

Research Article

Band Gap Engineering of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ Alloys

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Received 13 August 2013; Revised 3 February 2014; Accepted 2 March 2014; Published 13 May 2014

Academic Editor: Velimir Radmilovic

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The structural and electronic properties of the ternary $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ alloys have been calculated using the full-potential linear muffin-tin-orbital (FP-LMTO) method based on density functional theory within local density approximation (LDA). The calculated equilibrium lattice constants and bulk moduli are compared with previous results. The concentration dependence of the electronic band structure and the direct and indirect band gaps are investigated. Moreover, the refractive index and the optical dielectric constant for $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ are studied. The thermodynamic stability of the alloys of interest is investigated by means of the miscibility. This is the first quantitative theoretical prediction to investigate the effective masses, optical and thermodynamic properties for $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ alloy, and still awaits experimental.

1. Introduction

In recent years, the wide-gap II–VI compounds are widely investigated because of the attractive applications in fabricating blue-green and blue optoelectronic devices, such as light-emitting diodes and laser diodes [1–4]. The applications include the use of II–VI compound based materials as light sources, in full colour displays, and for increasing the information density in optical recording [5, 6]. The beryllium containing II–VI compounds had been found to possess an enhanced ability to significantly reduce the defect propagation due to a greater prevalence of strong covalent bonding and lattice hardening in the materials [7, 8]. The strong covalent bonding in beryllium-based II–VI compounds achieves a considerable lattice hardening, which avoids multiplication of defects during the operation of II–VI semiconductor laser devices [9, 10]. $\text{Be}_x\text{Cd}_{1-x}\text{Se}$ alloys have attracted great attention because they are promising for the fabrication of full-colour visible optical devices due to a large difference in the energy gaps E_g of the binary constituents (CdSe, $E_g = 1.74$ eV; BeSe, $E_g = 5.5$ eV) [11].

In the present theoretical work, band gap of zinc-blende CdSe is varied systematically by alloying with Be. In order to investigate the optoelectronic nature of these alloys, their

structural, electronic, and optical properties are calculated. All calculations are based on density functional full-potential linear muffin-tin orbital (FP-LMTO) method with perdwang local density approximation (LDA).

2. Method of Calculations

The calculations reported here were carried out using the *ab initio* full-potential linear muffin-tin orbital (FP-LMTO) method [12–15] as implemented in the Lmtart code [16]. The exchange and correlation potential was calculated using the local density approximation (LDA) [17]. The FP-LMTO is an improved method compared to previous LMTO techniques, and it treats muffin-tin spheres and interstitial regions on the same footing, leading to improvements in the precision of the eigenvalues. At the same time, the FP-LMTO method, in which the space is divided into an interstitial region (IR) and nonoverlapping muffin-tin spheres (MTS) surrounding the atomic sites, uses a more complete basis than its predecessors. In the IR regions, the basis set consists of plane waves. Inside the MT spheres, the basis set is described by radial solutions of the one particle Schrödinger equation (at fixed energy) and their energy derivatives multiplied by spherical harmonics.

TABLE 1: Lattice constants a and bulk modulus B of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ compared with experimental results, Vegard's law, and other theoretical calculations.

x	Lattice constant a (Å)				Bulk modulus B (GPa) [B']		
	This work	Exp.	Vegard's law	Other calc.	This work	Exp.	Other calc.
0	6.06	6.052 ^a		6.025 ^b	55.05 [4.17]	55 ^c	54 ^d
0.25	5.90		5.82		57.72 [3.93]		
0.5	5.71		5.58		63.19 [4.15]		
0.75	5.46		5.34		66.6 [3.85]		
1	5.10	5.14 ^e		5.13 ^f -5.04 ^g	81.25 [3.77]	92 ^e	77 [3.55] ^f -80 [3.11] ^g

^aRef [25], ^bRef [26], ^cRef [27], ^dRef [28], ^eRef [29, 30], ^fRef [31], ^gRef [32].

The charge density and the potential are represented inside the MTS by spherical harmonics up to $l_{\max} = 6$. The integrals over the Brillouin zone are performed up to 35 special k -points for binary compounds and 27 special k points for the alloys in the irreducible Brillouin zone (IBZ) using Blochl's modified tetrahedron method [18]. The self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-6} Ry. In order to avoid the overlap of atomic spheres, the MTS radius for each atomic position is taken to be different for each composition. We point out that the use of the full-potential calculation ensures that the calculation is not completely independent of the choice of sphere radii.

Structural properties of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ are calculated using Murnaghan's equation of state [19] as follows:

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

where E_0 is the total energy of the supercell, V_0 is the unit volume, B_0 is the bulk modulus at zero pressure, and B'_0 is the derivative of bulk modulus with pressure.

Optical properties of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ are calculated using a fine k mesh of 1500 points for the present calculation. The dielectric function of a crystal depends on the electronic band structure and its investigation by optical spectroscopy which is a powerful tool in the determination of the overall optical behavior of a compound. It can be divided into two parts, real and imaginary as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \quad (2)$$

The imaginary part of the complex dielectric function, $\varepsilon_2(\omega)$, in cubic symmetry compounds can be calculated by the following relation [20, 21]:

$$\varepsilon_2(\omega) = \frac{8}{2\pi\omega^2} \sum_{mn} \int \left| p_{nn'}(k) \right|^2 \frac{dSk}{\nabla\omega_{mn'}(k)}, \quad (3)$$

while $\varepsilon_1(\omega)$ is used to calculate the real part of the complex dielectric function as follows:

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

Refractive index is calculated in terms of real and imaginary parts of dielectric function by the following relation

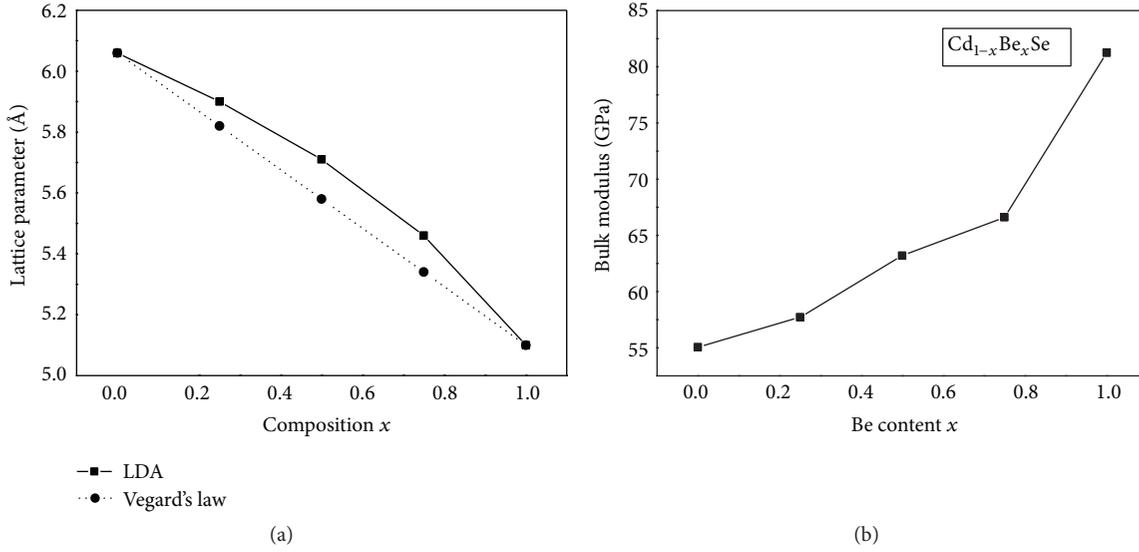
$$n(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2 \right\}^{1/2} + \varepsilon_1(\omega) \right]^{1/2}. \quad (5)$$

3. Result and Discussion

In order to study the structural properties of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ ($0 < x < 1$), alloys are modeled at various compositions of Be with a step of 0.25. Structure optimization of each compound is performed by minimizing the total energy with respect to the unit cell volume and c/a ratio using Murnaghan's equation of state [19]. The crystal structure of CdSe and BeSe zinc-blende with space group $F\bar{4}3m$ (no. 216). Structural parameters such as lattice constant, a (Å), are calculated from the stable volume and are presented in Table 1. It is clear from the table that our calculated results for the binary compounds are in good agreement with the available experimental and calculated data.

Figures 1 and 2 show the variation of the calculated equilibrium lattice constant and bulk modulus as a function of concentrations x for the $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ alloy. The obtained results for the composition dependence of the calculated equilibrium lattice parameter almost follow Vegard's law [22]. In going from CdSe to BeSe, when the Be-content increases, the values of the lattice parameters of the $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ alloy decrease. This is due to the fact that the size of the Be atom is smaller than the Cd atom. On the opposite side, one can see from Figure 2 that the value of the bulk modulus increases as the Be concentration increases.

The calculated band structure and partial density of states for $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ ($0 < x < 1$) are presented in Figure 3. It is clear from the figure that $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ ($0 < x < 1$) is a direct band gap material. The substitution of Be does not affect the direct band gap nature of the compound but increases the gap, which is clear from Figure 2(d). The direct band gap varies from 0.39 to 4.45 eV and the indirect band gap also increases from 1.89 to 3.71 eV with the increase in Be concentration between 0.25 and 0.75. It is obvious from the data presented in Table 2 that our calculated values for the band gaps of CdSe and BeSe are closer to the experimental results than the other calculated ones. The reason for our better results is the use of effective Perdew and Wang potential in the LDA scheme [17] and high k -points (1500). DFT always underestimates the band gaps; the origin of band structures is

FIGURE 1: Variation in lattice constants a and bulk modulus B of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ as a function of composition x .TABLE 2: Fundamental direct and indirect band gaps of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ compared with the experimental and other calculations.

x	Direct energy band gap, $E_g^{\Gamma-\Gamma}$			Indirect energy band gap, $E_g^{\Gamma-X}$			Band gap bowing
	This work	Exp.	Other calc.	This work	Exp.	Other calc.	
0	0.39	1.75 ^a	0.34 ^b , 0.26 ^c	2.31	5.4 ^d	5.4 ^e , 3.82 ^f , 3.79 ^g	
0.25	0.84	2.12 ^h , 2.56 ^h [$x = 0.2$] 2.65 ⁱ [0.24], 2.45 ^j [$x = 0.35$]		1.89			3.41
0.5	1.44	2.65 ^j [$x = 0.46$]		2.74			2.44
0.75	2.47			3.71			6.32
1	4.45		4.72 ^k -4.04 ^l	2.47	4-4.5 ^m	2.39 ^k , 2.31 ^l	

^aRef [33], ^bRef [26], ^cRef [27], ^dRef [34], ^eRef [35], ^fRef [36], ^gRef [37], ^hRef [38], ⁱRef [39], ^jRef [40], ^kRef [41], ^lRef [42], ^mRef [43].

presented in Figure 3. In general, the band structures of these three compositions x (0.25, 0.5, 0.75) are very similar. The uppermost valence band is mainly formed by Se 4p states.

The valence band maximum appears to be almost degenerate at the Γ and X k points for three concentrations (0.25, 0.5, and 0.75), the energy at X being (1.04, 1.29, and 1.24) eV lower than that at Γ , respectively. On the other hand, the conduction band minimum occurs at Γ , so there is a direct gap of 0.84, 1.44, and 2.47 eV at Γ and an indirect $\Gamma-X$ gap of 1.89, 2.74, and 3.71 eV for three concentrations (0.25, 0.5, and 0.75), respectively. To the best of our knowledge, there are no theoretical or experimental data on the energy band gaps for $x = 0.25, 0.5,$ and 0.75 available in the literature to make a meaningful comparison. It is clear from the results that the conduction band is mainly composed of Be-2p state for all ternary alloys. Figures 3(a) and 3(b) show that the lower part of the valence band is composed of Cd-4d and the upper part is mainly dominated by Se-4p state. This is due to the nature of bonding. At $x = 0.25, 0.5,$ and 0.75 partial covalent bond is stronger so the charge is shared by Se-4p and Be-2s states.

The calculated band gap versus concentration was fitted by a polynomial equation. The results are shown in Figure 2(d) and are summarised as follows:

$$\text{Cd}_{1-x}\text{Be}_x\text{Se} \longrightarrow \begin{cases} E_{\Gamma-\Gamma} = 0.466 - 0.088x + 3.99x^2 \\ E_{\Gamma-X} = 1.978 + 2.593x - 1.737x^2 \end{cases} \quad (6)$$

The variation in the band gap of $\text{Cd}_{1-x}\text{Be}_x\text{Se}$ provides promising results of the use of the compound in optoelectronic devices working in visible to ultraviolet regions. Depending on the need and requirement of a particular application, any desired band gap between 0.39 and 4.45 eV can be achieved.

We have calculated the frequency dependent imaginary dielectric function and real dielectric function. The effects of using k points in the BZ have already been discussed in the earlier work by Khan et al. [23]. The knowledge of both the real and the imaginary parts of the dielectric function allows the calculation of important optical functions. In this work, we also present and analyse the refractive index $n(\omega)$ given by (4).

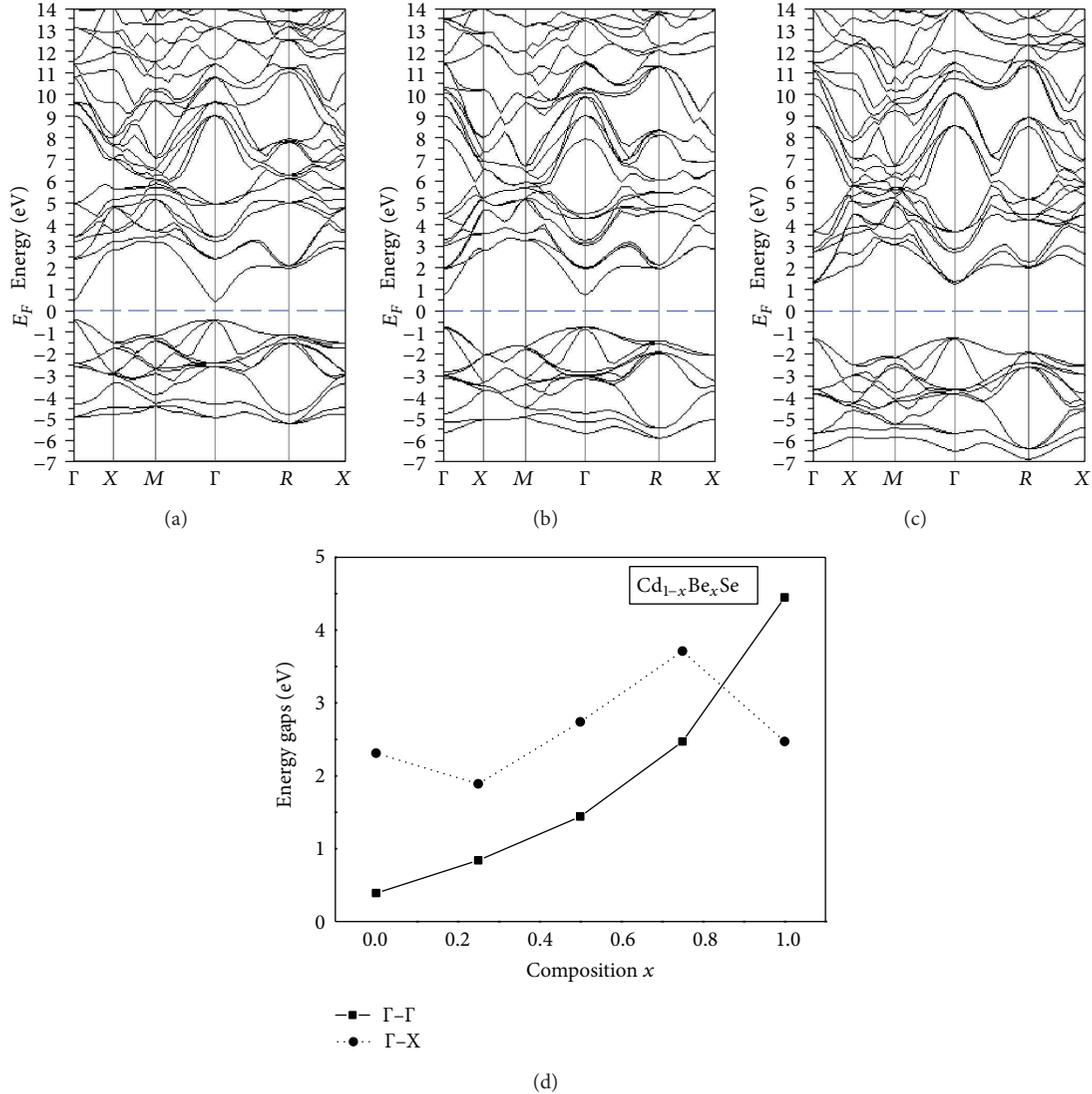


FIGURE 2: Calculated band structure of (a) Cd_{0.75}Be_{0.25}Se, (b) Cd_{0.5}Be_{0.5}Se, (c) Cd_{0.25}Be_{0.75}Se, and (d) band gap as a function of x .

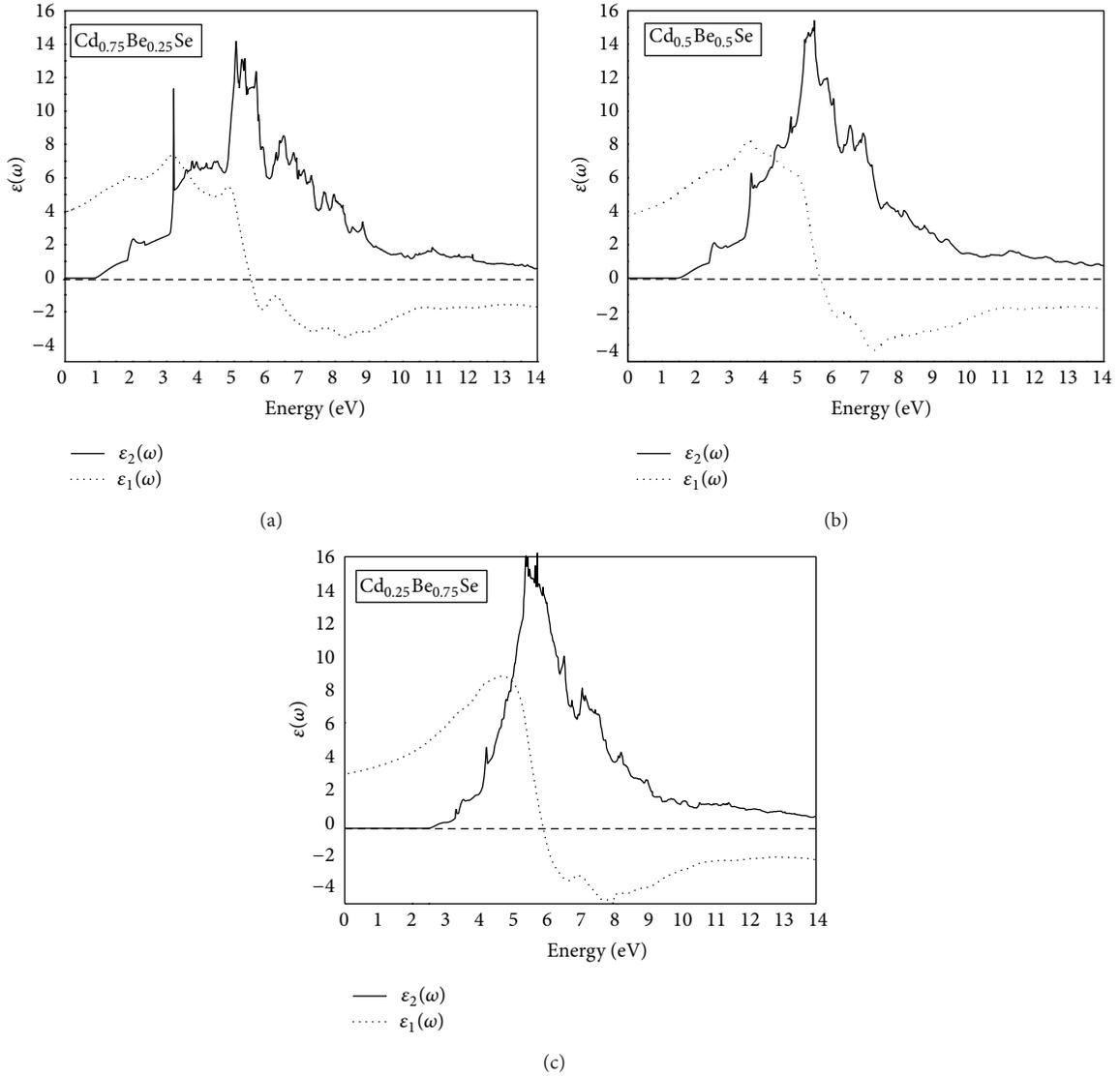
The calculated imaginary part of the dielectric function for Cd_{1-x}Be_xSe ($x = 0.25, 0.5$ and 0.75) in the energy range 0–12 eV is shown in Figure 3. It is clear from the figure that for $x = 0.25, 0.50, 0.75$, and 1.0 the critical points in the imaginary part of the dielectric function occur at about 0.85, 1.45, 2.48, and 4.45 eV, respectively. These points are closely related to the direct band gaps $E_G^{\Gamma-\Gamma}$; 0.84, 1.44, 2.47, and 4.45 eV of Cd_{1-x}Be_xSe for the corresponding values of $x = 0.25, 0.50, 0.75$ and 1 .

The calculated real parts of the complex dielectric function $\epsilon_1(\omega)$ for Cd_{1-x}Be_xSe are presented in Figure 3. It is clear from the figure that the static dielectric constant, $\epsilon_1(\omega)$, is strongly dependent on the band gap of the compound. The calculated values of $\epsilon_1(\omega)$ for Cd_{1-x}Be_xSe at $x = 0, 0.25, 0.50, 0.75$ and 1.0 are 4.35, 3.94, 3.74, 3.57, and 3.42 for corresponding direct band gaps 0.39, 0.84, 1.44, 2.47, and 4.45 eV, respectively. These data explain that the smaller energy gap yields larger $\epsilon_1(0)$ value. This inverse relation of

$\epsilon_1(\omega)$ with the band gap can be explained by the Penn model [24] as follows:

$$\epsilon_1(0) \approx 1 + \left(\frac{\hbar\omega_p}{E_g} \right)^2. \quad (7)$$

The calculated values of the optical dielectric constant $\epsilon(\omega)$ and refractive index $n(\omega)$ are listed in Table 3; comparison with the available data has been made where possible. As compared with other calculations, it seems that the values of $n(\omega)$ obtained from FP-LMTO method for the end-point compounds (i.e., CdSe and BeSe) are in good agreement with the theoretical results, together with the refractive index $n(\omega) = \sqrt{\epsilon}$ at zero pressure. Note that ϵ is obtained from the zero-frequency limit of $\epsilon_1(\omega)$, and it corresponds to the electronic part of the static dielectric constant of the material, a parameter of fundamental importance in many aspects of materials properties. It is clear from Figure 4 that

FIGURE 3: Frequency dependent imaginary part and real part of dielectric functions of $Cd_{1-x}Be_xSe$.TABLE 3: Refractive index, optical dielectric constant of $Cd_{1-x}Be_xSe$ alloys for different compositions x .

x	Refractive index n			Optical dielectric constant ϵ		
	This work	Exp.	Other calc.	This work	Exp.	Other calc.
0	2.08	2.64 ^a	2.47 ^b	4.36	5.2 ^c	5.05 ^d , 4.89 ^e
0.25	1.98			3.947		
0.5	1.93			3.74		
0.75	1.89			3.57		
1	1.85			3.43	6.1 ^f	6.09 ^g

^aRef [44], ^bRef [45], ^cRef [46], ^dRef [47], ^eRef [48], ^fRef [48], ^gRef [49].

the refractive index of the material decreases with the increase in the Be concentration.

Figure 4 shows the variation of the computed static optical dielectric constant and static refractive index versus composition for $Cd_{1-x}Be_xSe$ alloys. The computed static optical dielectric constant and static refractive index versus

composition were fitted by polynomial equation. The results are summarized as follows:

$$Cd_{1-x}Be_xSe \longrightarrow \begin{cases} \epsilon(0) = 4.3400 - 1.5610x + 0.6662x^2 \\ n(0) = 2.0745 - 0.3685x + 0.1485x^2. \end{cases} \quad (8)$$

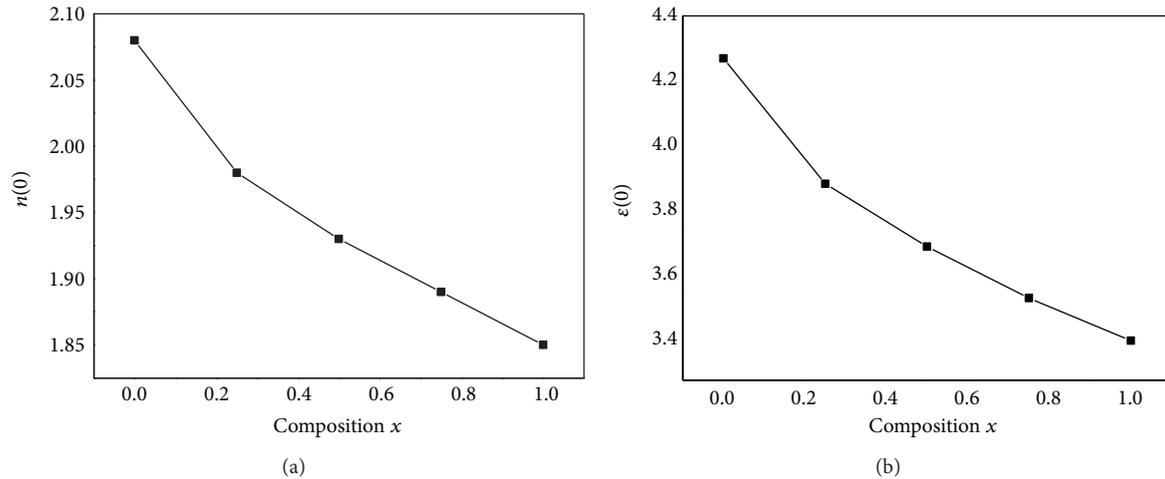


FIGURE 4: Computed static optical dielectric constant and static refractive index as function of composition for $\text{Cd}_{1-x}\text{Be}_x\text{Se}$.

4. Conclusions

Density functional calculations are carried out for the first time to investigate structural and optoelectronic properties $\text{Cd}_{1-x}\text{Be}_x\text{Se}$. Structure as well as bonding nature of the material significantly varies with Be concentration. The lattice constant of the crystal decreases linearly with x . The calculated band structure predicts that the alloys have direct band gaps, which increase with the increase in x . On the basis of wide range of fundamental direct band gaps (0.39–4.45 eV) and indirect band gaps (1.89–3.71 eV) between 0.25 and 0.75, it can be concluded that the material can be used in optoelectronic devices working in the IR, visible, and UV regions of the spectrum.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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