

# Mechanical stability and optoelectronic behavior of BeXP<sub>2</sub> (X = Si and Ge) chalcopyrite

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## ARTICLE INFO

### Keywords:

Chalcopyrite compounds  
Mechanical properties  
DFT  
Optoelectronic properties

## ABSTRACT

We have conducted a first-principles study on the structural, electronic, optical and elastic properties of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds. Using the density functional theory (DFT), implemented in both full potential linear muffin-tin orbital (FP-LMTO) and Vienna Ab initio simulation (VASP) packages. The FP-LMTO is used for the determination of the structural, electronic and optical properties, while the VASP is used to determine the elastic constants that give indications about the material stability. The obtained equilibrium structural parameters are in good agreement with available results. An investigation of the band gap indicates that our compounds possess a semiconductor behavior with direct band gap for BeSiP<sub>2</sub> and with an indirect band gap for BeGeP<sub>2</sub>. The energy band gaps decreased by changing Be atoms from Si to Ge. We have calculated the dielectric function  $\epsilon(\omega)$ . The obtained results show that these materials are promising semiconductors for photovoltaic applications. For the elastic properties, the single-crystal elastic constants  $C_{ij}$ , shear anisotropic factors  $A$ , as well as polycrystalline bulk, shear and Young's modulus ( $B$ ,  $G$  and  $E$ ) and Poisson's ratio  $\nu$  have been predicted. The generalized elastic stability criteria for a tetragonal crystal are well satisfied, indicating that BeSiP<sub>2</sub> and BeGeP<sub>2</sub> are mechanically stable in the chalcopyrite structure.

## 1. Introduction

Ternary chalcopyrite compounds are currently an interesting technologically; they are promising materials for electronic, optoelectronic and photonic fields, because of their potential and excellent electronic, linear and non-linear optic properties. This type of material is recently widely used for light-emitting diodes, solar cells, photovoltaic detectors, optical-light eliminators, lasers and modulators [1–3].

The ABC<sub>2</sub> chalcopyrite compounds of type I-III-VI<sub>2</sub> with chalcogenide anions and II-IV-V<sub>2</sub> with pnictide anions are still the subject of numerous studies due to their high potential applications [4–14]. They are the most preferable materials for photovoltaic technologies. These Chalcopyrite-type materials are well-known semiconductors with energy band gap ranging from 1–3 eV [15, 16]

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<https://doi.org/10.1016/j.cjph.2020.01.007>

Received 14 November 2019; Received in revised form 1 January 2020; Accepted 13 January 2020

Available online 24 January 2020

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which is suitable for the preparation of high quality solar cells because of its high capability of absorbing the visible light spectrum [17]. Some works experimental consolidate the technological interest of its materials in the nonlinear and optoelectronic field, among these experimental works, Phosphorus-containing nonlinear and optoelectronic crystal, such as 2D GeP as a Novel Broadband Nonlinear Optical Material [18], 2D Black Phosphorus [19], Black Phosphorus Photodetectors [20], recent advances in black phosphorus-based photonics devices [21].

The I-III-VI<sub>2</sub> and II-IV-V<sub>2</sub> chalcopyrite compounds crystallize in the chalcopyrite structure with a tetrahedral space group I-42d ( $D_{2d}^{12}$ ) [5–14]. They have a crystalline structure analogous to ternary semiconductors II–VI and III–V, respectively. They have almost the same arrangement of the zincblende anion atoms, but differ in the order of distribution of the cationic atoms (A and B) which cause the tetragonal unit cell to have a c-axis approximating double the a-axis of the unit zinc blende cell. A binary analogue can be defined for each ternary compound ABC<sub>2</sub> by taking the cation from the column between the A and B atoms in the periodic table.

Chalcopyrite compounds have tetragonal (coordination 4) structures in which each atom is associated with four neighboring close atoms forming a more or less regular tetrahedron. Each anion (C) is linked to two cations (A) and two cations (B) while each cation is bound to four anions forming the above-mentioned tetrahedron.

More recently, the development of beryllium (Be) based chalcopyrite compounds shows magnificent properties, which have great potential applications [22,23]. Otherwise, previous works have confirmed that these compounds are potential candidates for spintronic devices application because they exhibit magnetic properties when doped with transition elements [24,25]. All Be-based compounds are thermodynamically stable because they possess negative enthalpies of formation [23]. A few theoretical calculations have been performed on the BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite materials [22,23]. However, the information on these compounds is incomplete which motivated us to calculate for the first time some of the parameters for the considered materials.

In order to fully take advantage of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> compounds in the chalcopyrite phase properties for eventual technological applications, a theoretical investigation is necessary. For this purpose, we have conducted that investigation on the structural, electronic, optical and elastic properties of the BeSiP<sub>2</sub> and BeGeP<sub>2</sub> in the chalcopyrite structure. The organization of the paper is as follows. In Section 2, we have described the employed method and the details of the calculations. Results and discussions of the structural, electronic, optical and elastic properties are presented in Section 3. Finally, conclusions and remarks are given in Section 4.

## 2. Calculation methodology

In this study, the calculations are performed using the Lmrt computer code, to study the structural, electronic and optical properties BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite compounds at thermodynamic equilibrium. The Lmrt computer code uses full-potential linear muffin-tin orbital (FP-LMTO) method [26,27], which is based on the DFT formalism (Density functional theory) [28,29], The generalized gradient approximation (GGA-PBE) of Perdew et al. [30] has been used as an exchange and correlation potential.

In order to achieve energy eigenvalues convergence, the charge density and potential inside the MTSs are represented by spherical harmonics up to  $l_{max} = 6$ . The self-consistent calculations are considered to be converged when the total energy of the system is stable at  $10^{-5}$  Ry. The  $k$  integration over the Brillouin zone is performed using the tetrahedron method [31]. To avoid the overlap of atomic spheres, the MTSs radii for each atomic position are taken differently for each composition. We point out that the using of the full-potential calculation ensures that the calculation is not completely independent of the choice of spheres radii. The values of the spheres radii (MTSs), used in our calculation, are summarized in Table 1.

The elastic properties were performed using the Vienna ab initio simulation package (VASP) with a plane wave basis-set and ultrasoft pseudopotentials [32,33]. Exchange and correlation potentials were included using the generalized gradient approximation (GGA-PBE) of Perdew et al. [30]. The atomic relaxation was stopped when the forces acting on atoms were less than 0.02 eV/Å. The Brillouin zone (BZ) integration was performed by the linear tetrahedron method with Blochl corrections [31]. An energy cutoff of 500 eV was applied, while the  $10 \times 10 \times 10$  mesh of Monkhorst-Pack points was used. The convergence in the total energy of the unit cell was better than  $10^{-5}$  eV/atom.

## 3. Results and discussion

### 3.1. Structural properties

The BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds structure is closely related to the zincblende structure and contains four formula

**Table 1**  
The muffin-tin radius (RMT in atomic units) for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

Compound	BeSiP <sub>2</sub>	BeGeP <sub>2</sub>
R <sub>MT</sub> (Be)	2.107	2.158
R <sub>MT</sub> (S,Ge)	2.431	2.485
R <sub>MT</sub> (P)	2.263	2.410

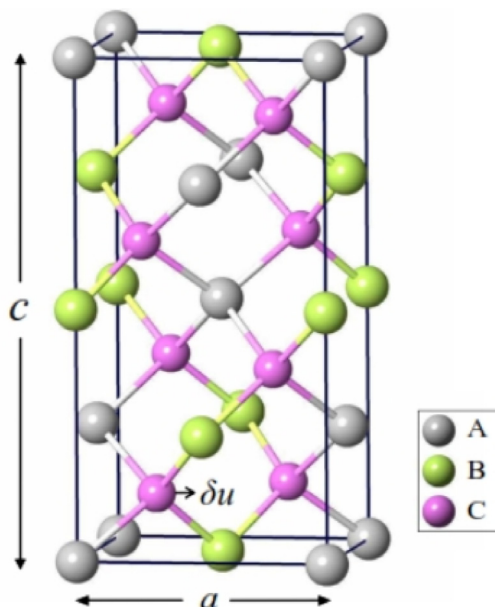


Fig. 1. Crystal structure of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors. (A = Be, B = Si or Ge, C = P).

units in each unit-cell, with the Be, Si(Ge) and P atoms occupying Wyckoff positions 4a (0,0,0), 4c (0,0,0.5) and 8d ( $u, 0.25, 0.125$ ), respectively. Generally, the chalcopyrite lattice is characterized by three structural parameters: the lattice constants  $a$  and  $c$ , as well as the dimensionless anionic displacement parameter  $u$  which is often called the internal parameter.

To determine the structural properties of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds, we performed a self-consistent calculation of the total energy as a function of three variables, the lattice constants ( $a$ ), the ratio ( $c/a$ ) and the anionic displacement ( $u$ ), in a way to calculate the lattice constants ( $a$ ), at ideal values of the ratio ( $c/a$ ) and the anionic displacement ( $u$ ) (such that  $u_{\text{ideal}} = 0.25$  and  $c/a_{\text{ideal}} = 2$ ). Then we optimize the ratio ( $c/a$ ) to  $a_{\text{op}}$  and  $u_{\text{ideal}}$ . Following, determine  $u$  using the ratio  $(c/a)_{\text{op}}$  and  $a_{\text{op}}$ . Finally, for accuracy using the optimized values, the lattice constants ( $a$ )<sub>op</sub>, the anionic displacement  $u$ <sub>op</sub> and the ratio  $(c/a)$ <sub>op</sub>, we recalculate the equilibrium anionic displacement  $u$ , the ratio ( $c/a$ ) and the lattice constant of equilibrium cell (Fig. 1).

The equilibrium lattice constants  $a$ , bulk modulus ( $B$ ) and its pressure derivatives ( $B'$ ) of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds are optimized by an adjustment of the total energy obtained as a function of cell volume  $E_{\text{Total}}(V)$  using the fitting Murnaghan equation of state [34]. However, the  $c/a$  ratio and the anionic displacement  $u$  are optimized by an adjustment of their total energies obtained in terms of  $c/a$  and  $u$  ( $E_{\text{Total}}(c/a)$  and  $E_{\text{Total}}(u)$ ) using a polynomial fitting.

The results and optimal values of  $a$ ,  $c$ ,  $c/a$  and  $u$  are listed in the Table 2. The structural parameters obtained are in good agreement with the other theoretical data existing in the literature [35]. It can be noted that the approximation method used to calculate these structural parameters, namely, GGA-PBE overestimate the computed data relative to the other works. It can also be seen that the structure of these compounds is quite similar to that of two superimposed ideal zincblende structures, characterized by its ratio  $c/a = 2$  and its internal structural parameter  $u = 0.25$ , which, one and the other, describe the position of atoms (Si/Ge).

### 3.2. Electronic properties

In this part, we are interested in the calculations of energy band structures and electronic density of states, relating to the BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds, using the optimized mesh parameters. The calculations were made along the different high

Table 2

Calculated equilibrium lattice constant ( $a$ ,  $c$  in Å),  $c/a$  ratio, distortion parameter ( $u$ ), equilibrium volume  $V(\text{a.u.})^3$ , bulk modulus  $B_0(\text{GPa})$  and its first derivative  $B'$  for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

		$a_0$	$c$	$c/a$	$u$	$V(\text{a.u.})^3$	$B$	$B'$	$E_0(\text{Ry})$
BeSiP <sub>2</sub>	Present cal	5.16	10.27	2.018	0.236	935.072	92.96 98.14 <sup>b</sup>	4.41	-3955.97
	Other cal	5.12 <sup>a</sup>	10.21 <sup>a</sup>	1.995 <sup>a</sup>	0.235 <sup>a</sup>	–	–	–	–
BeGeP <sub>2</sub>	Present cal	5.30	10.69	1.998	0.224	1006.52	82.96	4.12	-11,192.11
	Other cal	5.20 <sup>a</sup>	10.45 <sup>a</sup>	2.008 <sup>a</sup>	0.221 <sup>a</sup>	–	–	–	–

<sup>a</sup> Ref [35].

<sup>b</sup> Ref [38].

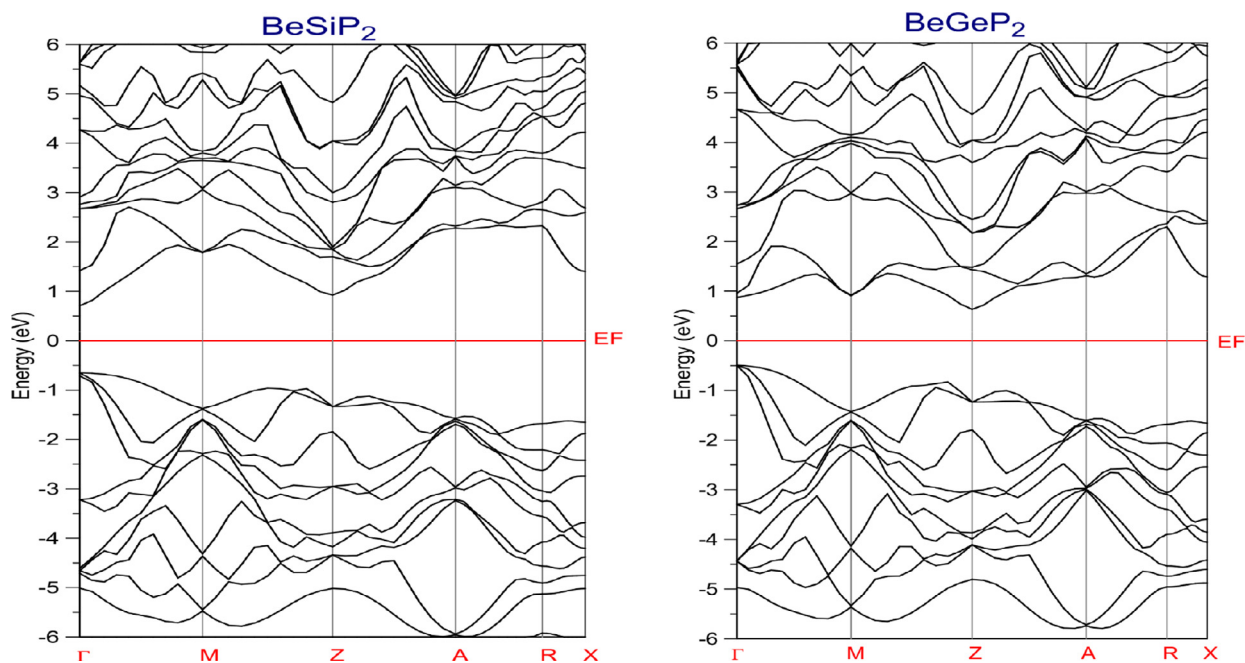


Fig. 2. Band structures along high-symmetry directions of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

symmetry points and directions in the first Brillouin zone in order to determine the energy gap values and nature of these materials. Calculations were made using the GGA-PBE approximation. The electronic band structures with the total and partial densities of state are given in Figs. 2 and 3 respectively.

At first, we note that the compounds studied have semiconductors behavior with direct bandgap for BeSiP<sub>2</sub> and indirect bandgap for BeGeP<sub>2</sub>, since the valence band maximum (VBM) is located at  $\Gamma_v$  point for the both compounds, and that the conduction band minimum (CBM) is located at  $\Gamma_c$  point for BeSiP<sub>2</sub> and  $Z_c$  point for BeGeP<sub>2</sub>. Furthermore, Shaposhnikov et al., categorized BeSiP<sub>2</sub> as direct band gap material, whereas BeGeP<sub>2</sub> was categorized as indirect band gap material [35]. The calculated band gaps along with other available data are presented in Table 3. From Table 3, it is clear that the band gaps decreased by changing the cation B from Si to Ge.

Secondly, Fig. 3 show that the electronic density of state can be divided into two distinct regions, below the maximum of the valence band (VBM), for both BeSiP<sub>2</sub> and BeGeP<sub>2</sub> compounds. The lowest region is included in the energy range ( $-7 \rightarrow -5.8$  eV for BeGeP<sub>2</sub>) and between ( $-7 \rightarrow -5.2$  eV for BeSiP<sub>2</sub>), it is dominated by the contribution of (Ge<sub>s</sub> and P<sub>s,p</sub>) states for BeGeP<sub>2</sub> and it is dominated by the contribution of (Si<sub>s</sub> and P<sub>s,p</sub>) states for BeSiP<sub>2</sub>. The second region is located between  $-5.2$  eV and the Fermi energy (EF), the latter region is itself divided into two sub-bands: the first one going from ( $-5.2 \rightarrow -2.2$  eV) and is, essentially, dominated by (Ge<sub>p</sub>, P<sub>p</sub>) states for BeGeP<sub>2</sub> and is, essentially, dominated by (Si<sub>p</sub>, P<sub>p</sub>) states for BeSiP<sub>2</sub> with a small contribution of (Be<sub>s</sub>, p) states in both compounds. The second sub-band is formed with significant contributions of (Be<sub>p</sub>, P<sub>p</sub>) states for both BeGeP<sub>2</sub> and BeSiP<sub>2</sub> compounds with a small contribution of (Be<sub>s</sub>, Ge<sub>p</sub>) states for BeGeP<sub>2</sub> and (Be<sub>s</sub>, Si<sub>p</sub>) states for BeSiP<sub>2</sub>. The conduction band, consists mainly of a mixture of states of type (Be/Ge/P<sub>s,p</sub>) for BeGeP<sub>2</sub> and (Be/Si/P<sub>s,p</sub>) for BeSiP<sub>2</sub>.

### 3.3. Optical properties

The knowledge of the different ways and forms of the interaction of light with matter in solid state physics is of great importance. The study of the optical properties of solids is an important tool for understanding the electronic properties of materials. In some particular structures, the energetic dependence of properties, mentioned above, on the band structure is very important. Critical information on eigenvalues as well as eigenfunctions is needed to calculate the frequency/energy dependent on optical properties.

The dielectric function of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds were calculated and presented with the GGA-PBE approximation. The magnitude, or the largest measurable quantity that we are interested here, is the dielectric function  $\epsilon(\omega)$  of the system, which is a complex quantity. The optical properties are deduced from the dielectric function of the semiconductor given by  $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ , where  $\epsilon_1(\omega)$  and  $\epsilon_2(\omega)$  are the real and imaginary parts of the dielectric function, respectively [36,37]. The imaginary part of the dielectric function is a necessary and crucial quantity. It indicates the evolution of inter-band transitions in the semiconductor [38].

For the studied materials of chalcopyrite structures, the dielectric function is solved in two components,  $\epsilon_x(\omega)$  which is represented by ordinary polarization spectra along direction x ( $E_{\perp c}$ -axis) and  $\epsilon_z(\omega)$  corresponding to the extraordinary polarization along the direction of z ( $E // c$ -axis). Fig. 4 illustrate the imaginary and real parts of the electronic dielectric function spectrum for a

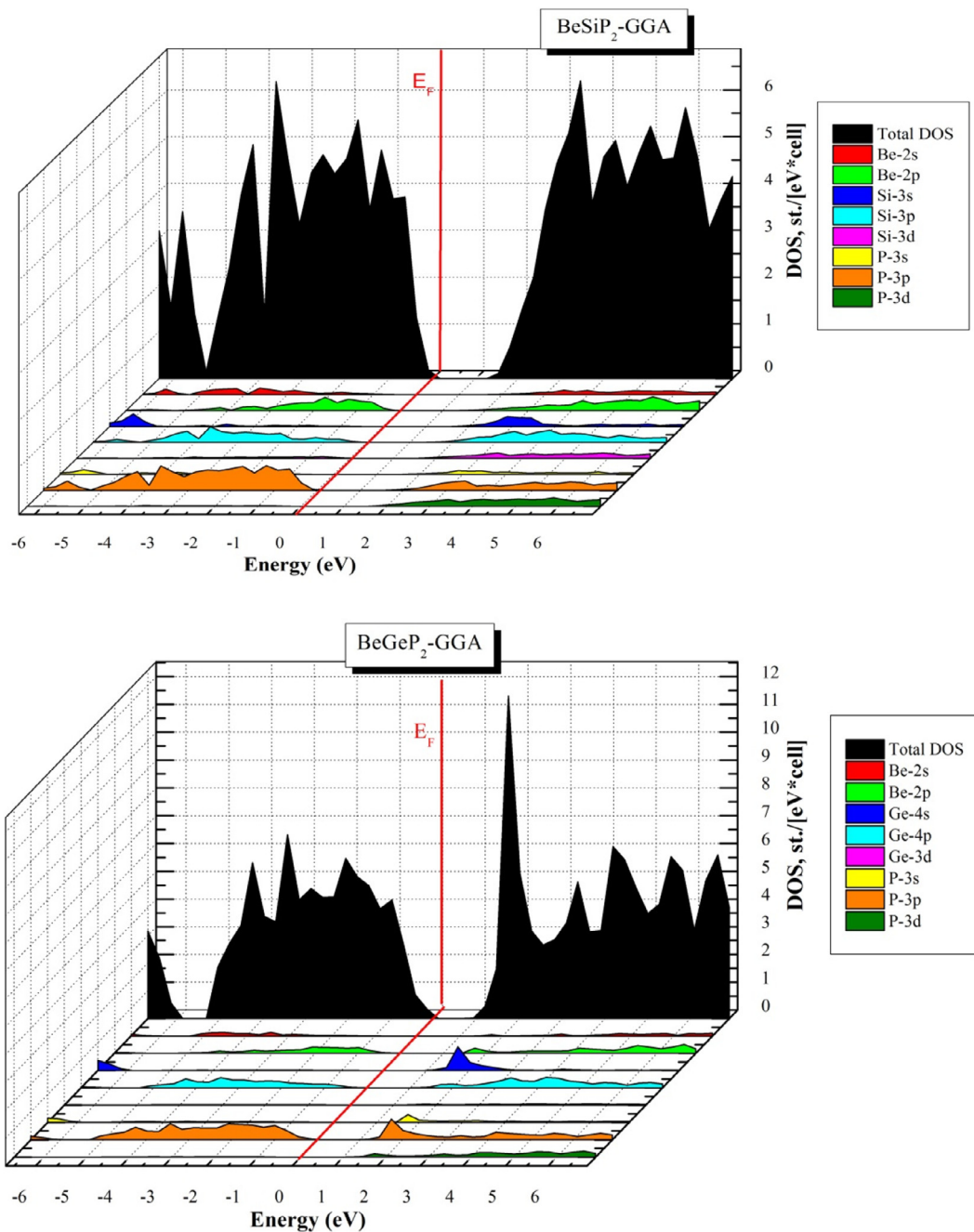


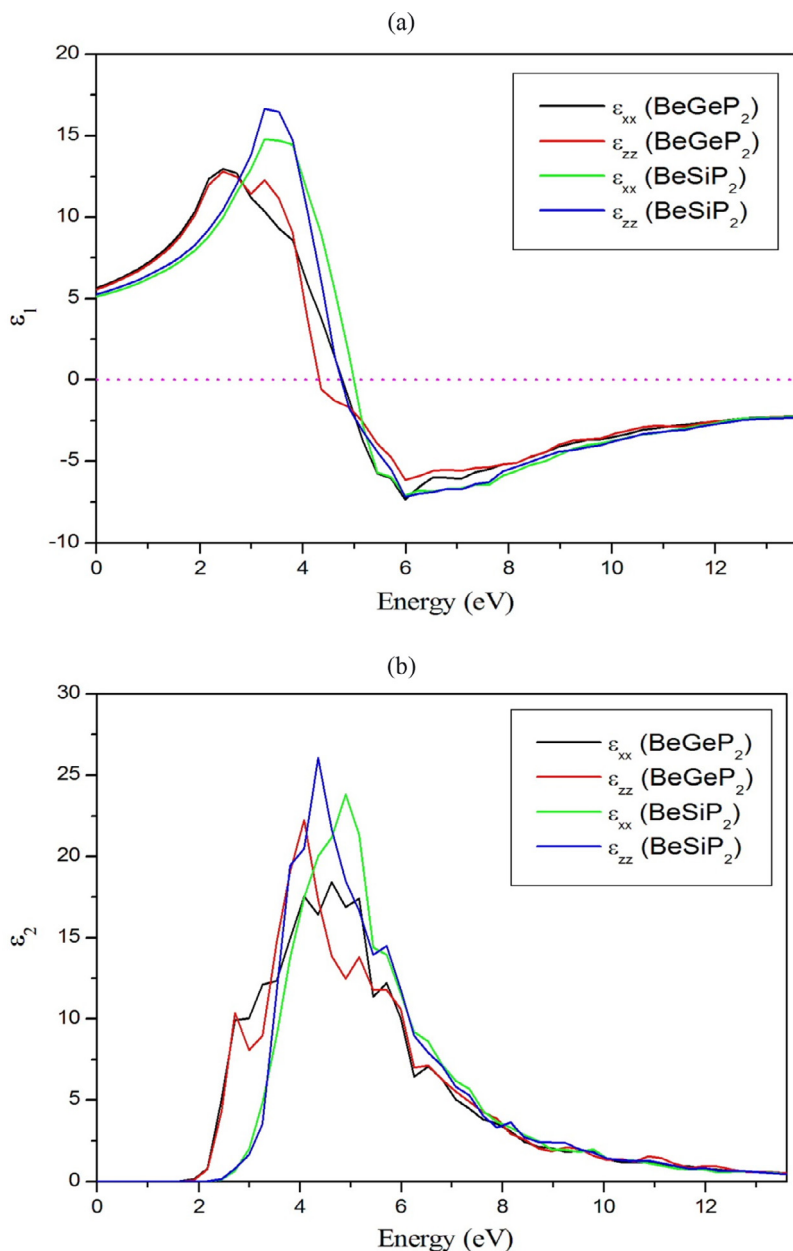
Fig. 3. Total and partial density of states of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

Table 3

Calculated energy band gap( $E_g$  in eV) compared with other theoretical values B' for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

Compound	Present cal	Other cal	Gap nature
BeSiP <sub>2</sub>	1.36	1.20 <sup>a</sup>	Direct
BeGeP <sub>2</sub>	1.12	0.85 <sup>a</sup>	Indirect

<sup>a</sup> Ref [35].



**Fig. 4.** Calculated dielectric functions of imaginary  $\epsilon_2(\omega)$  and real  $\epsilon_1(\omega)$  parts of the dielectric function for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite Compounds: real(a) and imaginary(b).

radiation up to 13.6 eV.

If we look at the real parts of the dielectric function, the main peaks are attributed to about 3.26 and 2.44 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub>, respectively, for both  $\epsilon_{1x}$  and  $\epsilon_{1z}$ . We can clearly see that the real part of the dielectric function becomes null for  $\epsilon_{1x}$  at the energy value 5 and 4.76 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> respectively, and it becomes null for  $\epsilon_{1z}$  to about 4.76 and 4.28 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> respectively, the minimum of these spectra corresponds to the energies 5.98 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> in all directions. Then the spectra of  $\epsilon_1$ , slowly increase to zero at high energy for all configurations. The static dielectric constants obtained in this study are about 5.15 and 5.6 for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> respectively in all directions.

Also our analysis of Fig. 4 for the curves of the imaginary parts of the dielectric functions  $\epsilon_2$ , shows that the first critical point of the dielectric function occurs at the energy of 1.63 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> for both  $\epsilon_{2x}$  and  $\epsilon_{2z}$ . This value corresponds to the electronic transition value ( $\Gamma_v \rightarrow \Gamma_c$ ). This point represents the fractionation  $\Gamma_v \rightarrow \Gamma_c$  which gives the threshold of the direct optical transitions between the highest state of the valence band and the lowest state of the conduction band. This is known as the fundamental absorption edge. Beyond these points, the curve increases rapidly for our two compounds. This is due to the fact that the

number of points contributing to  $\varepsilon_2$  increases sharply. The main peaks in the  $\varepsilon_{2x}$  spectra are located at 4.89 and 4.62 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> respectively, and it is located in the  $\varepsilon_{2z}$  at 4.35 and 4.08 eV for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> respectively.

### 3.4. Elastic properties

The linear response of an elastic crystal of arbitrary symmetry to infinitely small deformation is determined by the elastic constants. These form a tensor of rank four, which can be reduced to a  $6 \times 6$  matrix. Taking into account the symmetry of the directions of the deformation as well as by using the Voigt notation, and according to the principle in Neumann, the particular symmetry of a crystalline cell may impose additional restrictions on the elements of the elastic matrix. Since our chalcopyrites belong to the group of symmetry space of type I42d (122d D), with the class of Laue 42 m. A tetragonal material has seven elastic constants noted:  $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{16}$ ,  $C_{33}$ ,  $C_{44}$  and  $C_{66}$  ( $C_{16} = 0$  for a space group tetragonal material I-42d) and to be stable, these constants must satisfy the stability criteria generalized at zero pressure of a tetragonal structure, given by [39]:

$$M_1 = C_{11} > 0$$

$$M_2 = C_{44} > 0$$

$$M_3 = C_{66} > 0$$

$$M_4 = C_{11} - C_{12} > 0$$

$$M_5 = (C_{33})(C_{11} + C_{12}) - 2(C_{13})^2 > 0$$

Several other mechanical quantities can be determined by the elastic constants, in particular the Young's modulus E, the shear modulus G, the Poisson's ratio  $\nu$ , the compressibility modulus B and the anisotropic parameter by using the following relations [40]:

$$G = \frac{G_V + G_R}{2}$$

$$B = \frac{B_V + B_R}{2}$$

$$A = \frac{C_{33} - C_{13}}{C_{11} + C_{12} - C_{33}}$$

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

$$\nu = \frac{3B - 2G}{6B + 2G}$$

With:

$$G_R = 15 \left[ \frac{18B_V}{C^2} + \frac{6}{C_{11} - C_{12}} + \frac{6}{C_{44}} + \frac{3}{C_{66}} \right]^{-1}$$

$$G_V = \frac{1}{30} [M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66}]$$

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13}$$

$$C^2 = (C_{11} + C_{12}) C_{33} - 2C_{13}^2$$

$$B_V = \frac{1}{9} [2(C_{11} + C_{12}) + C_{33} + 4C_{13}]$$

$$B_R = \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}}$$

From where;  $G_R$ ,  $G_V$ ,  $B_V$  and  $B_R$  are respectively the shear module and the module of compressibility of Voigt and Reuss approximations Board.

The calculated elastic constants  $C_{ij}$  are summarized in Table 4, the shear modulus G, the Young's modulus E, Anisotropy factor and the Poisson's ratio are summarized in Table 5. The calculated values are the closest to compared to the calculated values available in the literature [23]. Our materials are stable, so we can synthesize them since the stability criteria are checked.

We conclude also that our compounds are more resistant to unidirectional compression to sheared formation due to the value  $C_{11} > C_{12}$  and  $C_{11} > C_{44}$ . The Zener anisotropy factor A shows the degree of elastic anisotropy in solids, we remarks that this factor his value is greater than unity which indicate the alloys are entirely anisotropic. From Table 4, we notice that the values of  $C_{44}$  and  $C_{66}$  are almost equal this shows that these compounds have the same shear along [100] (010) and [100] (001).

Table 5 show that our calculated bulk modulus of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> are 85,58 GPa and 63,92 GPa, respectively, which are in reasonable agreement with Ouahrani's [38] and with Fahad's [23] theoretical values. Both BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite studied

**Table 4**Calculated single-crystal elastic constants ( $C_{ij}$ , in GPa) for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

		$C_{11}$	$C_{12}$	$C_{13}$	$C_{33}$	$C_{44}$	$C_{66}$
BeSiP <sub>2</sub>	Present cal	155,38	54,60	48,19	157,57	79,45	79,61
	OTHER cal	164.7 <sup>a</sup>	49.8 <sup>a</sup>	50.2 <sup>a</sup>	167 <sup>a</sup>	85.7 <sup>a</sup>	85.7 <sup>a</sup>
BeGeP <sub>2</sub>	Present cal	174.27 <sup>b</sup>	61.23 <sup>b</sup>	63.08 <sup>b</sup>	178.82 <sup>b</sup>	91.32 <sup>b</sup>	90.60 <sup>b</sup>
	Other cal	124,98	31,47	33,08	130,33	63,36	61,62
		165.04 <sup>b</sup>	58.64 <sup>b</sup>	61.46 <sup>a</sup>	163.02 <sup>b</sup>	83.63 <sup>b</sup>	87.51 <sup>b</sup>

<sup>a</sup> Ref. [22].<sup>b</sup> Ref. [23].**Table 5**Calculated shear anisotropic factor (A), polycrystalline bulk modulus, shear modulus and Young's modulus (B, G and E, in GPa), B/G ratio and Poisson's ratio ( $\nu$ ) for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> ternary chalcopyrite semiconductors.

	A	B	G	E	$\nu$	B/G
BeSiP <sub>2</sub>	2086	85,582	67,482	160,311	0,187	1268
BeGeP <sub>2</sub>	3723	63,929	55,955	129,951	0.176 <sup>a</sup>	1.142

<sup>a</sup> Ref. [22].

are more resistive to volume compression than to shear due to  $B > G$ . The Young's modulus E is defined as the ratio of the tensile stress to the corresponding tensile strain. The obtained E values for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> are 160,31 GPa and 129.35 GPa, respectively, indicating BeSiP<sub>2</sub> compound has the higher stiffness than BeGeP<sub>2</sub> in the chalcopyrite structure.

Mechanical properties such as ductility and brittleness of semiconductor materials are very important for their technological applications. Considering that B and G represent the resistance to fracture and plastic deformation, respectively, the B/G ratio of polycrystalline phase is treated as an indication of ductile or brittle character [41]. The critical value which separates ductile and brittle materials is 1.75, corresponding to  $\nu = 0.26$ . If  $B/G > 1.75$ , the material behaves in a ductile manner, otherwise, it does in a brittle manner. As seen from Table 5, the values of the B/G ratio for BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrite compounds are smaller than the critical value, thus they may be classified as brittle materials.

#### 4. Conclusion

Chalcopyrite compounds are promising materials for some technological applications in electronics, optoelectronics and photonics because of their potential and excellent electronic, linear and nonlinear optical properties. This manuscript presents a theoretical investigation of structural, electronic, optical and elastic properties of BeSiP<sub>2</sub> and BeGeP<sub>2</sub> chalcopyrites. The different results obtained are summarized in the following points:

- The lattice constants and the equilibrium volume increased as we moved from Si to Ge, whereas the c/a ratio decreased by replacing B from Si to Ge. Also, the internal parameters decreased by changing A from Si to Ge. The structural properties of the ground state (a, c / a and u) obtained from our calculations are in good agreement with other theoretical calculations.
- The investigation of the band gap suggested that BeSiP<sub>2</sub> has a direct band gap compound, whereas BeGeP<sub>2</sub> has indirect band gap compound. The band gaps decreased by changing B from Si to Ge. The obtained results stayed in good agreement other theoretical data.
- Concerning the optical properties, we studied the imaginary part  $\epsilon_2$  and the real part  $\epsilon_1$  of the dielectric function to reproduce the dielectric constant  $\epsilon_0$ . The results obtained show that these materials are promising semiconductors for optoelectronic applications and above all as good candidates for photovoltaic applications.
- For the elastic properties, the single-crystal elastic constants  $C_{ij}$ , shear anisotropic factors A, as well as polycrystalline bulk, shear and Young's modulus (B, G and E) and Poisson's ratio  $\nu$  have been predicted. The generalized elastic stability criteria for a tetragonal crystal are well satisfied, indicating that BeSiP<sub>2</sub> and BeGeP<sub>2</sub> are mechanically stable in the chalcopyrite structure against elastic deformations. Moreover, chalcopyrite BeSiP<sub>2</sub> and BeGeP<sub>2</sub> should be classified as brittle materials.

#### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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