Optoelectronic properties of XYAs$_2$ (X=Zn, Cd; Y=Si, Sn) chalcopyrite compounds

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First principle calculations are performed to predict the electronic and optical properties of XYP$_2$ (X=Zn, Cd; Y=Si, Ge, Sn) semiconductors chalcopyrite. Our calculated results are in excellent agreement with the available experimental values. The bandgap values decrease by changing the cations X from Zn to Cd as well as Y from Si to Ge to Sn in XYAs$_2$. The Zn and Cd-d states contribute significantly in the density of states. The distribution of thevalence charge density indicates theexistence ofthe covalent bonding between cations and anion. Optical properties of these compounds are described in terms of refractive index and reflectivity. The predicted refractive indexes are in excellent agreement with the measured ones.CdGeAs$_2$ possess a high birefringence compared to the other compounds.Reflectivity is above 50% in the visible and ultraviolet regions of energy spectrum. The nature of the direct band gap in these compounds and their high reflectivity in visible and ultraviolet (UV) regions, make them promising candidate for optoelectronic, photonic and optic applications.

1. Introduction

XYAs$_2$ chalcopyrites had attracted more attention since few decades. Tremendous experimental and theoretical works have been done to these compounds because of their importance in electronics, spintronics, LED and solar cell applications. XYAs$_2$ (X=Zn, Cd and Y=Si, Ge, Sn) chalcopyrites have tetragonal symmetry with space group $I\overline{4}2d(D_{2D}^{12})$ [1-6]. Among these chalcopyrites, the CdGeAs$_2$ is the cheapest candidate for nonlinear optical frequency convertor [7, 8]. It has very high second-order nonlinear coefficient with a wide infrared transparency range (2.3-18μm), which makes it very promising candidate for mid-infrared frequency generator in C$_2$ laser and optical parametric oscillator device fabrication [9]. ZnGeAs$_2$is a good candidate in opto-electronics for high efficient multi-junction solar cell applications [10]. The natural deformation in CdSiAs$_2$ leads to strong the crystallographic anisotropy which makes the compound attractive for nonlinear optoelectronicsand solar cell applications [11]. ZnSnAs$_2$ gets interest in spintronics applications because it becomes ferromagnetic when it is doped with Mn at room temperature [12].

XYAs$_2$ chalcopyrite semiconductors have been the subject of manyexperimental and theoretical studies. On experimental side Clarence *et al*., studied the thermo and electro reflectance of ZnSiAs$_2$as a function of temperature [13]. Optical spectra of these alloys were reported by Stokowski [14]. Shy *et al*., reported the growth and electrical properties of these compounds [1]. Highefficiency second harmonic generation with CdGeAs$_2$ was reported by Menyuk *et al*. [15]. Osinsky *et al*., studied the sulfur doping effect on optical anisotropy of CdSiAs$_2$ [11]. After the pioneer work of Medvedkin*etal*. [16], the magnetic properties of II-IV-V$_2$ compounds were reported in Refs. [17, 18, 19]. Magomedov *et al*., reported the thermal and electrical conductivity of CdSnAs$_2$ in both solid and liquid states [20]. Although the electronic structure of semiconductors could be obtained experimentally [21], however the structural and electronic properties of ZnGeAs$_2$ were theoretically studied by Janotti *et al*., [10]. Ab initio study onthe linear and nonlinear optical properties of CdGeAs$_2$was done by Yu *et al*., [22]. In this latter study, the calculated band gap energy of 0.43 eV was much less than the measured one.

From the above literature it is clear that there is considerable experimental works on XYAs$_2$ (A=Zn, Cd; B=Si, Ge, Sn) compounds. There are no earlier detailed first-principle calculations on the optoelectronic properties of this family of compounds have been done. The current work carries the calculations of the electronic and optical properties of the XYAs$_2$ (A=Zn, Cd; B=Si, Ge, Sn) compounds. These properties are calculated by using the density functional theory (DFT) [23, 24].

2. Computational details

Present calculations were performed using the full potential linearized augmented plane wave plus local orbitals (FP-LAPW+lo) method [25] based on Density Functional Theory (DFT) [23, 24] as implemented in wien2K package [26]. The exchange-correlation potential was treated withEngel and Vosko GGA scheme (GGA-EV)[27].

In the present self-consistent calculations, the muffin-tin model for the crystal potential is assumed and the unit cell is divided into two regions, within and outside the muffin-tin sphere. The electrons are paired into two groups, namely the core electrons whose charge densities are confined within the muffin-tin spheres and the valence electrons. The core electron states are treated fully relativistically by solving the Dirac equation, whereas the valence electrons are treated non-relativistically. In both regions of the unit cell, different basis sets are used to expand the wave function, charge density and potential inside the non-overlapping spheres of muffin-tin radius (R_{MT}) around each atom. Linear combination of radial solution of the Schrödinger equation times the spherical harmonic is used while the plane wave basis set is used in the interstitial region. R_{MT} is chosen in such a way that there is no charge leakage from the core and total energy convergence is ensured. The R_{MT} values for Si, Ge, Sn, Zn, Cd, and As are 2.16, 2.19, 2, 2.30, 2.2 and 2.05 a.u., respectively. The maximum value of angular momentum l_{max} = 10 is taken for the wave function expansion inside the atomic spheres. The plane wave cut-off value of R_{MT} K_{max}= 7 is used. On the basis of convergence test a mesh of 726 k-points (in the irreducible wedge of the first Brillouin zone (IBZ) that has been explored within the tetrahedron method [28]) and G_{max} = 12 are used for well converged results. The self-consistency was achieved up to 0.001 Ry.

3. Results and discussion

All the XYAs₂ (X=Zn, Cd; Y=Si, Ge, Sn) compounds crystallize in the chalcopyrite structure at normal growth conditions. The chalcopyrite structure of XYAs₂ compounds is shown in Fig. 1. It is seen from the figure that 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 As atom occupies (u, 1/4, 1/8), (-u, 3/4,1/8), (3/4, u, 1/8), (1/4, -u,7/8) sites. The electronic and optical properties are calculated at the experimental lattice parameters given in Table 1.
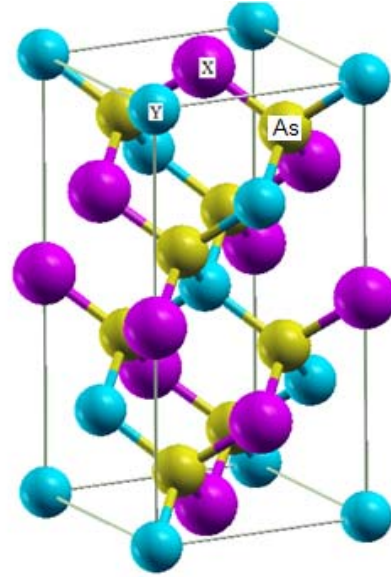

Fig. 1. Chalcopyrite structure of XYAs₂.

Table 1. Used lattice constants, R_{MT}, R_{MT}-K_{max}, l-max, and K-points.

Compound	Latt. Cons.		u(Exp.)
	a[A]ᵃ,ᵇ,ᶜ	c[A]ᵃ, ᵇ,ᶜ	
ZnSiAs₂	5.606	10.886	.26ᵇ
ZnGeAs₂	5.671	11.153	.264ᵇ
ZnSnAs₂	5.851	11.703	.239ᵇ
CdSiAs₂	5.885	10.881	.29ᵈ
CdGeAs₂	5.93	11.220	.28ᵈ,ᵇ
CdSnPₐₛ	6.08	11.928	.26ᵇ

ᵃRef.[1], ᵇRef. [36], ᶜRef.[29] , ᵈRef.[30]

The electronic properties of the herein studied chalcopyrite compounds are discussed via the calculated electronic band structures, density of states, and charge density distribution. Figs. 3 and 4, display the calculated band structure of ZnYAs₂ and CdYAs₂along some high symmetry lines in the Brillouin zone within the GGA-EV approximation. The zero energy is chosen to coincide with the top of the valence band. It is clear from these figures that the valence band maximum (VBM) and the conduction band minimum (CBM) are both occurs at the Γ point, resulting in a direct band gap nature (Γ- Γ) in all studied compounds. One can remark that the replacement of Si atom by Ge atom and by Sn atom decreases the energy band gap. One can also note that the energy band gap decrease when changing the X cations from Zn to Cd.The calculated band gap values for the herein investigated chalcopyrite compounds within the GGA and EV-GGA are listed in Table 2, along with the

experimental values and other previous theoretical calculations. From the results given in Table 2, it is clear that the computed energy band gap value using the GGA approximation are much lower than the experiment values. Thecomputedband gap values within the EV approximation are higher than the GGA onesand in very good agreement to the experimental band gap values [29-31]. The values of the calculated band gaps with EV-GGA

show a significant improvement over the results based on GGA [22, 30] compared to the experimental values, e.g. the previous predicted bandgap of $CdSnAs_2$ was 0.12 [30] which is quite less than experimental bandgap of 0.26 eV [36]. The GGA predicted bandgap of the compound is 0.02 eV while GGA-EV bandgap is 0.26 which is in excellent agreement to the experimental results. Same trend is seen for other compounds.
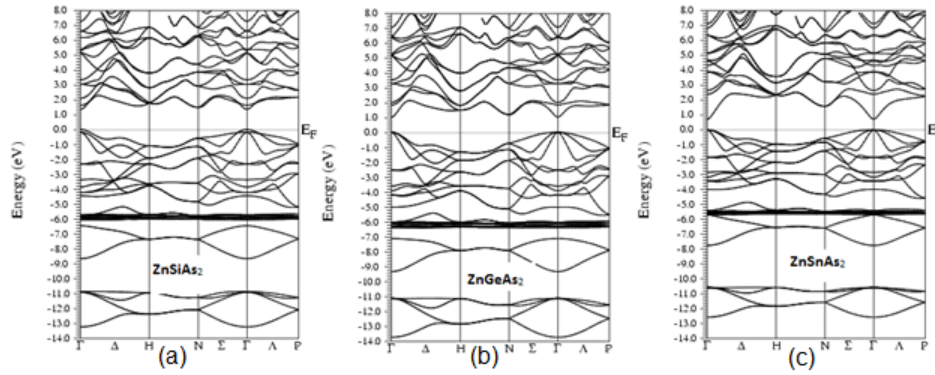

Fig. 2. Band structures of (a) $ZnSiAs_2$, (b) $ZnGeAs_2$ and (c) $ZnSnAs_2$.
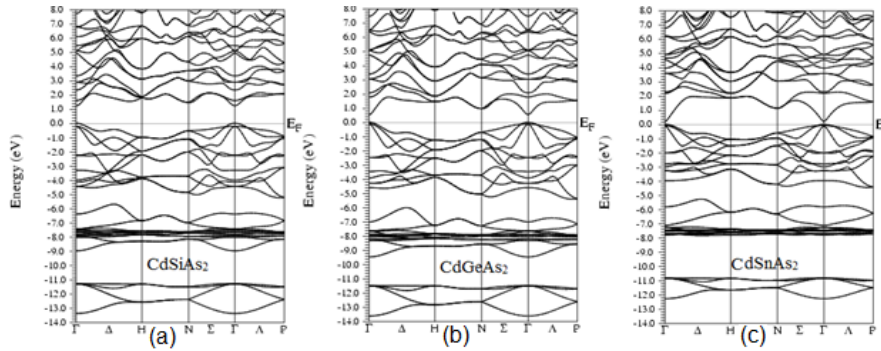

Fig. 3. Band structures of (a) $CdSiAs_2$, (b) $CdGeAs_2$ and (c) $CdSnAs_2$.

Table 2. Calculated bandgaps along with experimental and previous work.

Compounds	This work		Experimental	Other Works
	GGA	EV		
$ZnSiAs_2$	1.2	1.4	1.93[c],2.12[f]	
$ZnGeAs_2$	0.78	1.1	1.15[c,f]	
$ZnSnAs_2$	0.32	0.71	0.73[c],0.74[f]	
$CdSiAs_2$	0.98	1.27	1.55[c,d]	0.17[d], 0.73[d]
$CdGeAs_2$	0.2	0.56	0.57[c,f],0.50[d]	0.12[d],0.32[d]0.43[e], 0.09[d], 0.37[d]
$CdSnAs_2$	0.02	0.26	0.26[c,d,f]	0.10[d], 0.12[d]

[c]Ref.[29] , [d]Ref.[30] , [e]Ref.[22], [f]Ref.[31]

The contribution of different states in the band structure can be studied from the density of states (DOS). Total and partial density of states of $ZnYAs_2$ and $CdYAs_2$ are plotted in Fig. 4 and Fig. 5, respectively. The pattern of

the DOS is almost the same in all compounds. The first band from the left is mainly composed of the As-4p state. Next band below the Fermi level (E_F) is the valence band (VB). Lower part of this band is formed due to the d states

of X (Zn, Cd) cations in $ZnYAs_2$ and $CdYAs_2$, respectively. Upper part of the VB mainly composed of the As-$4p$ state. Next band above E_F, is the conduction band (CB).This band is composed of s and p states of Y cations and As-$4s$ state.
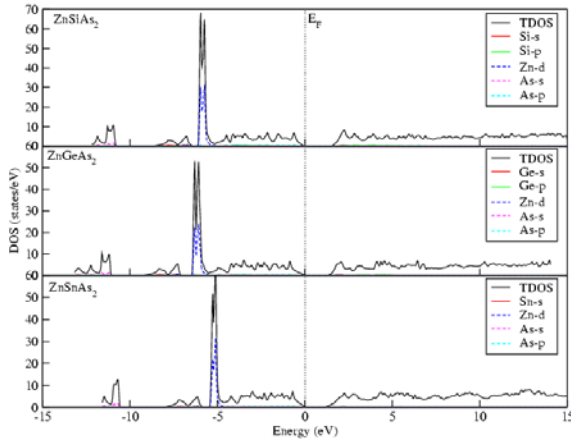

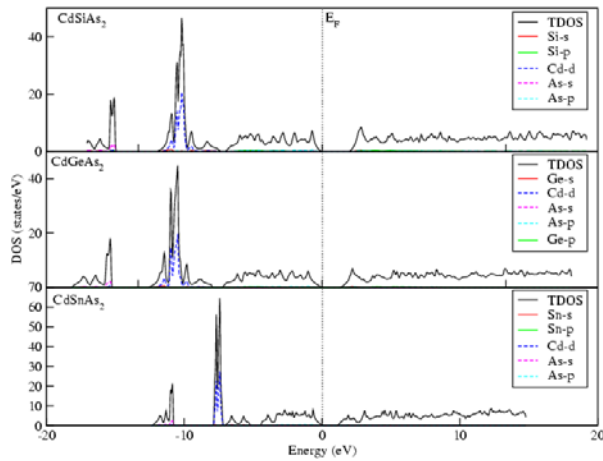Fig. 4. *Total and partial density of states of* $ZnYAs_2$.

Fig. 5. *Total and partial density of states of* $CdYAs_2$.

Electronic charge density distributions serve as a complementary tool to achieving a proper understanding of the nature of chemical bond of the system being studied [32, 33]. The electronic charge density in the (111) plane is plotted in Fig. 6 for $XYAs_2$. The distribution of electronic density of the cations and anions reveals that there is sharing of charge, hence the compounds are covalent in nature. This covalent bonding is mainly due to the pd-hybridization of the anions and cations as seen from Figs. 4 and 5. It is further noticed that the covalent behavior decreases among XAs as we replace the cations from Si to Ge to Sn, while increases among YAs as we replace the cations from Si to Ge to Sn.
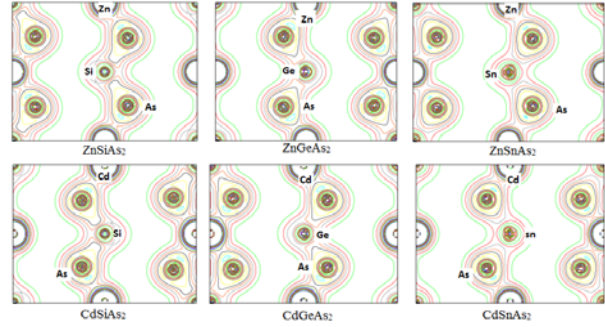

Fig. 6. *Electron density of* $XYAs_2$ *in (111) plane.*

Optical response of these compounds is studied using the optical code of Claudia et al.[34]implemented in Wien2k package [26]. Complex refractive index ($\tilde{n}(\omega) = n(\omega) + ik(\omega)$) describes the refraction and absorption of the compounds. It consists of two parts; the real part, $n(\omega)$, is just the ordinary refractive index while the other part, $k(\omega)$, is the extinction coefficient which describe the loss of photon energy as it propagate through the optical medium. As these compounds have tetragonal symmetry, only two tenser components (parallel and perpendicular to the **c**- axis corresponding to the electric field) are required to completely describe the optical properties. The parallel and perpendicular components of refractive index ($n^{\parallel}$ and $n^{\perp}$) and extinction coefficient ($k^{\parallel}$ and $k^{\perp}$) as a function of energy are plotted in Figs. 7 and 8 for $ZnYP_2$ and $CdYP_2$ (Y=Si, Ge, Sn) compounds. From Fig. 7, it can be seen that $n^{\parallel}(0)$ and $n^{\perp}(0)$ at zero frequency show the static refractive indices. They increase beyond the zero frequency limits and reached to their maximum values. Beyond the maximum value they start to decrease and with few oscillations they go beyond unity. In this region (n<1) the phase velocity of the photons increases to universal constant (C). However the group velocity always less than the C, therefore the relativity relations not effected [35]. The peaks in the spectra shift towards lower energy by changing the cations from Si to Ge to Sn. The variation is in accordance to the decrease in the bandgaps. The calculated values of zero frequency refractive index ($n^{\parallel}(0)$ and $n^{\perp}(0)$), their maxium values ($n^{\parallel}(\omega)_{Max.}, n^{\perp}(\omega)_{Max.}$), birefringence ($\Delta n(0)$) and anisotropy among the parallel and perpendicular parts of the refractive index are given in Table 3. It is further noted that the birefringence $\Delta n(0)$ is maximum in $CdGeAs_2$ compared to other compounds of this family. Also our calculated refractive indices are in agreement with the Ref. [31].
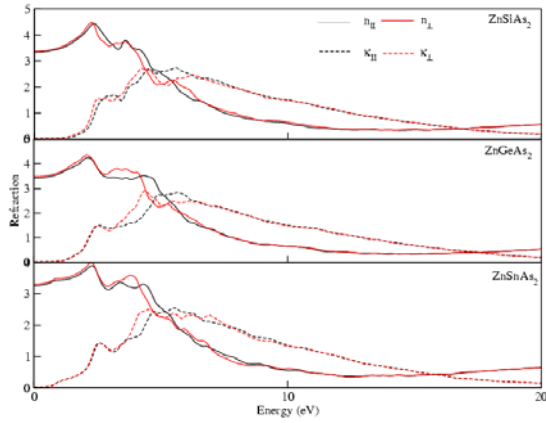
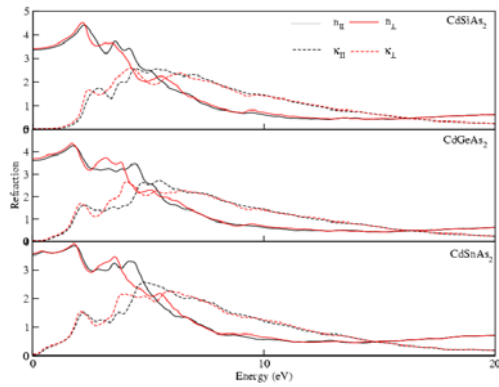*Fig. 7. Refractive index as a function of energy for ZnYAs$_2$ (Y=Si, Ge, Sn).*

Fig. 8. Refractive index as a function of energy for CdYAs$_2$ (Y=Si, Ge, Sn).

Extinction coefficient $k(\omega)$ shows the absorption of compounds. It is seen from the figure that the absorption edge of ZnSiAs$_2$, ZnGeAs$_2$, ZnSnAs$_2$, CdSiAs$_2$, CdGeAs$_2$ and CdSnAs$_2$ occurs at 1.42, 1.26, 0.62, 1.36, 0.54, and 0.27 eV for $k_{\parallel}$ and at 1.47, 1.26, 0.62, 1.31, 0.59, 0.275 eV for $k_{\perp}$, respectively. They are in accordance with the variation of the bandgap which decreases by changing the cation X as well Y from top to bottom of the periodic table. The absorption edges correspond to the transitions of electrons from the top of the valence band (Γ) to the bottom of the conduction band (Γ). Beyond the critical points, the absorption increases and become maximum at some particular energy, and then it decreases with small oscillations. Different absorption peaks in the spectra are due to the transition of the electrons from the valence and lower bands to the unoccupied states of the conduction band. The compounds ZnSiAs$_2$, ZnGeAs$_2$, ZnSnAs$_2$, CdSiAs$_2$, CdGeAs$_2$ and CdSnAs$_2$ show high absorption in the range 2.56-10.80eV, 2.51-11.12 eV, 2.56-10.58 eV, 2.29-10.52 eV, 1.79-10.90 eV and 1.85-9.98 eV, respectively. In these energy ranges a large anisotropy is seen, while the parallel and perpendicular parts are

isotropic outside this energy range. It is further noted that the absorption shifts towards lower energy by changing the cations from Si to Ge to Sn for both ZnYAs$_2$ and CdYAs$_2$ (Y=Si, Ge, Sn).

Frequency dependent reflectivity $R(\omega)$ of the compounds is calculated and depicted in Figs. 9 and 10 for ZnYP$_2$ and CdYP$_2$ along parallel $R^{\parallel}(\omega)$ and perpendicular $R^{\perp}(\omega)$ to the **c**- axis corresponding to the electric field. The reflectivity spectra of the compounds start from the zero frequency which is the static part of the reflectivity. Beyond the zero frequency limit it increases and with some oscillations it become maximum and then decreases and vanishes at high energy. The reflectivity spectra of the compounds shift towards lower energy by changing the cations from Si to Ge to Sn in XYP$_2$. The zero frequency limits and its maximum values are given in Table 4 along with the energy ranges in which these are maximum and highly anisotropic. It is clearly seen from the figures that the reflectivity is high in the visible and ultraviolet region of the energy spectrum. Therefore these compounds can be used as Bragg's reflectors.
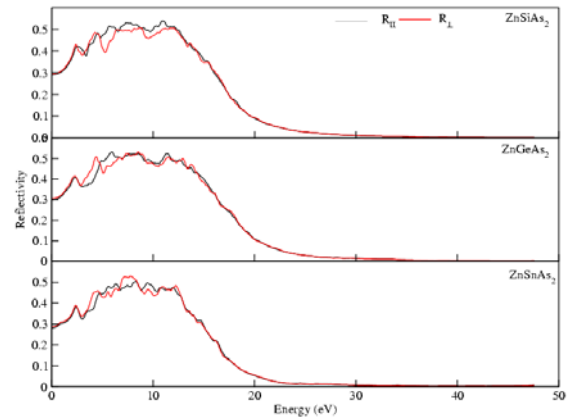

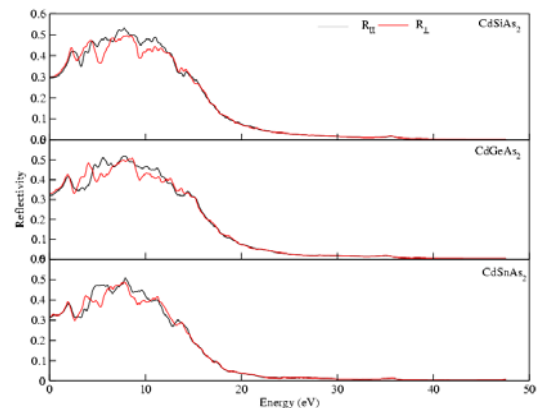*Fig. 9. Reflectivity as a function of energy for ZnYAs$_2$ (Y=Si, Ge, Sn)*

Fig. 10. Reflectivity as a function of energy for CdYAs$_2$ (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	$n^{\parallel}(0)$	$n^{\perp}(0)$	$\Delta n(0)$	$n^{\parallel}(\omega)_{Max.}$	$n^{\perp}(\omega)_{Max.}$	Anisotropy range
ZnSiAs₂	3.3442,(3.10)	3.3690	0.024	4.443	4.4805	0.95-8.70
ZnGeAs₂	3.4219,(3.50)	3.4802	0.0583	4.2537	4.3568	0.39-6.76
ZnSnAs₂	3.2586	3.3052	0.0466	3.8985	3.991	0.21-9.07
CdSiAs₂	3.3602,(3.50)	3.414	0.0508	4.415	4.5275	0.45-8.35
CdGeAs₂	3.612,(3.40)	3.699	0.087	4.2816	4.3735	0.021-6.87
CdSnAs₂	3.5369,(3.70)	3.579	0.0421	3.861	3.9285	1.46-6.56

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

Compounds	$R^{\parallel}(0)\%$	$R^{\perp}(0)\%$	Max. $R^{\parallel}(\omega)$ %	Max. $R^{\perp}(\omega)$ %	Max. $R(\omega)$ range	Anisotropy range
ZnSiAs₂	29.12	29.40	53.90	50.70	2.12-14.61	2.23-15.48
ZnGeAs₂	29.99	30.64	53.19	53.25	1.58-15.64	2.97-15.97
ZnSnAs₂	28.13	28.67	50.322	52.92	2.18-13.52	2.78-12.75
CdSiAs₂	29.30	29.91	53.04	49.59	1.63-13.35	0.49-15.53
CdGeAs₂	32.08	32.99	51.77	50.45	1.30-13.08	0.10-14.94
CdSnAs₂	31.26	31.73	50.56	48.30	1.52-12.26	1.85-14.61

4. Conclusions

We applied the highly accurate full potential linearized augmented plane wave plus local orbitals method within the generalized gradient approximation of Englo-Vosko to predict the electronic, chemical bonding and optical properties. The conclusions are; the calculated bandgap values show better agreement with the experimental data than the previous theoretical ones. d-states of the Zn and Cdhave high density of states. Compounds possess strong covalent bonding. The computed refractive indices are in excellent agreement with the experimental measured ones. The birefringence is highest in CdGeAs₂. The very high reflectivity of these compounds in visible and ultraviolet (UV) regions, make them promising candidate for optoelectronic, photonic and optic applications.

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