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THEORETICAL INVESTIGATION OF STRUCTURAL, ELECTRONIC, AND OPTICAL PROPERTIES OF $ZnSnP_2$ SEMICONDUCTOR

M. Ouledali [1, 2], B. Amrani [3], S. Daoud [4, *], S. Louhibi-Fasla [1], H. Rekab-Djabri [1,5], N. Beloufa [1], S. Bekheira [6], I. Ouadha [7]

[1]*Laboratory of Micro and Nanophysics (LaMiN), National Polytechnic School Oran, ENPO-MA, BP 1523, El M'Naouer, 31000, Oran, Algeria*
[2] *Faculty of Science and Technology, University of Amed Draia, Adrar, Algeria.*
[3]*Laboratory of Theory and Simulation of Materials, Faculty of Exact and Applied Sciences, University of Oran 1 Ahmed Ben Bella, BP 1514, El Menouer, 31000, Oran, Algeria.*
[4]*Laboratory of Materials and Electronic Systems, Mohamed El Bachir El Ibrahimi University of Bordj Bou Arreridj, 34000, Bordj Bou Arreridj, Algeria*
[5]*Faculty of Nature and Life Sciences and Earth Sciences, Akli Mohand-Oulhadj University, 10000, Bouira, Algeria*
[6]*Laboratory of Materials (LabMat), ENP-Oran, Algeria*
[7]*Magnetic Materials Laboratory, Faculty of Exact Sciences, University of Djillali Liabès, Sidi Bel-Abbès, 22000, Algeria*
**Corresponding author E-mail: salah_daoud07@yahoo.fr*

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Abstract

The structural, electronic, and optical properties of $ZnSnP_2$ compound were determined using the first principles calculations. We applied the full-potential enhanced plane wave method (FP-LAPW) within the framework of density functional theory (DFT) as implemented in the Wien2k package. The exchange-correlation potential term was treated using the local density approximation (LDA), the generalized gradient approximation (GGA), the Engel–Vosko generalized gradient approximation (EV–GGA) and GGA plus modified Becke–Johnson (mBJ). The lattice parameters of the $ZnSnP_2$ obtained by minimizing the total energy are consistent well with the existing theoretical and experimental results. The Dugdale and MacDonald Grüneisen parameter was found to be 1.43 from the GGA and 1.44 from the LDA, respectively.

According to the electronic properties, the band structure analysis of $ZnSnP_2$ shows that it has a direct band gap in the (Γ-Γ) direction with a value of 1.43 eV. We have investigated the optical properties of $ZnSnP_2$ semiconducting compound. The data of the dielectric functions shown that the peaks are positioned at around 2.41, 3.21, 3.83 and 4.09 eV, respectively.

1. Introduction

Advances in solar photovoltaic (PV) power generation are critical to addressing global energy needs [1, 2]. The optimization of different parameters, especially: the band gap *Eg*, dimensions,….etc of the solar cell material for best values are parameterized in research and compared at different time [3]. Improving the power output by further optimizing device performance may be contributed to the reduction of production cost of solar cells [4].

In this field, $ZnSnP_2$ ternary compound has developed into a promising photovoltaic absorber material due to its suitable optical property: a direct band gap of 1.68 eV [5], which gives a high theoretical photovoltaic conversion efficiency approaching 33.7% in AM 1.5G sunlight at the Shockley-Queisser limit [6]. $ZnSnP_2$ material shows p-type conductivity [7, 8]. Theoretically, Scanlon and Walsh [9] attempted to reduce the band gap of $ZnSnP_2$ to the optimal value of 1.5 eV to increase the photoelectric conversion efficiency, and found that controlling the cation distribution could adjust its band gap. Yokayama *et al.* [10] alloyed $ZnSnP_2$ with another semiconductor with narrower band gap, $CdSnP_2$ found that the band gap of $Zn_{1-x}Cd_xSnP_2$ decreases with increasing *x*.

The electronic structure of different materials can be tuned by the application of high pressure as has been demonstrated in the literature [11-15]. Xu *et al.* [16] investigated the effects of the strain on the electronic structure of $ZnSnP_2$ ternary compound using an *ab-initio* calculation. They found that the biaxial tensile strain reduces the value of the band gap from 1.3 to 1.0 eV for $ZnSnP_2$ compound.

In this contribution, we have used the full potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT) to investigate the structural parameters, electronic structure and optical properties of $ZnSnP_2$ ternary compound.

The paper is organized as follows: in the second section, we present the details of the calculation, while the results and discussions are presented in the third section. Finally, a conclusion is given in the fourth section.

2. Computational details

The full potential linearized augmented plane wave (FP-LAPW+lo) method [17, 18] with the local density approximation (LDA), the generalized gradient approximation (GGA) [19], Engel-vosko generalized gradient approximation (EV-GGA) [20], and the Modified Becke-

Johnson (mBJ) exchange potential [21], as implemented in the Wien2K computer software [22] are used for studying $ZnSnP_2$ semiconductor.

The band gaps and electronic dispersion curves are usually under-estimated by the GGA method [23], while the mBJ exchange potential has very accurate electronic band structures for various types of semiconductors and insulators.

In the FP-LAPW method, the unit cell is divided into a muffin-tin sphere and interstitial regions. Within the so-called muffin-tin sphere, the wave function is expanded into spherical harmonics and the maximum quantum number for wave function expansion into the atomic spheres has been constrained to $l_{max} = 10$. The plane wave cutoff of $K_{max} = 7.0$, RMT (RMT is the smallest muffin-tin radius in the unit cell) is selected for expansion of the wave functions in the interstitial region (IR) while the charge determination is Fourier expanded to $G_{max} = 12$ $Ryd^{-1/2}$. The calculations were done using 500 k-points in the Brillouin zone (ZB).

3. Discussion of results

3. 1. Structural properties

The crystal structure of $ZnSnP_2$ ternary chalcopyrite is a body centered tetragonal (BCT) with space group $I\bar{4}2d$ [24, 25]. This structure is characterized by two lattice parameters *a* and *c*, and the internal parameter *u* [16]. The atomic positions of different elements constituted $ZnSnP_2$ material are: Zinc (0 0 0; 0 1/2 1/4), Tin (1/2 1/2 0; 1/2 0 1/4) and Phosphorus (u 1/4 1/8; -u 3/4 1/8; 3/4 -u 7/8; 1/4 u 7/8), respectively. It is clearly seen that the atomic positions of phosphorus depend on the internal parameter *u*.

The parameters of the structure for the $ZnSnP_2$ have been calculated using an energy optimization procedure. In this procedure, the experimental lattice constant is chosen and varies in its neighborhood. Therefore, the volume of the unit cell varies and hence the density depends on the energy of the unit cell is the ground state of the system and the volume corresponding to the minimum energy is the optimized volume [26, 27]. The total energies were then calculated as a function of volume and the obtained data fitted to the Murnaghan equation of state [28-30].

$$E(V) = \frac{B_0 V}{B'_0}\left[\frac{(V_0/V)^{B'_0}}{B'_0 - 1} + 1\right] + E_0 - \frac{V_0 B_0}{B'_0 - 1} \quad (1)$$

where B_0 is the bulk modulus ($B_0 = \partial^2 E/\partial V^2$), and B'_0 is the pressure derivative of the bulk modulus. The *c/a* ratio has also been optimized at a constant volume.

Our results have shown that the most stable structure of $ZnSnP_2$ material occurs when the axial ratio $c/a = 2.00$ and $u = 0.227$. The structural properties and bulk parameters are listed in Table 1, and compared to other data of the literature [5, 24, 31 - 34]. It can be seen that our values agree well with the experimental and other theoretical results, indicating that the methods used in our work are reliable and reasonable. The deviation between our value (65.98 GPa) of the bulk modulus B and the experimental one (67.5 GPa) [32] is only around 2.25 %. Furthermore, our values of the pressure derivative of the bulk modulus calculated from both LDA and GGA are almost the same (~ 4.86). This later value is also in good agreement compared to the theoretical result (4.67) reported by Sahin *et al.* [24].

Table 1. Lattice constants a and c, internal parameters u, bulk modulus B_0 and its pressure derivative B'_0 for $ZnSnP_2$ compared to other theoretical [5, 24] and experimental [31 - 34] values.

Method		a (Å)	c (Å)	c/a	u	V (Å^3)	E (eV)	B (GPa)	B'_0
Pres. work	GGA	5.731	11.486	2.00	0.232	377.25	- 471273.56	65.98	4.85
	LDA	5.603	11.243	2.00	0.227	352.96	- 470720.12	79.52	4.87
Theo. work	[5]	5.666	11.399	2.00	0.232	-	-	-	-
	[24]	5.638	11.228	1.99	0.25			73.69	4.67
Expe.	[31]	5.651	11.476	2.00	0.239	-	-	67.5 [32]	-
	[33]	5.65	11.30	2.00	0.227	-	-	-	-
	[34]	5.652	11.305	2.00	0.229	-	-	-	-

The Dugdale and MacDonald Grüneisen parameter γ_{D-M} was estimated as follow [35]:

$$\gamma_{D-M} = \left(\frac{1}{2}B' + \frac{2}{9}\left(\frac{p}{\mathrm{B}}\right) - 1\right) \Big/ \left(1 - \frac{2p}{3\mathrm{B}}\right) \qquad (2)$$

where B is the bulk modulus, p is the pressure and B' is the first-order pressure derivative of B.

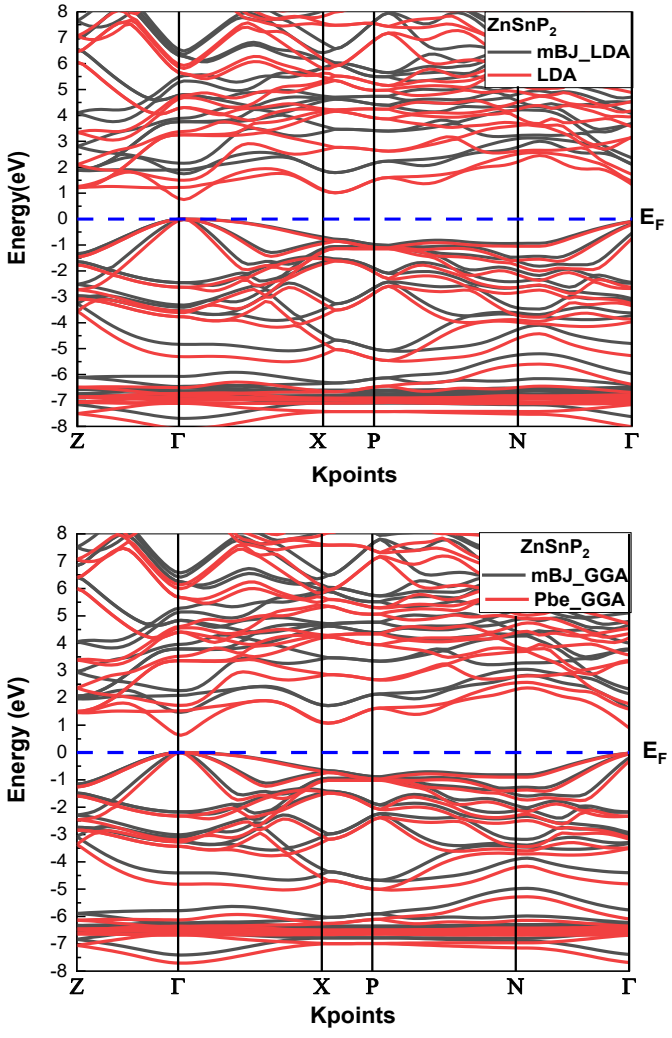
At zero-pressure, the Dugdale and MacDonald Grüneisen parameter γ_{D-M} of $ZnSnP_2$ compound was predicted and found to be 1.43 from the GGA and 1.44 from the LDA, respectively. In comparison with other theoretical data, we can observe that our obtained values of γ_{D-M} for $ZnSnP_2$ compound are lower than the value (2.18) of the thermodynamic Grüneisen parameter γ calculated at T= 300 K and P = 0 GPa [36].

3.2. Electronic properties

The electronic properties of $ZnSnP_2$ semiconducting compound are discussed by

calculating the band structure, and the total and partial density of states (DOS). The calculated band structure of $ZnSnP_2$ along the lines of high symmetry of the first Brillouin zone is shown in Fig. 1. It can be seen that the top and bottom of the valence and conduction bands are located at the same points of symmetry Γ, which is consistent with previous theoretical studies [16, 37]. The self-consistent scalar relativistic band structure of the $ZnSnP_2$ compound was obtained at equilibrium volume in the GGA, EV and mBJ schemes. The usual problem of reducing the DFT gap with experimental results prompts researchers to find a suitable solution; mBJ is a modified version of the interchangeability proposed by Becke and Johnson [16, 21].

The agreement with the experiment is very good for various semiconductors and is of the same order of agreement as that obtained with the hybrid functions or the GW methods [38]. This semi-local exchange potential mimics the behavior of the orbit-dependent potentials very well and leads to calculations which are barely more expensive than GGA calculations. Therefore, it can be applied to very large systems efficiently.



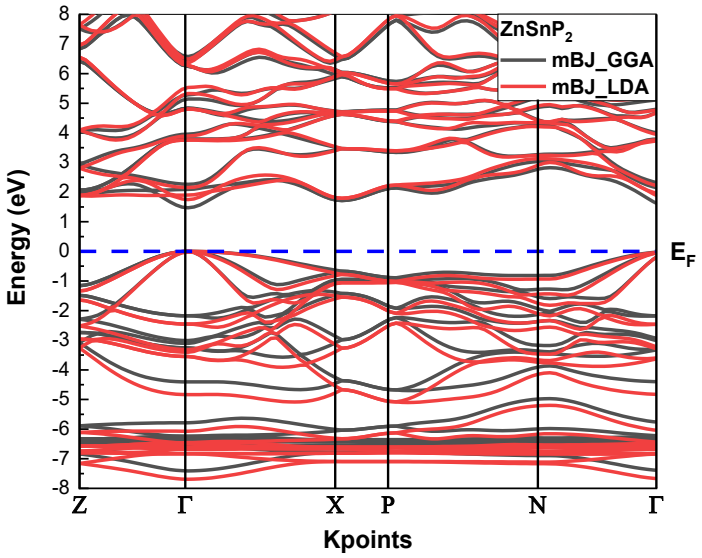


Figure 1. Band structures of $ZnSnP_2$ compound, calculated along high symmetry directions

Table 2 shows the band gap *Eg* predicted using the LDA, GGA, Table 2 shows the band gap *Eg* predicted using the LDA, GGA, EV and mBJ approaches. As shown in Table 2, we observe clearly that our calculated values of *Eg* were improved using the mBJ approach with both the LDA and the GGA. Our calculated values (1.43 and 1.71 eV) of *Eg* are in good agreement with the experimental data (1.68 eV) [39] and other theoretical values [16, 40]. The deviation between our value (1.71 eV) of *Eg* and the value (1.68 eV) [39] is less than 1.80 %.

Table 2. Calculated band gap energy Eg (eV) values of chalcopyrite $ZnSnP_2$ compound, using GGA, Engle-vosko (EV) and mBJ methods. The results are compared with the experimental [39] and other theoretical [16, 40] values.

	Present work					Other works		
Method	LDA	PBE-GGA	EV-GGA	mBJ (LDA)	mBJ (GGA)	Exp. [39]	Theo[16]	Theo [40]
	0.71	0.61	0.37	1.71	1.43	1.68	1.31	1.06

The density of states (DOS) is an important physical quantity, which helps on the understand the nature of the electronic band structure and magnetic properties of materials [41]. Furthermore several electronic transport properties of semiconducting materials are determined based on knowledge of the density of states. Thus, it makes it possible to know the nature of the chemical bonds in the material and therefore the transfer of charges between the orbital and the atoms. The total and partial densities of states (TDOS, PDOS) spectra for $ZnSnP_2$ are shown in Fig. 2.

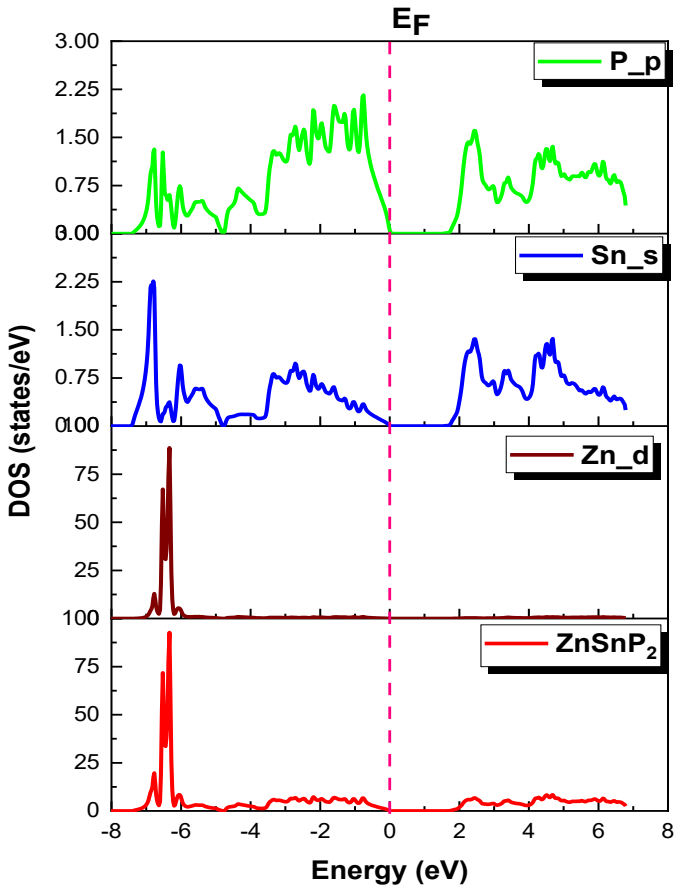


Figure 2. Total and partial density of states for $ZnSnP_2$ material

It is clearly seen that the lower part of the valance band is mainly due to the d-states of Zn, while the extended region at the top of the valance band is made up of s-states. From PDOS, hybridization between the s and p states can be clearly observed. The p states of P mainly contribute to the bottom of the conduction bands.

3.3. Optical properties

We have investigated the optical properties of $ZnSnP_2$ semiconducting compound. The dielectric function ε (ω) can be used to describe the linear response of the system to electro-magnetic radiation, which concerns the interaction of photons with electrons [42].

It is well known that the imaginary part $\varepsilon_2(\omega)$ of the dielectric function can be calculated with the momentum matrix elements between the occupied and unoccupied wave functions within the selection rules [41, 43-45]:

$$\varepsilon^{ij}{}_2(\omega) = \frac{4\pi^2 e^2}{\Omega m^2 \omega^2} \sum_{knn'\sigma} \langle kn\sigma | p_i | kn'\sigma \rangle \langle kn'\sigma | p_j | kn\sigma \rangle f_{kn} (1 - f_{kn'}) \delta(e_{kn'} - e_{kn} - \hbar\omega) \qquad (3)$$

In Eq. (3), e is the electron charge, Ω is the crystal volume, m is mass of the electron, and f_{kn} is the Fermi distribution. Moreover, $|kn\sigma\rangle$ is the crystal wave function corresponding to the n^{th} eigenvalue with crystal momentum k and σ spin. The real part of the dielectric function, $\varepsilon_1(\omega)$, is obtained from $\varepsilon_2(\omega)$ using the so-called Kramers–Kronig transformation written below [46, 47]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\eta \int_0^{\infty} \frac{\varepsilon_2(\omega')\omega'}{\omega'^2 - \omega^2} d\omega' \tag{4}$$

where ω is the frequency, and η is the so-called Cauchy principal value.

The refractive index, n (ω) is obtained directly from the relation [24]:

$$n(\omega) = \left(\left(\left(\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2\right)^{1/2} + \varepsilon_1(\omega)^2 \right)/2 \right)^{1/2} \tag{5}$$

In the present contribution, all the spectra are plotted with the incident radiation polarized both perpendicular and parallel to the tetragonal c-axis of the crystal.

Fig. 3 shows the real part $\varepsilon_1(\omega)$ calculated in mBJ of the dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The main real part peak for $ZnSnP_2$ material is at around 2.37 eV, which is slightly higher than that (2.275 eV) reported for $Sc_{0.5}Ga_{0.5}P$ ternary semiconducting alloy [41]. From the quantitative point of view, similar behavior of the real part $\varepsilon_1(\omega)$ for $ZnSnP_2$ material was obtained by Sahin *et al.* [24] using pseudo-potential plane-wave (PP-PW) approach.

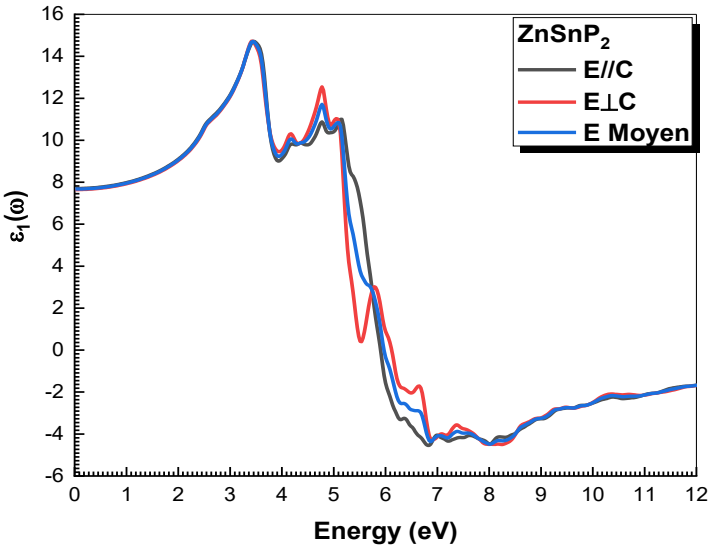


Figure 3. The calculated real part $\varepsilon_1(\omega)$ of dielectric constant for $ZnSnP_2$

It should be noted that the so-called imaginary part $\varepsilon_2(\omega)$ of the dielectric function $\varepsilon(\omega)$ is the fundamental factor described the optical properties for any material [24]. Fig. 4 displays $\varepsilon_2(\omega)$ calculated in mBJ as a function of the photon energy for $ZnSnP_2$ material. There are four main peaks for $ZnSnP_2$, the peaks are positioned at 2.41, 3.21, 3.83 and 4.09 eV, respectively.

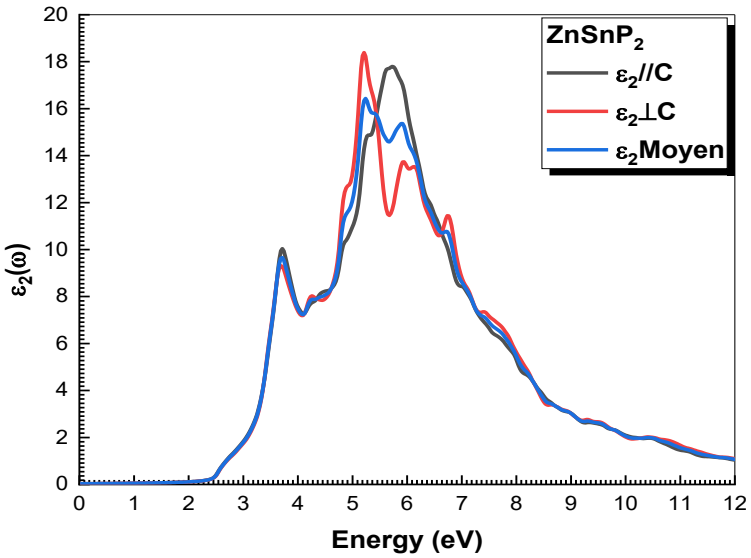


Figure 4. The calculated imaginary part $\varepsilon_2(\omega)$ of complex dielectric constant for $ZnSnP_2$

It should be noted that both ε_1 and ε_2 display isotropic behaviors except the intermediate energies for the $ZnSnP_2$. The zero-frequency limits $\varepsilon_1(0)$ is the electronic part of the static dielectric constant. Table 3 summarizes some important optical properties for $ZnSnP_2$ compound.

It can be seen that our value (7.68) of the zero-frequency limit ε_{moy} is lower than the results 10.08 and 12.68 reported in Refs. [24] and [48], respectively. Although our value (2.78) of the refractive index is lower than the theoretical one (3.16) reported by Sahin *et al.* [24], it is in general in agreement with the experimental one (2.9) [49].

Table 3. Zero-frequency limit ε_0 and refractive index n_0 for $ZnSnP_2$ crystal, in comparison with other data of the literature [24, 48].

Parameter		$\varepsilon_1^{//}(0)$	$\varepsilon_1^{\perp}(0)$	ε_{moy}	$n_1^{//}(0)$	$n_1^{\perp}(0)$	n_{moy}	Δn
Present work	mBJ	7.65	7.70	7.68	2.77	2.78	2.78	0.0096
Other works	[24]			10.08			3.16	
	[48]	12.68	12.75	12.72	3.56	3.57	3.57	0.0105

Before it is absorbed, the light of a given wavelength penetrates into the material for a certain distance. This later can be determined by the optical absorption coefficient [50]. One of the main reasons for the success of the solar photovoltaic material is its high optical absorption

coefficient. The corresponding absorption spectra are produced from the different inter-band transitions and can be calculated using the equation as followed [51]:

$$\alpha(\omega) = \sqrt{2}\omega \left(\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} - \varepsilon_1(\omega) \right)^{1/2} \quad (6)$$

where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary parts of the dielectric function, respectively.

Fig. 5 shows the absorption coefficient calculated for $ZnSnP_2$ compound as a function of the photon energy. The photon energy absorbed by an electron to excite itself from valence band (VB) to conduction band (CB) was used to define the optical band gap of semiconducting material.

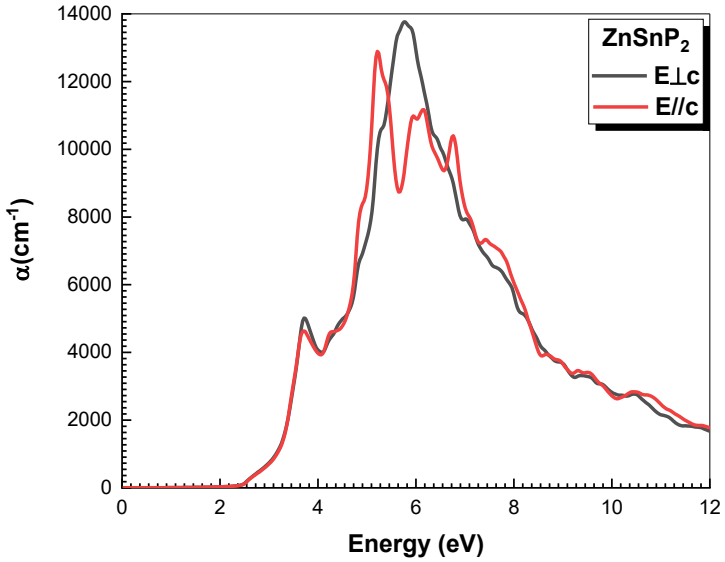


Figure 5. The calculated absorption coefficient α(ω) for $ZnSnP_2$ compound

The absorption threshold for $ZnSnP_2$ compound was found to be 1.48 eV, corresponding to their forbidden bands. This value is slightly higher than direct optical transition value (1.443 eV) reported for $Sc_{0.5}Ga_{0.5}P$ ternary semiconducting alloy [41].

4. Conclusion

In conclusion, we performed systematic *ab initio* first principle calculations of the structural, electronic and optical properties of $ZnSnP_2$ chalcopyrite semiconductor using the DFT. The calculated structural parameters such as the lattice constants, the anion internal parameter (u) and the bulk modulus of chalcopyrite are in good agreement with other available theoretical and experimental works. The values of the pressure derivative of the bulk modulus

calculated from both LDA and GGA are almost the same (~ 4.86).

Our value 1.43 (1.44) of the Dugdale and MacDonald Grüneisen parameter γ_{D-M} of $ZnSnP_2$ is lower than the theoretical one (2.18) of the thermodynamic Grüneisen parameter γ of the literature.

Analysis of the chalcopyrite band structure indicates the existence of a direct band-gap in the (Γ-Γ) direction with a value of *Eg* = 1.43 eV using mBJ (GGA) calculation and *Eg* = 1.71 eV using mBJ (LDA) approach, respectively. Our value (1.71 eV) of *Eg* deviates from the experimental one (1.68 eV) by around 1.80 %.

We have investigated the optical properties of $ZnSnP_2$ semiconducting compound. The analysis of the dielectric function shown that the peaks are positioned around 2.41, 3.21, 3.83 and 4.09 eV, respectively, while the absorption threshold was found to be 1.48 eV.

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