, optical properties of RhBiSe are very convenient for the optoelectronic applications. In the last part of the study, the elastic features are investigated. In the light of that investigation on elastic features, it was exhibited that, RhBiSe is an mechanically stable, elastically anisotropic and fragile material with high thermal conductivity property. We believe that this study will be very useful to the researchers on the future studies on RhBiSe compound since all the results throughout the study are very consistent with each other.

Appendix A. –Atomic Positions of RhBiSe Crystal.

Table 4. The atomic positions of the atoms in the unit cell of RhBiSe crystal.

	Wyckoff	x	y	z
Bi (1)	1a	0.130137	0.630137	0.869863
Bi (2)	1a	0.630137	0.869863	0.130137
Bi (3)	1a	0.869863	0.130137	0.630137
Bi (4)	1a	0.369863	0.369863	0.369863
Rh (1)	1a	0.485515	0.985515	0.514485
Rh (2)	1a	0.985515	0.514485	0.485515
Rh (3)	1a	0.514485	0.485515	0.985515
Rh (4)	1a	0.014485	0.014485	0.014485
Se (1)	1a	0.879743	0.379743	0.120257
Se (2)	1a	0.379743	0.120257	0.879743
Se (3)	1a	0.120257	0.879743	0.379743
Se (4)	1a	0.620257	0.620257	0.620257

References

[1]   N. N. Rosman, R. M. Yunus, L. J. Minggu, K. Arifin, M. N. I. Salehmin, M. A. Mohamed, and M. B. Kassim, "Photocatalytic properties of two-dimensional graphene and layered transition-metal dichalcogenides based photocatalyst for photoelectrochemical hydrogen generation: An Overview," International Journal of Hydrogen Energy, vol. 43, pp. 18925-l8945, 2018.

[2]   U. Caliskan , S. Kahraman and T. Koçyiğit , "Multi-Scale Modeling of Graphene/Polymer Nanocomposites-Molecular Interfacial Interactions", International Scientific and Vocational Studies Journal, vol. 5, no. 2, pp. 124-134, 2021.

[3]   D. Monga, S. Sharma, N. P. Shetti, S. Basu, K. R.Reddy, and T. M. Aminabhavi, "Advances in transition metal dichalcogenide-based two-dimensional nanomaterials," Materials Today Chemistry, vol.19, pp. 100399, 2021.

[4]   L. Feng, R. A. B. Villaos, Z. Huang, C. HsiuHsu, and F. Chuang, "Layer-dependent band engineering of Pd dichalcogenides: a first-principles study," New Journal of Physics, vol. 22, pp. 053010, 2020.

[5]   F. Hulliger, and E. Mooser, "Semiconductivity in Pyrite, Marcasite and Arsenopyrite Phases," Journal of Physics and Chemistry of Solids, vol. 26, pp. 429-433, 1965.

[6]   T. B. E. Grønbech, K. Tolborg, H. Svendsen, J. Overgaard, Yu-Sheng Chen, and B. B. Iversen, "Chemical Bonding in Colossal Thermopower FeSb2," Chemistry—A European Journal, vol. 26, pp. 8651 – 8662, 2020.

[7]   I. Dodony, M. Posfai, and P. R. Buseck, "Structural relationship between pyrite and marcasite," American Mineralogist, vol. 81, pp. 119-125, 1996.

[8]   F. Hulliger, and E. Mooser, "The Bond Description of Semiconductors: Polycompounds," Progress in Solid State Chemistry, vol. 2, pp. 330-377, 1965.

[9]   L. Liu, D. Wang, S. Lakamsani, W. Huang, C. Price, and H. L. Zhuang1 "Dimension engineering of single-layer PtN2 with the Cairo tessellation," Journal of Appied Physics, vol.125, pp.204302, 2019.

[10]   R. Sun, M. K. Y. Chan, and G. Ceder, "First-principles electronic structure and relative stability of pyrite and marcasite: Implications for photovoltaic performance," Physical Review B vol. 83, pp.235311, 2011.

[11]   M. Pathak, D. Tamang, M. Kandasamy, B. Chakraborty, and C. S. Rout, "A comparative experimental and theoretical investigation on energy storage performance of CoSe2, NiSe2 and MnSe2 nanostructures," Applied Materials Today vol.19, pp.100568, 2020.

[12]   M. A. S. Adamson, P. Yox, T. Hernandez, F. Wang, and J. Vela, "Phase Evolution, Polymorphism, and Catalytic Activity of Nickel Dichalcogenide Nanocrystals," Chemistry of Materials, vol. 34, pp.746−755, 2022.

[13]   P. C. Sreeparvathy, and V. Kanchana "Giant thermopower in 'p' type OsX2 (X: S, Se, Te) for a wide temperature range: A first principles study," Journal of Physics: Condensed Matter, vol. 30, no. 29, pp. 295501, 2018.

[14]   C. Arrouvel, "Surfaces, Interfaces and Crystal Growth of Marcasite FeS2," Materials Research, vol. 24 no. 1 pp. e20200383, 2021.

[15]   I. Mahmudov, Y. Demir, Y. Sert, Y. Abdullayev, A. Sujayev, S. H. Alwasel, and I. Gulcin "Synthesis and inhibition profiles of N-benzyl- and N-allyl aniline derivatives against carbonic anhdrase and acetylcholinesterase – A molecular docking study," Arabian Journal of Chemistry, vol. 15, pp. 103645, 2022.

[16]   İ. Çapan, S. Servi, İ. Yıldırım, and Y. Sert, "Synthesis, DFT Study, Molecular Docking and Drug-Likeness Analysis of the New Hydrazine-1-Carbothioamide, Triazole and Thiadiazole Derivatives: Potential Inhibitors of HSP90," ChemistrySelect, vol. 6, pp. 5838 –5846, 2021.

[17]   X. Gonze, J. M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G. M. Rignanese, L. Sindie, M. Verstrate, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, P. Ghosez, J. Y. Raty, and D. C. Allan, "First-principles computation of material properties: the ABINIT software Project", Computational Materials Science, vol.25, pp.478-492, 2002.

[18]   Fuchs, M. and Scheffler, M. "Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory", Computer Physics Communications, 119: 67-98, (1999).

[19]   N. Troullier, and J. L. Martins, "Efficient pseudopotentials for plane-wave calculations," Physical Review B, vol. 43, pp. 1993-2006, 1991.

[20]   W. Khon, and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects", Physical Review, vol. 140, pp. A1133-A1138, 1965.

[21]   M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos, "Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients", Reviews of Modern Physics, vol. 64, pp.1045-1098, 1992.

[22]   J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," Physical Review Letters, vol. 77, pp. 3865-3868, 1996.

[23]   J. H. Monkhorst, and J. D. Pack, "Special points for Brillouin-zone integrations", Physical Review B, vol. 13, pp. 5188-5192, 1976.

[24]   A. Jain*, S.P. Ong*, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson (*=equal contributions), "The Materials Project: A materials genome approach to accelerating materials innovation," APL Materials, vol. 1, no.1, pp. 011002, 2013.

[25]   K. Momma, and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data" Journal of Applied Crystallography, vol.44, pp.1272-1276, 2011.

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[26]   J. F. Nye, "Physical Properties of Crystals: Their Representation by Tensors and Matrices," Oxford University Press, United States, Chapter 8, 1985.

[27]   F. Mouhat, F.X. Coudert, "Necessary and sufficient elastic stability conditions in various crystal systems," Physical Review B, vol. 90, pp. 224104, 2014.

[28]   E. Kilit Dogan, and S. Erden Gulebaglan, "A computational estimation on structural, electronic, elastic, optic and dynamic properties of Li2TlA (A=Sb and Bi): First-principles calculations," Materials Science in Semiconductor Processing, vol.138, pp.106302, 2022.