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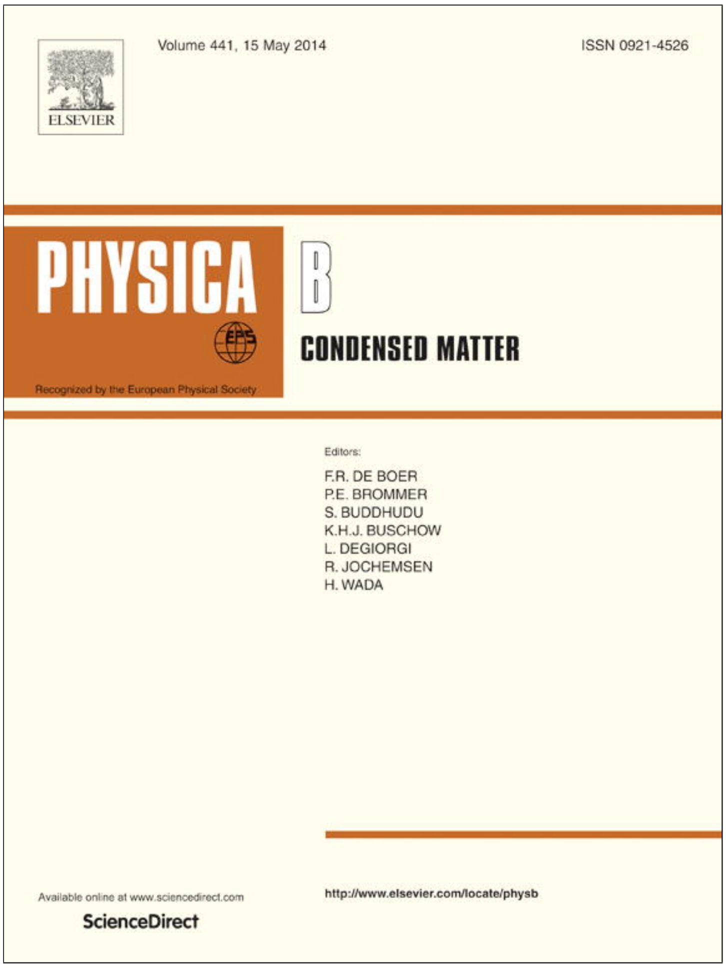

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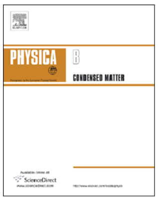

Towards from indirect to direct band gap and optical properties of XYP_2 ($X=Zn$, Cd; $Y=Si$, Ge, Sn)

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ABSTRACT

First principle calculations are performed to predict the electronic and optical properties of XYP_2 ($X=Zn$, Cd; $Y=Si$, Ge, Sn) compounds. The calculations show an excellent agreement with the available experimental results as compared to previous calculations. The band gap value decreases by changing the cations X from Zn to Cd as well as Y from Si to Ge to Sn in XYP_2. The d-states of the Zn and Cd contribute majorly in the density of states. Bonding nature in these compounds is analyzed from the electron density plots. Optical response of these compounds is noted from the complex refractive index and reflectivity spectra. The wide direct band gap and the high reflectivity in the visible and ultraviolet regions for these compounds make them potential candidates for optoelectronic and photonic applications.

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1. Introduction

XYP_2 ternary compound crystallize in tetragonal chalcopyrite structure providing a three dimensional network with space group$I\bar{4}2d(D_{2D}^{12})$. These compounds form a diverse group of semiconductors, offering a remarkable and promising properties making them potential materials for electronic and optoelectronic applications such as solar energy converters, light emitting and spintronic devices. Most of ternary chalcopyrite compounds are characterized by high nonlinear optical coefficients and considerable birefringence, some of them have a large absorption coefficient for solar cell, and others are efficient sources for spintronic [1–6]. $CdGeP_2$ and $ZnGeP_2$ compounds possess a ferromagnetic behavior when they are doped with the manganese at room temperature [7], which makes them candidate materials in spintronic applications. $ZnGeP_2$ is established as nonlinear optical (NLO) material with high nonlinear optical coefficients [8]. $CdGeP_2$ is also considered to be an important material for technological applications in the areas of optical parametric oscillators and up converters [9]. The $ZnSnP_2$ is a viable candidate as a light absorber in solar cells [10]. $CdSiP_2$ offers unique properties for parametric down-conversion into the mid-IR [11].

Tremendous experimental works on XYP_2 type semiconductors have been done. Stokowski reported the polarized-reflectance spectra and logarithmic derivative of the reflectance at 2 K of these compounds [12]. The growth and electronic properties of these compounds were reported by Shay and co-workers [1]. Gehlhoffa et al., studied the native point defects in $ZnSiP_2$ [8]. Optical and vibrational properties of $CdGeAs_2$ were reported by Choi and co-authors [5]. Medvedkin et al., reported on the ferromagnetism nature of $CdGeP_2$ when it is doped with Mn at room temperature [7]. Sato and co-workers reported on novel magnetic semiconductors based on II–IV–V_2 compounds and opened the golden eras regarding XYZ_2 type alloys for spintronic applications [13]. Zhang et al. [14] studied the thermal annealing effects on the infrared transmittance reported by Chalus et al. [11]. On the theoretical side, some attempts have been devoted to the herein studied compounds. Jiang et al. [15] reported the cation-related point defect in $ZnGeP_2$. Reddy and co-authors studied the correlations between energy gap, optical electronegtivity and electronic polarizibility for these materials [16]. Chiker and co-authors [17–19] studied the electronic and optical properties of the investigated compounds using the augmented plane wave method and the local density approximation (LDA). Rashkeev et al. [20] reported on the second harmonic and birefringence on some

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ternary pnictides semiconductor using the first principles linear muffin-tin orbitals (LMTO) method within the atomic sphere approximation. The obtained band gaps in the later studies are much smaller than the experimental results.

From the above it is clear that there is considerable experimental works have done on XYP_2 (X=Zn, Cd; Y=Si, Ge, Sn) compounds. Few theoretical studies using the common LDA within first principles technique have appear to consider this family of compounds for opto-electronic application. Therefore, we think it is timely to perform calculations on the optoelectronic properties for these compounds using the density functional theory (DFT) [21,22] with Engel and Vosko's GGA formalism which proven to yields better band gaps rather than the common LDA and GGA approximations, in order to complete the existing theoretical and experimental works on these compounds.

The paper is organized as follows. Section 2 briefly describes the computational techniques used in this work. Results and discussions of the structural, electronic and optical properties are presented in Section 3. Finally, conclusions and remarks are given in Section 4.

2. Computational details

Calculations were performed using the full potential linearized augmented plane wave plus local orbitals (FP-LAPW+lo) method [23] as implemented in Wien2K package [24]. The exchange-correlation potential was treated with Engel and Vosko GGA scheme [25]. The different computational parameters namely, $R_{MT}*K_{max}$, where R_{MT} denotes the smallest muffin-tin radii and K_{max} gives the magnitude of largest K vector in the plane wave basis, the charge density Fourier expansion parameter G_{max}, the expansion parameter l_{max} for the valence wave functions inside the atomic spheres, and the special K-points explored within the tetrahedron method [26] for integrating the irreducible first Brillouin zone (IBZ) are given in Table 1. The self-consistent calculations are considered to be converged when the total energy of the system is stable within 0.001 Ry. The electronic and optical properties are calculated using the experimental lattice parameters given in Table 1. The herein studied compounds crystallize in chalcopyrite structure at ambient conditions. The crystal structure of chalcopyrite XYP_2 compounds is shown in Fig. 1. The X atom occupies (0, 0, 0), (0, 1/2,1/4) sites, the Y cations occupies (0, 0, 1/2), (0, 1/2,3/4) sites, and P atom occupies (u, 1/4, 1/8), (−u, 3/4,1/8), (3/4, u, 1/8), (1/4, −u,7/8) sites.

3. Results and discussion

In this section we present the obtained results on the optoelectronic properties of the investigated compounds such us band structures, densities of states and optical spectra. The electronic band structure of XYP_2 (X=Zn, Cd; Y=Si, Ge, Sn) compounds are computed at the experimental lattice parameters within both GGA and EVGGA schemes. Figs. 2 and 3 illustrate the calculated band structures for $ZnYP_2$ and $CdYP_2$ compounds, respectively, within the EVGGA as a prototype since the band profiles are quite similar for both GGA and EVGGA with a small difference in details. The zero energy is chosen to coincide with the top of the valence band. It is seen that the pattern of the band structures (BS) in $ZnYP_2$ compounds is almost similar with a small difference in details. A clear similarity in the calculated band structures of $CdYP_2$ compounds is also observed. The overall calculated band profiles are in fairly good agreement with the previous theoretical results.

It is seen from Figs. 2 and 3 that the valence band maximum (VBM) is located at the Γ point in all compounds. However, the conduction band minimum (CBM) occurs along the Δ-direction near the H point for $ZnSiP_2$ and $CdSiP_2$ and at the Γ for the remained compounds, resulting in a direct band gap (Γ–Γ) for XYP_2 (X=Zn, Cd; Y=Ge, Sn) compounds and an indirect band gap ($\Gamma-\Delta_{min}$) for $ZnSiP_2$ and $CdSiP_2$. The results of our calculations are in agreement with the earlier calculations for the valence band configuration, predicting the valence band maximum (VBM) at the Γ point. However, there is some controversy on the position of the conduction band minimum (CBM) and consequently on the nature of the band gap either to be direct, pseudo direct or indirect. The pseudo direct nature meant that the gap is nominally direct but corresponds to a weak, almost forbidden, optical transition. Chiker and co-workers [18] and Rashkeev et al. [20] found that both $ZnSiP_2$ and $CdSiP_2$ are pseudo direct band gap materials with CBM location at the Γ-edge, in contrast to the study of Shay and Tell

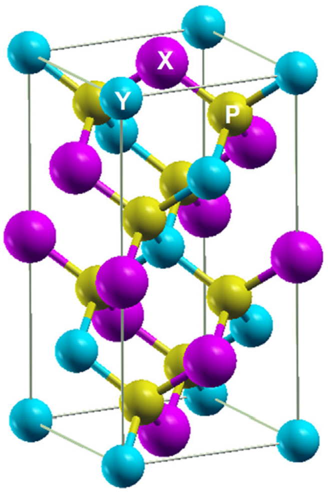

Fig. 1. Chalcopyrite structure of XYP_2.

Table 1
The lattice parameters, R_{MT}, $R_{MT}*K_{max}$, l_{max} and K-points, used in our calculations.

Compound	Latt. Const.		u (expt.)	R_{MT}	$R_{MT}*K_{max}$	l_{max}	K-points
	a[Ȧ][a,b]	c[Ȧ][a,b]					
$ZnSiP_2$	5.4	10.43	.269[b]	Si=1.99, Zn=2.16, P=1.91	7	10	726
$ZnGeP_2$	5.463	10.74	2582[b]	Ge=2, Zn=2, P=2	7	10	726
$ZnSnP_2$	5.652	11.305	.239[b]	Sn=2, Zn=2, P=2	7	10	726
$CdSiP_2$	5.67	10.431	.27[c]	Si=2.09,Cd=2.17, P=1.92	7	10	726
$CdGeP_2$	5.74	10.776	.28[c]	Ge=2, Cd=2, P=2	7	10	726
$CdSnP_2$	5.90	10.93	.26[c]	Sn=2.25, Cd=2.32, P=2.05	7	10	726

[a] Ref. [1].
[b] Ref. [33].
[c] Ref. [32].

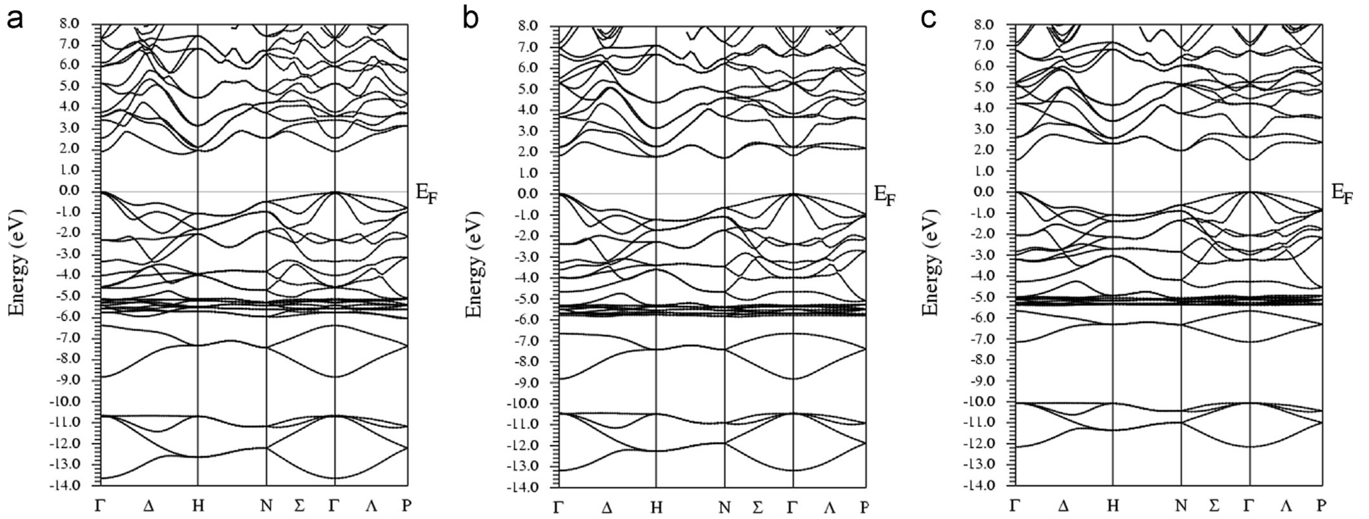

Fig. 2. EV-GGA electronic band structures of $ZnSiP_2$ (a), $ZnGeP_2$ (b) and $ZnSnP_2$ (c).

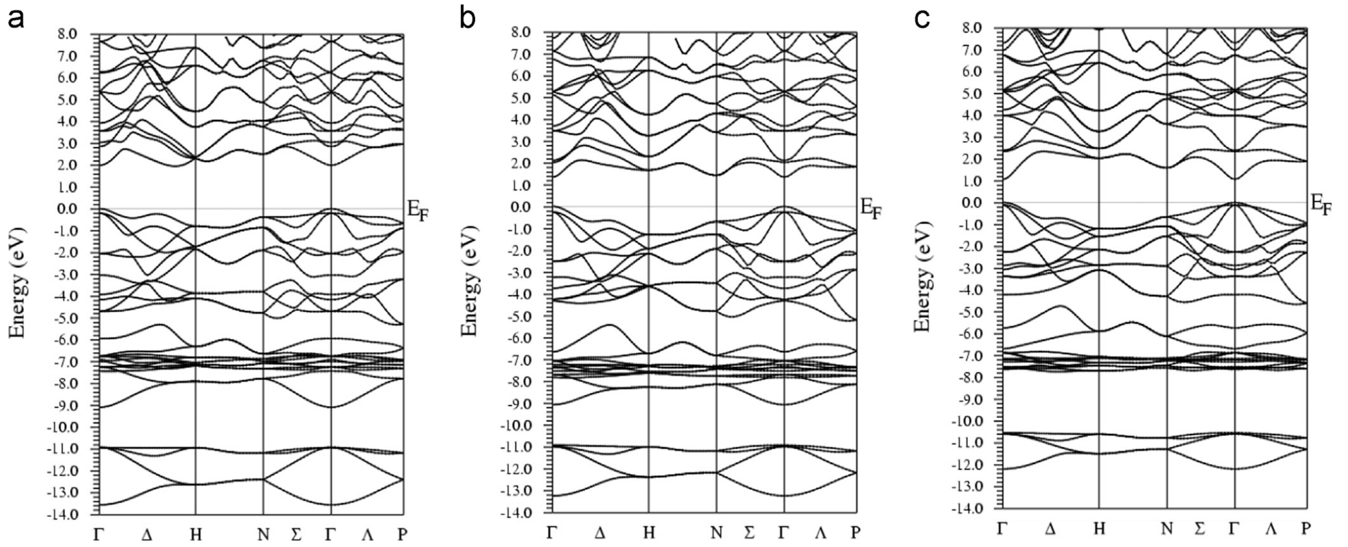

Fig. 3. EV-GGA electronic band structures of $CdSiP_2$ (a), $CdGeP_2$ (b) and $CdSnP_2$ (c).

Table 2
The calculated band gaps together with other theoretical and experimental gaps. All energies are in eV.

Compounds	This work		Experimental	Previous works
	GGA	EVGGA		
$ZnSiP_2$	1.44	1.98	2.07[h], 2.07[c]	1.22[i], 1.135[a]
$ZnGeP_2$	1.50	1.82	2.05[h]	1.16[i], 1.079[a]
$ZnSnP_2$	1.10	1.58	1.66[c]	0.776[a]
$CdSiP_2$	1.50	2.00	2–2.45[h],2.20[g]	1.30[d], 1.38[d], 1.10[e], 1.19[f],1.273[b]
$CdGeP_2$	1.00	1.40	1.72[h],1.67[g]	0.43[d], 0.73[d], 0.95[e], 0.75[f],0.954[b]
$CdSnP_2$	0.72	1.04	1.14[g]	0.09[d], 0.37[d],0.366[b]

[a] Ref. [18] .
[b] Ref. [19].
[c] Ref. [1].
[d] Ref. [32].
[e] Ref. [17].
[f] Ref. [20].
[g] Taken from Refs. [1,32].
[h] Ref. [34].
[i] Ref. [35].

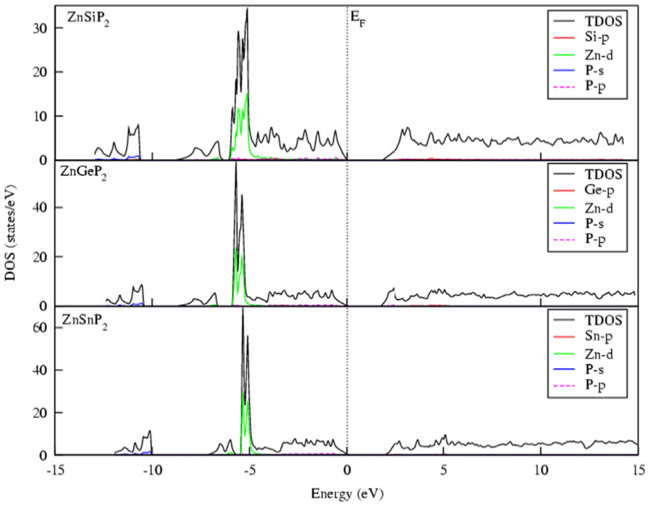

Fig. 4. Calculated total and partial densities of states of $ZnYP_2$.

study [27] who found a direct band gap for these compounds. Our results for $CdSnP_2$ and $ZnSnP_2$ along with those of Chicker et al. [18,19], show the CBM at the Γ point, predicting that both compounds are direct band gap materials (Γ–Γ). For $ZnGeP_2$ compound, Varea De Alvarez and Cohen [28,29] found a direct band gap (Γ–Γ) using the empirical pseudo potential method. While, the calculations of Rashkeev et al. [20] using the first principles linear muffin-tin orbitals (LMTO) method showed an indirect band gap for $ZnGeP_2$ with the CBM occurred at the N point. Limpijumnong et al. [30] found several close lying CBM of which the lowest one is at a low symmetry point of the Brillouin zone, and they showed that their results may account for the available experimental data and point out some problems with the traditional pseudo-direct gap interpretation. The electronic band structure calculation of Chiker et al. [18] determines the CBM at the T-point predicting $ZnGeP_2$ is an indirect band gap material (Γ–T). It is further seen that by changing the cations from Si to Ge to Sn the conduction band minima shifts to the Γ symmetry point making the $ZnGeP_2$ and $ZnSnP_2$ compounds a direct band gap materials. Similar trend has seen for the $CdYP_2$ compounds (Fig. 3 (a–c)). The computed GGA and EVGGA band gaps values of the herein studied compounds are given in Table 2 along with the existing experimental findings for the sake of comparison. It is clearly seen that the band gaps predicted by GGA are lower than the experiment values. This well-known underestimation of the band gap is mainly due to the fact that the simple form of GGA is not sufficiently flexible for accurately reproduce both exchange-correlation energy and its charge derivative. Engel and Vosko [25] constructed a new functional form of the GGA, namely EVGGA, which proved to improve the results for quantities that depend on the energy eigenvalues, including the band gaps [31]. The calculated EV-GGA band gap values show a significant improvement

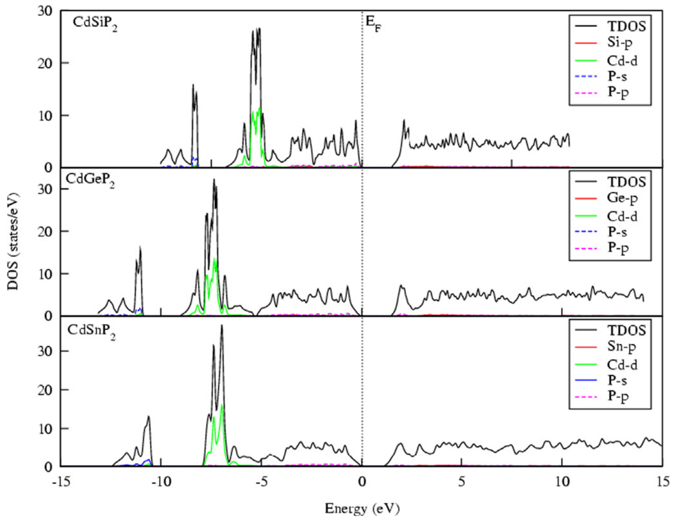

Fig. 5. Calculated total and partial densities of states of $CdYP_2$.

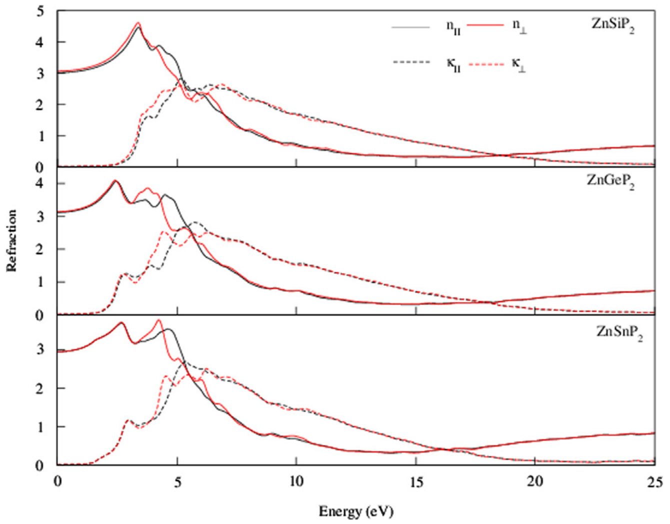

Fig. 7. Calculated refractive index$n(\omega)$spectra for $ZnYP_2$ (Y=Si, Ge, Sn).

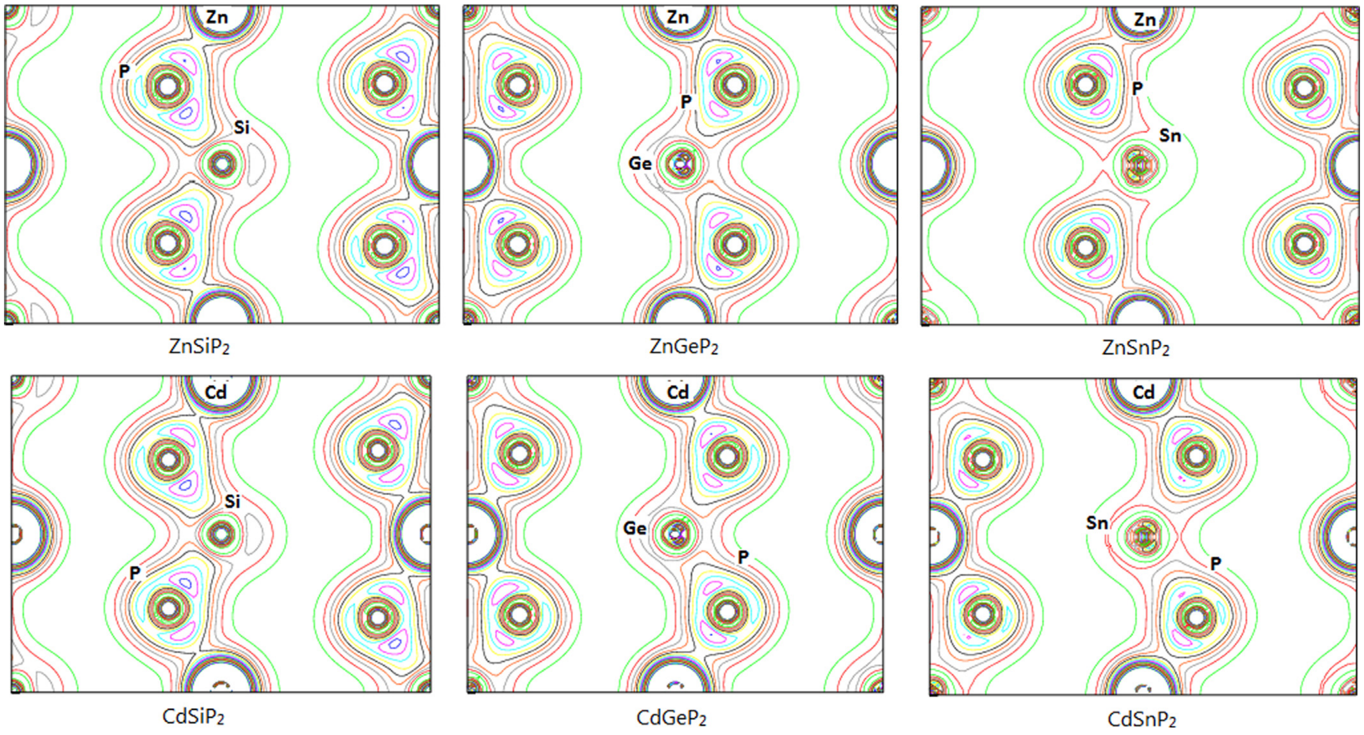

Fig. 6. Electron density plots of XYP_2 in the (1 1 1) direction.

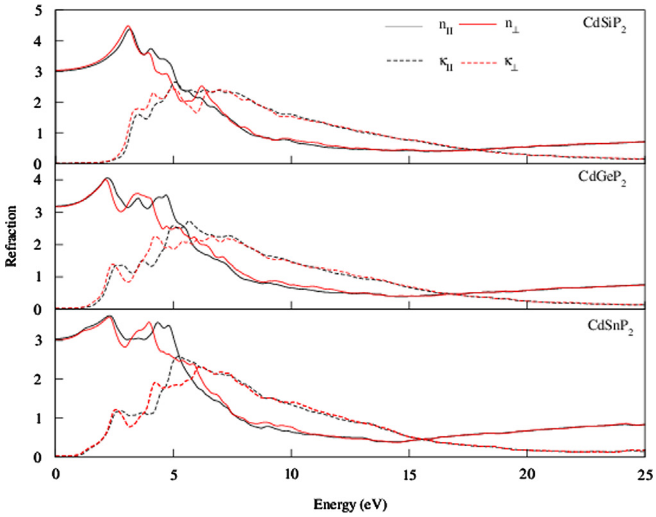

Fig. 8. Calculated refractive index$n(\omega)$spectra for $CdYP_2$ (Y=Si, Ge, Sn).

Table 3
Calculated zero frequency refractive index, $n(0)$, birefringence $\Delta n(0)$, maximum refractive index, $n(\omega)$, and anisotropy range.

Compounds	$n^{II}(0)$	$n^{\perp}(0)$	$\Delta n(0)$	$n^{II}(\omega)_{\mathrm{Max.}}$	$n^{\perp}(\omega)_{\mathrm{Max.}}$	Anisotropy range
$ZnSiP_2$	3.018, (3.40)[a]	3.069	0.051	4.460	4.615	3.85–7.0
$ZnGeP_2$	3.117, (3.10) [a]	3.142	0.025	4.0647	4.0965	3.14–6.69
$ZnSnP_2$	2.942, (2.90 [a])	2.943	0.001	3.678	3.767	3.36–7.29
$CdSiP_2$	3.017, (3.10) [a]	3.047	0.03	4.379	4.487	1.36–12.25
$CdGeP_2$	3.193, (3.30) [a]	3.167	−0.026	4.057	4.016	2.11–12.25
$CdSnP_2$	3.040, (3.10) [a]	3.006	−0.034	3.63	3.594	1.19–10.85

[a] Ref. [16].

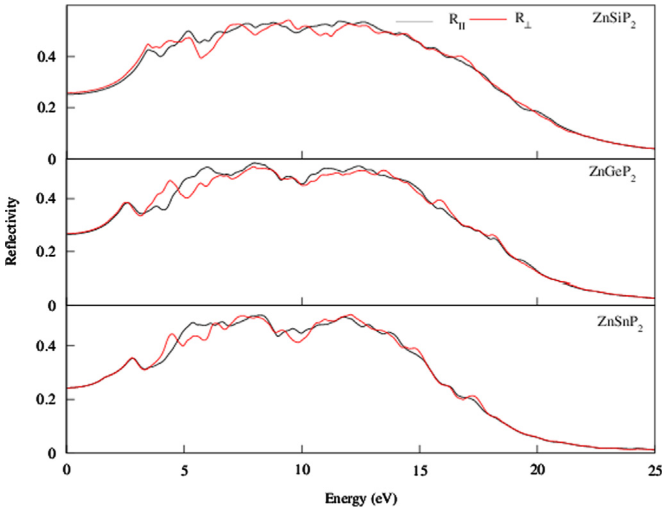

Fig. 9. Calculated reflectivity $R(\omega)$ spectra for $ZnYP_2$ (Y=Si, Ge, Sn).

over the present GGA results and previous calculations [17–20,35] compared to the experimental data [1,34].

In order to get an insight into the electronic nature and chemical bonding of the studied compounds, the total partial densities of states (TDOS and PDOS) diagrams are plotted in Figs. 4 and 5. The pattern of the DOS is almost the same in both types of the compounds. The first band from the left is mainly occupied by P-3s states. The next band is the upper valence band (UPV) which is divided into two parts. The lower part is composed from "d" states of X (Zn, Cd) cations. The higher part is due only to the P-3p states. The bands above the Fermi level E_F, are the conduction bands (CB) which are composed of "p" states of Y cations.

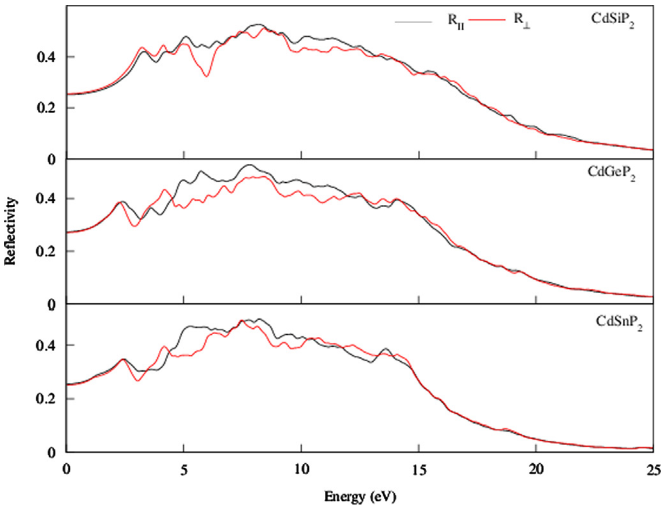

Fig. 10. Calculated reflectivity $R(\omega)0$ spectra for $CdYP_2$ (Y=Si, Ge, Sn).

Table 4
Calculated zero frequency reflectivity, $R^{II}(0)$ and $R^{\perp}(0)$, maximum reflective index, maximum reflectivity of $R^{II}(\omega)$ and $R^{\perp}(\omega)$, and anisotropy range.

Compounds	$R^{II}(0)\%$	$R^{\perp}(0)\%$	Max. $R^{II}(\omega)$ %	Max. $R^{\perp}(\omega)$ %	Max. $R(\omega)$ range	Anisotropy range
$ZnSiP_2$	25.23	25.85	53.77	54.24	3.25–17.52	3.22–17.36
$ZnGeP_2$	26.45	26.74	53.49	52.04	2.38–16.82	2.96–18.32
$ZnSnP_2$	24.27	24.28	51.26	51.58	2.0–15.88	3.44–17.88
$CdSiP_2$	25.21	25.59	52.70	51.18	2.0–15.18	2. 6–15.96
$CdGeP_2$	27.35	27.04	52.86	48.36	2.18–14.58	1.39–16.05
$CdSnP_2$	25.55	25.07	49.71	49.37	2.48–14.20	1.74–14.78

The nature of bonding among the cations and anions can be studied from the electronic charge density [36,37]. The electronic charge density in the (1 1 1) plane is plotted in Fig. 6 for XYP_2 compounds. The distribution of electronic density of the cations and anions reveals that there is some sharing of charge, hence the compounds are partially covalent and ionic in nature. The covalence is mainly because of pd-hybridization of the anions and cations, while the ionic bonding is due to transfer of charge from the X and Y cations to P anion. It is further noticed that the ionic behavior among XP decreases as we change the cations from Si to Ge to Sn, while it increases in YP when we replace the cations Si by Ge and by Sn.

Using the optical code of Ambrosch and Sofo [38] implemented in Wien2k package [24], we have calculated the complex refractive index ($\tilde{n}(\omega)=n(\omega)+ik(\omega)$). $n(\omega)$ and $k(\omega)$ are the real and imaginary components of the refractive index, respectively. The real part, $n(\omega)$, is just the ordinary refractive index while the imaginary part, $k(\omega)$, is the extinction coefficient which describes the loss of photon energy when it propagate through the optical medium. Due to the tetragonal symmetry of the herein studied compound, all the optical spectra are plotted for electrical field vector $\vec{E}$ of the incident radiation polarized both perpendicular ($\vec{E} \perp c$) and parallel ($\vec{E} \perp c//c$) to the tetragonal c-axis of the crystal.

Figs. 7 and 8 display the calculated refractive index ($n^{II}$and$n^{\perp}$) and extinction coefficient ($k^{II}$and$k^{\perp}$) for a radiation up to 25 eV of the chalcopyrite $ZnYP_2$ and $CdYP_2$ (Y=Si, Ge, Sn), respectively. The zero frequency refractive index $n^{II}(0)$ and $n^{\perp}(0)$ of the herein studied compounds along with the available experimental indices are listed in Table 3. From the table it is clear that the calculated refractive indices are in very good agreement to the experimental indices [16]. The refractive index spectra increase from the static value to attain a maximum then decrease with few oscillations to go below unity. In the region where the refractive index is smaller than the unity ($n<1$) the phase velocity of the photons increases beyond the universal constant (C). However, the group velocity always less than the C and therefore the relativity relations not effected [39]. It is seen from the refractive index spectra that the replacement of Si by Ge in these compounds shifts the positions of the peaks towards the lower energy. In contrary the positions of the peaks are shifted towards the higher energy when Ge is replaced by Sn. The birefringence $\Delta n(0)$ decreases by changing the cation Y from Si to Ge to Sn (see Table 3).

Extinction coefficient $k(\omega)$describes the absorption of compounds. It is seen from both $k^{II}$and$k^{\perp}$spectra that the absorption edge occurs at about 2.35, 1.9, 1.48, 2.34, 1.30 and 1.03 eV for $ZnSiP_2$, $ZnGeP_2$, $ZnSnP_2$, $CdSiP_2$, $CdGeP_2$ and $CdSnP_2$, respectively. They are in accordance with the variation of the band gap which decreases by changing the cation X as well Y from the top to the bottom of the periodic table. Beyond the critical points, the absorption increases to reach its maximum value at some particular energy then decreases with small oscillations. $ZnSiP_2$, $ZnGeP_2$, $ZnSnP_2$, $CdSiP_2$, $CdGeP_2$ and $CdSnP_2$ show a high absorption in the energy range 3.28–9.61 eV, 2.76–6.30 eV, 3.3–7.3 eV, 3.27–8.16 eV, 2.34–7.96 eV and 2.50–7.52 eV, respectively. In these energy ranges a considerable anisotropy between the parallel and perpendicular components of the absorption spectra is clearly observed. Further, one can notice that the absorption edge is shifted to the lower energy in going from Si to Ge to Sn for both $ZnYP_2$ and $CdYP_2$ (Y=Si, Ge, Sn) compounds.

Figs. 9 and 10 show the frequency dependent parallel and perpendicular reflectivity spectra (R^{II},$R^{\perp}$) against energy for $ZnYP_2$ and $CdYP_2$ (Y=Si, Ge, Sn) compounds. It is evident that these compounds behave like semiconductors since the $R(\omega)$ values are not approach to the unity towards zero energy. Beyond the zero frequency limits, the reflectivity spectra increase with some oscillations up to reach the maximum of about 54% and then start to decrease smoothly and vanish at high energy. Peaks pointing around the maximum of reflectivity arise from the inter band transition. The computed zero frequency reflectivity, $R^{II}(0)$ and $R^{\perp}(0)$, maximum reflective index, maximum reflectivity of $R^{II}(\omega)$ and $R^{\perp}(\omega)$, and the anisotropy range are quoted in Table 4.

4. Conclusions

We applied the highly accurate full potential linearized augmented plane wave plus local orbitals method within the generalized gradient approximation of Engel and Vosko to predict the electronic, chemical bonding and optical properties. The most relevant conclusions are summarized as follows: (i) The computed band gaps show better agreement with the experimental ones then the previous calculations. (ii) The Zn and Sn "d" states have high density of states. (iii) Compounds possess partial ionic and covalent bonding. (iv) The calculated refractive indexes are in excellent agreement with the measured ones. (v) The birefringence $\Delta n(0)$ decreases by changing the cations Y from Si to Ge to Sn in XYP_2. (vi) The high reflectivity in visible and ultraviolet regions of energy spectrum makes these materials useful in the domain of photonics, optoelectronics and optics.

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