

Physical Properties of the $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ Alloys: *Ab-Initio* Method

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ABSTRACT

The present work performs self-consistent *ab initio* full-potential linear muffin-tin orbital (FP-LMTO) method to study the structural and electronic properties of the ternary $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy, based on density functional theory (DFT). In this approach, both the local density approximation (LDA) and the generalized gradient approximation (GGA) were used for the exchange-correlation potential calculation. The ground-state properties are determined for the bulk materials CdSe, ZnSe and their alloy in cubic phase. In particular, the lattice constant, bulk modulus, electronic band structures and effective mass. We mainly showed deviation of the lattice parameter and bulk modulus from Vegard's law of our alloys. We also presented the microscopic origins of the gap bowing using the approach of Zunger *et al.* The results are compared with other theoretical calculations and experimental data and are in reasonable agreement.

Keywords: FP-LMTO; *Ab-Initio*; Approach of Zunger; Effective Mass

1. Introduction

In recent years II-VI semiconductors have received much attention because of their technological potential applications, ranging from optoelectronic devices such as light emitting diodes [1,2], solar cells [3,4], displays [5,6], photovoltaic cells [7,8] to luminescence biological tags [9,10]. Their mixed II-VI ternary semiconductors are used in optoelectronic devices ranging from blue to near-ultraviolet spectral region [9-11]. These materials are also used for manufacturing X-ray, γ -ray detectors [12, 13]. Cd based compounds can also be used as an alternative material for short and medium wavelength infrared focal plane arrays [13,14]. Among them, ZnSe and CdSe which are members of the II-VI semiconductors are technologically important materials due to their direct and rather large gap. ZnSe compounds have cubic (zinc blende) structure [15,16], whereas CdSe compounds depending on the growth condition may have both zinc blende and wurtzite (hexagonal) structures at normal conditions. Theoretical studies indicate that CdSe compounds are stable in both zinc blende and wurtzite structures [17-19], we choose the zinc-blende phase, since it has fewer atoms in unit cell, and is therefore computationally easier to treat. The structural and electronic properties of these compounds have been investigated,

both experimentally and theoretically during the past 50 years. $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ mixed crystals have recently been studied theoretically [20,21] and experimentally [22,23]. With different methods for example, Suzuki and Adachi [24] have calculated the optical constants of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ (for $x = 0, 0.47, 0.53, 1$) using the first-principle methods. Electronic and optical properties of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ (for $x = 0, 0.25, 0.75, 1$) have been investigated using the empirical pseudopotential method (EPM) by Benosman *et al.* [21]. Kim *et al.* [22] have investigated optical properties of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ films grown on GaAs. Samarth *et al.* [23] have studied the composition (x) dependence of the fundamental gap of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ based on the reflection spectroscopy.

In this work, we have aimed to provide some additional information to the existing data on disorder effect of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ mixed crystals using the FP-LMTO method [25,26] to have an idea about their behaviors. The physical origins of gap bowing are calculated following the approach of Zunger and co-workers, all first we compare and investigate the structural, and electronic properties of ZnSe and CdSe compound using LDA, GGA.

The paper is organized as follows: Section 2 describes briefly the method used, in Section 3 we present our results concerning structural, electronic, bowing parameters, effective masses and we make a comparison with values reported in the literature, a final Section 4 presents our conclusions.

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2. Method of Calculations

In order to calculate the structural and electronic properties of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloys, we have employed the FP-LMTO method to solve the Kohn Sham equations. We have performed our calculations by Lmtart code [27] within the framework of density functional theory (DFT) [28] that has been shown to yield reliable results for the electronic and structural properties of various solids. For the exchange-correlation potential we have used both the local density approximation (LDA) [29] and the generalized gradient approximation (GGA) based on Perdew *et al.* [30]. The FP-LMTO method treats muffin-tin spheres (MTS) and interstitial regions (IR) 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 (IR) and non overlapping (MTS) surrounding the atomic sites, uses a more complete basis than its predecessors. In the IR regions, the basis functions are represented by Fourier series. Inside the MTS, the basis functions are represented in terms of numerical solutions of the radial Schrödinger equation for the spherical part of the potential multiplied by spherical harmonics. The charge density and the potential are represented inside the MTS by spherical harmonics up to $l_{\text{max}} = 6$. There is a parameter must be defined whenever a DFT calculation is performed the cut-off energy E_{cut} . In many ways, this parameter is easier to define than k points. The integrals over the Brillouin zone are performed up to 22 special k -points for binary compounds, 24 special k -points for the $x = 0.25$, $x = 0.75$ and 46 special k -points $x = 0.5$ of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloys in the

irreducible Brillouin zone (IBZ), using the Blöchl's modified tetrahedron method [31]. The self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-5} Ry. In order to avoid the overlap of atomic spheres the MTS radius for each atomic position is taken to be different for each case. Both the plane waves' cut-off is varied to ensure the total energy convergence. The values of the sphere radii MTS, number of plane waves (NPLW), and cut-off energy E_{cut} used in our calculation are summarized in **Table 1**.

3. Results and Discussion

3.1. Structural Properties

At first, a set of total energy calculation versus unit cell volume E (V), for binary compounds CdSe, ZnSe structure and their ternary alloys in zinc-blende were carried out in order to determine the structural parameters. We model the alloys at some selected compositions $x = 0.25$, 0.5 and 0.75, with ordered structures described in terms of periodically repeated supercells containing eight atoms. The corresponding values are fitted with the Murnaghan equation of state [32]. The equilibrium structural properties such as the lattice constants a_0 and bulk modulus B_0 were obtained for both binary compounds and their alloys, the results are given in **Table 2**. Considering the general trend that GGA usually overestimates the lattice parameters [33] on the other side are underestimated through local density approximation (LDA). The results obtained in this work are in close agreement with those obtained experimentally and are better than results

Table 1. The plane wave number PW, energy cut-off (in Ry) and muffin-tin radius (RMT) (in a.u.) used in calculation for binary CdSe, ZnSe and their alloys in Zinc-blende structure.

x	PW		$E_{\text{cut total}}(\text{Ry})$			RMT (a.u.)	
	LDA	GGA	LDA	GGA		LDA	GGA
0	5064	1205	87.333	144.4309	Cd	2.561	2.470
					Se	2.561	2.470
0.25	33400	65266	123.6696	181.4858	Cd	2.446	2.524
					Zn	2.446	2.524
					Se	2.446	2.524
					Cd	2.404	2.478
0.50	33400	65266	128.0740	188.2040	Zn	2.404	2.478
					Se	2.404	2.478
					Cd	2.354	2.427
					Zn	2.354	2.427
0.75	33400	65266	133.500	196.3489	Se	2.354	2.427
					Zn	2.273	2.205
					Se	2.463	2.389
1	5064	1205	101.000	168.8865			

Table 2. Calculated lattice parameter (a_0), bulk modulus (B) and its pressure derivative (B') compared to experimental and theoretical values of CdSe, ZnSe and $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy.

x	Lattice constant a_0 (Å)			Bulk modulus B (GPa)			B'	
	This work		Theo.	This work		Theo.	This work	Theo.
	LDA	GGA		LDA	GGA		LDA	GGA
0	6.037	6.262	6.05 ^{a,b,c,d}	58.9	44.55	53 ^{a,e} 69 ^f	3.16	3.01
			6.19 ^g 6.084 ^h 6.15 ⁱ 6.07 ^{j,k} 6.017 ^m			45.94 ^g 66 ^j 65.12 ^b 57.20 ^l 59.2 ^k 58.68 ^m		4.20 ^b 5.12 ^m 4.58 ^j
0.25	5.98	6.172		56.9	43.67		3.34	3.63
0.5	5.876	6.058		59.7	46.46		3.47	3.126
0.75	5.755	5.933		62.37	49.40		3.41	3.335
1	5.616	5.789	5.667 ^{n,o} 5.650 ⁿ 5.670 ^p	68.37	55.43	64.7 ⁿ 69.3 ^o 62.5 ^p	3.03	3.01
			5.624 ^q 5.79 ^s 5.681 ^u 5.730 ^g 5.57 ^g			71.82 ^q 59.01 ^s 59 ^r 66 ^u 70.93 ^g		4.77 ⁿ 4.88 ^q 6.53 ^s 5.41 ^t 3.8 ^r

^aRef. [40], ^bRef. [41], ^cRef. [42], ^dRef. [43], ^eRef. [44], ^fRef. [45], ^gRef. [46], ^hRef. [47], ⁱRef. [48], ^jRef. [49], ^kRef. [50], ^lRef. [51], ^mRef. [52], ⁿRef. [53], ^oRef. [54], ^pRef. [55], ^qRef. [56], ^rRef. [57], ^sRef. [58], ^tRef. [59], ^uRef. [60].

obtained using other methods. It can be seen that the lattice constant of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy linear decreases as the composition x increases. Also, the order of compressibility from high to low is: CdSe > Cd_{0.75}Zn_{0.25}Se > Cd_{0.5}Zn_{0.5}Se > Cd_{0.25}Zn_{0.75}Se > ZnSe. This diminution may stem from the lower mass of Zn atom than that of the Cd atom. For these configurations, the largest value of bulk modulus (68.37 GPa; 55, 43 GPa) with LDA and GGA respectively, was obtained for ZnSe, therefore it has the higher compressibility and it may be a more compressible compound. Usually, in the treatment of alloys, it is assumed that the atoms are located at the ideal lattice sites and the lattice constant varies linearly with the composition x according to the so-called Vegard's law [34]:

$$a(A_xB_{1-x}C) = xa_{AC} + (1-x)a_{BC} \quad (1)$$

where a_{AC} and a_{BC} are the equilibrium lattice constants of the binary compounds AC and BC, respectively, and $a(A_xB_{1-x}C)$ is the alloy lattice constant. However, deviation from Vegard's law has been observed in semiconductor alloys both experimentally [35] and theoretically [36,65]. Hence, the lattice constant can be written as:

$$a(A_xB_{1-x}C) = xa_{AC} + (1-x)a_{BC} - x(1-x)b \quad (2)$$

where the quadratic term (b) is the bowing parameter.

Figures 1 and 2, shows the calculated lattice constants and bulk modulus for each x of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ along with Vegard's law (v.z. the lattice constant of alloys should

vary linearly with composition x [35]). Our calculated lattice parameters at different compositions of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy were found to vary almost linearly with a marginal upward bowing parameter. Using the LDA approximation equals to -0.206 Å and 15.21 GPa for the lattice constant and bulk modulus, respectively. While, the GGA approximation gave values of -0.139 Å and 15.96 GPa for the bowing lattice parameter and the bulk modulus, respectively. Hence the Vegard's law is valid for this alloy. The physical origin of this marginal bowing parameter should be mainly due to the weak mismatches of the lattice constants of ZnSe and CdSe compounds.

3.2. Electronic Properties

To investigate the electronic properties of ZnSe and CdSe compounds as well as their alloy, we have calculated the band structure the high symmetry directions in the first Brillouin zone in the cubic phase structures within LDA and GGA using calculated equilibrium lattice constants as obtained previously. The valence band maximum (VBM) and the conduction band minimum (CBM) occur at the Γ point; hence these compounds are semiconductors with direct energy band gaps Γ - Γ . This direct energy band gap increased from CdSe ($x = 0$) to Zn ($x = 1$). The results of this calculation are compared with experimental values and results from other works in **Table 3**, the band gaps are smaller than the experimental

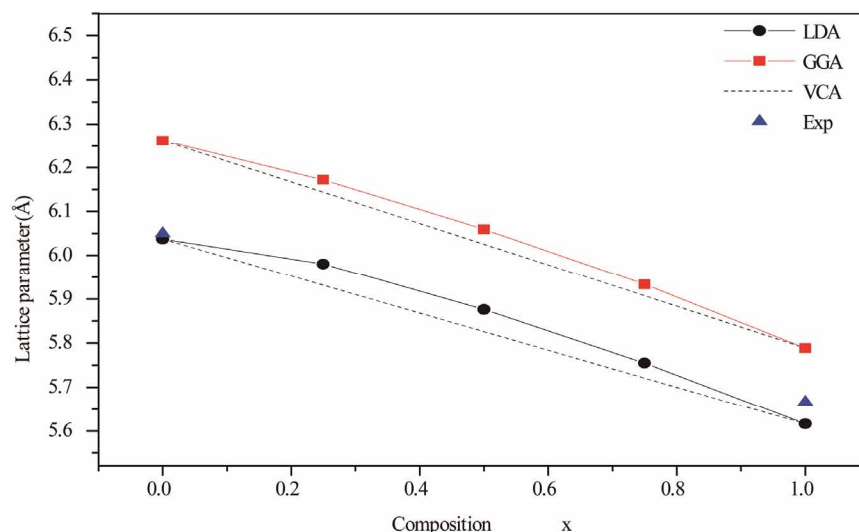


Figure 1. Composition dependence of the calculated lattice constants within LDA (solid circle) and GGA (solid square) of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy compared with experimental (solid triangle).

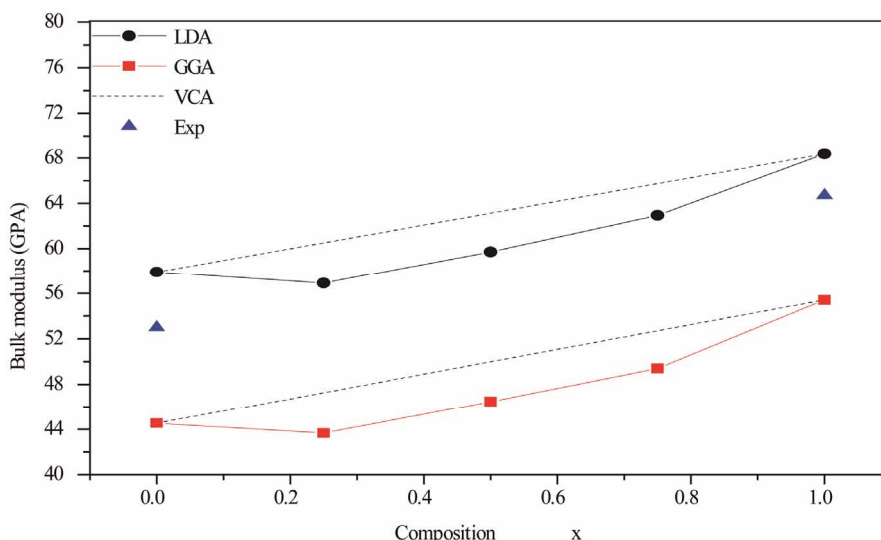


Figure 2. Composition dependence of the calculated bulk modulus within GGA (solid square) and LDA (solid circle) of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy compared with experimental (solid triangle).

values, one can note that the GGA approach underestimates the experimental values of the band gaps for all materials of interest. This is an expected result since the GGA usually underestimates the energy band gaps [37]. The GGA has a simple form which is not sufficiently flexible for accurately reproducing both exchange-correlation energy and its charge derivative.

The variation of the concentration (x) versus the value of the band structure (direct $E_{\Gamma-\Gamma}$ and indirect $E_{\Gamma-X}$ band gaps) with both LDA and GGA approximations is given in **Figure 3**. Afterwards this figure we notice the wide difference of direct and indirect band gaps of the composition x . has a behavior linear. The study of the polynomial function represents that our alloy has a direct gap with different concentration (0.25, 0.5 and 0.75), this

alloy $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ is different compared with other alloys, stabilizes and is not subject to change.

And obey the following variations:

$$\text{Zn}_x\text{Cd}_{1-x}\text{Se} \rightarrow \begin{cases} E_{\Gamma-\Gamma} = 0.42 + 0.036x + 0.04x^2, \\ E_{\Gamma-X} = 4.68 - 0.93x + 0.27x^2, \end{cases} \text{ (GGA)} \quad (3)$$

$$\begin{cases} E_{\Gamma-\Gamma} = 0.421 + 0.015x + 0.05x^2 \\ E_{\Gamma-X} = 4.8 - 0.61x + 0.18x^2 \end{cases} \text{ (LDA)} \quad (4)$$

The overall bowing coefficient at each composition x measures the change in the band gap according to the formal reaction

$$x AC(a_{AC}) + (1-x) BC(a_{BC}) \rightarrow A_x B_{1-x} C(a_{eq}) \quad (5)$$

Table 3. Direct (Γ - Γ) and indirect (Γ -X) band gaps of CdSe and ZnSe and their alloy at different concentrations (all values are in eV).

x	Energy gap (eV) (Γ - Γ)				Energy gap (eV) (Γ -X)			
	This work		Expt	Other cal	This work		Expt	Other cal
	LDA	GGA			LDA	GGA		
0	0.42	0.41	1.9 ^a	1.9 ^c 1.08 ^d 0.71 ^e 1.48 ^f 0.47 ^g 0.75 ^g 0.76 ^h 2.01 ^h 2.65 ⁱ	4.95	4.87	5.4 ^a	5.4 ^b
0.25	0.48	0.49			4.26	3.89		
0.5	0.62	0.58			4.29	3.94		
0.75	0.83	0.76			4.73	4.36		
1	1.18	1.00	2.80 ^a 2.82 ^a	2.8 ^j 1.39 ^c 2.76 ^k 1.176 ^g 1.86 ^l 1.6 ^m 1.2 ⁿ	5.11	5.06	4.5 ^a – 4.3 ^b	4.49 ^j 4.54 ^k 3.5 ^m 2.5 ^o

^aRef. [61], ^bRef. [62], ^cRef. [63], ^dRef. [40], ^eRef. [46], ^fRef. [64], ^gRef. [65], ^hRef. [50], ⁱRef. [66], ^jRef. [67], ^kRef. [68], ^lRef. [69], ^mRef. [70], ⁿRef. [52].

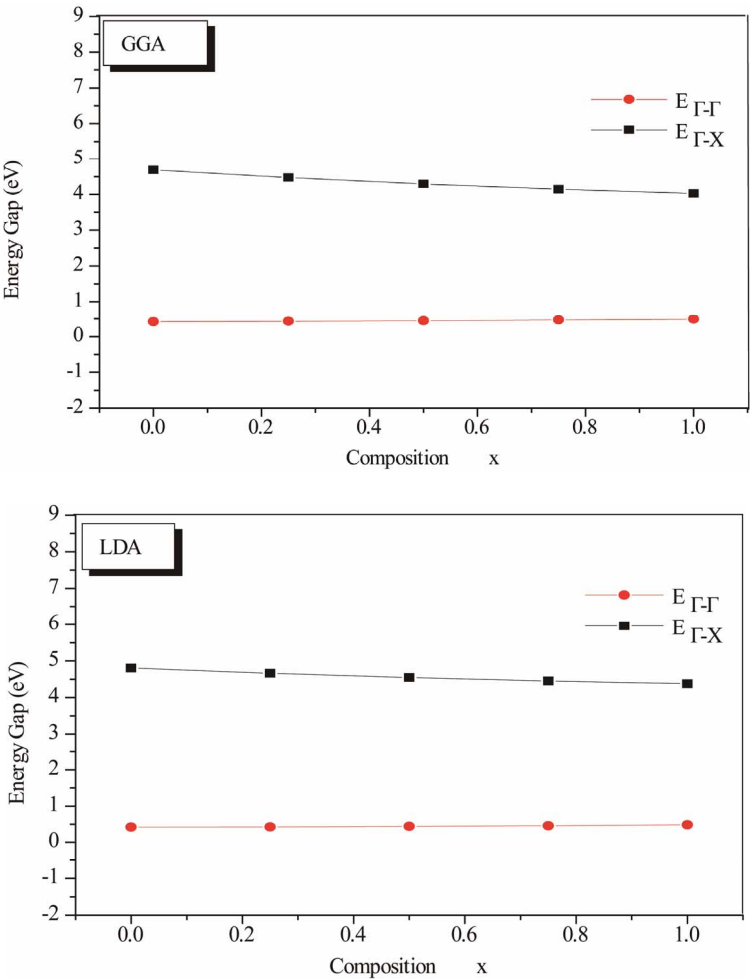


Figure 3. Energy band gap of $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy as a function of Se composition using LDA and GGA approximations.

where a_{AC} and a_{BC} are the equilibrium lattice constants of the CdSe, ZnSe compounds and a_{eq} is the equilibrium lattice constant of the $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy with the average composition x .

The physical origins of the bowing gap were investigated following the approach of Zunger and co-workers [38,39], which decompose it into three contributions:

$$AC(a_{AC}) + BC(a_{BC}) \rightarrow AC(a) + BC(a) \quad (6)$$

$$xAC(a) + (1-x)BC(a) \rightarrow A_xB_{1-x}C(a) \quad (7)$$

$$A_xB_{1-x}C(a) \rightarrow A_xB_{1-x}C(a_{eq}) \quad (8)$$

The first step measures the volume deformation (*VD*) effect on the bowing. The corresponding contributions b_{VD} to the bowing parameter represents the relative response of the band structure of the binary compounds *AC* and *BC* to hydrostatic pressure, which here arises from the change of their individual equilibrium lattice constants to the alloy value $a = a(x)$. The second contribution, the charge exchange (*CE*) contribution b_{CE} , reflects the charge transfer effect which is due to the different (averaged) bonding behaviour at the lattice constant a . The last contribution, the so called “structural relaxation” (*SR*), measures changes in passing from the unrelaxed to the relaxed alloy by b_{SR} . Consequently, the total bowing parameter is defined as:

$$b = b_{VD} + b_{CE} + b_{SR} \quad (9)$$

The general representation of the composition dependent band gap of the alloy in terms of the binary compounds gaps is $E_{\text{CdSe}}(a_{\text{CdSe}})$, $E_{\text{ZnSe}}(a_{\text{ZnSe}})$, and the total bowing parameter b is given by

$$E_g(x) = xE_{AC}(a_{AC}) + (1-x)E_{BC}(a_{BC}) - bx(1-x) \quad (10)$$

where E_{AC} and E_{BC} corresponds to the energy gap of ZnSe and CdSe for the $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy. This allows a splitting of the total bowing b into three contributions according to

$$b_{VD} = \frac{E_{AC}(a_{AC}) - E_{AC}(a)}{1-x} + \frac{E_{BC}(a_{BC}) - E_{BC}(a)}{x} \quad (11)$$

$$b_{CE} = \frac{E_{AC}(a)}{1-x} + \frac{E_{BC}(a)}{x} - \frac{E_{ABC}(a)}{x(1-x)} \quad (12)$$

$$b_{SR} = \frac{E_{ABC}(a) - E_{ABC}(a_{eq})}{x(1-x)} \quad (13)$$

All of these energy gaps occurring in expressions (11)-(13) have been calculated for the indicated atomic structures and lattice constants.

The calculated bowing coefficients b calculated at molar fractions $x = 0.25, 0.50$ and 0.75 for $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy are listed in **Table 4** using FP-LMTO method within

LDA and GGA approximations we notice that the structural relaxation effect is the smaller for the studied compositions $x = 0.25, 0.50$ and 0.75 and the main contribution to the band gap bowing is essentially due to the charge exchange (*CE*) contribution for $x = 0.25, 0.5$ and 0.75 . It is clearly seen that our LDA values for total bowing parameters are better than the corresponding with in GGA. **Figure 4** shows the variation of the band gap bowing versus concentration. It is shown that the optical bowing decreases slightly from 0.25 to 0.5 , and beyond 0.5 it increases rapidly, to the best of our knowledge, there are no theoretical or experimental data on the band gap bowing to check our predicted results.

3.3. Effective Masses

Although the effective mass approximation is used extensively throughout the literature, the actual electron and hole effective masses for the alloys in the whole range of x , are unknown. The transport and optical phenomena usually are governed by the band structures in the immediate vicinity of the Brillouin zone center. Thus the effective mass approximation turns to be an appropriate method to make the analysis of the electronic energy band curvatures. Generally, the effective mass is a tensor with nine components, however for the much

Table 4. Decomposition of optical bowing into volume deformation (*VD*), charge exchange (*CE*) and structural relaxation (*SR*) contributions (all values in eV).

		This work	
x		LDA	GGA
0.25	b_{VD}	0.3980	0.3461
	b_{CE}	5.6990	5.4295
	b_{SR}	0.3082	0.1657
	b	6.4052	5.9413
0.5	b_{VD}	0.42625	0.3832
	b_{CE}	5.5010	4.9792
	b_{SR}	0.2784	0.1665
	b	6.2056	5.5289
0.75	b_{VD}	0.4571	0.4029
	b_{CE}	9.5785	8.706
	b_{SR}	0.3350	0.2103
	b	10.3706	9.3192

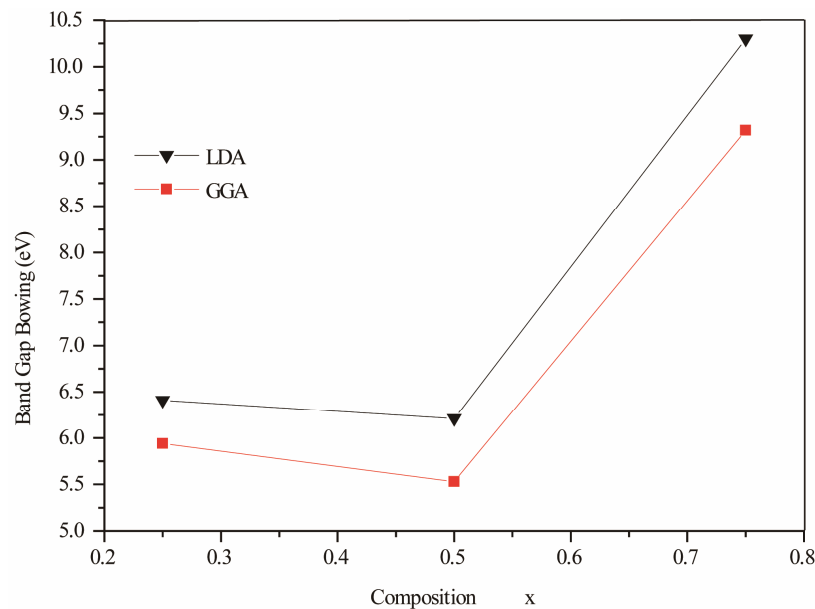


Figure 4. Calculated band gap bowing parameter as a function of Se concentration within GGA (solid square) and LDA (solid triangle).

Table 5. Electron (m_e^*), light hole (m_{lh}^*) and heavy hole (m_{hh}^*) effective masses (in units of free electron mass m_0) of the ternary alloy $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ compared with the available experimental data and theoretical result.

m_e^*			m_{hh}^*			m_{lh}^*				
This work		Expt	Other calc	This work		Other calc	This work		Other calc	
x	LDA	GGA		LDA	GGA		LDA	GGA		
0	0.100	0.007		0.240	0.360		0.160	0.230		
0.25	0.198	0.260		0.130	0.180		0.300	0.410		
0.5	0.300	0.400		0.135	0.185		0.330	0.440		
0.75	0.190	0.240		0.110	0.150		0.240	0.320		
1	0.100	0.008	0.147 ^a	0.112 ^b 0.214 ^c	0.160	0.230	1.024 ^b 0.265 ^c	0.100	0.140	0.104 ^b 0.064 ^c

^aRef. [71], ^bRef. [72], ^cRef. [65].

idealized simple case, where the E - k diagram can be fitted by a parabola $E = \hbar^2 k^2 / 2 m^*$, the effective mass becomes a scalar at high symmetry point in Brillouin zone. We have computed the electron effective mass at the conduction band minima (CBM) and the hole effective mass at the valence band maxima (VBM) for CdSe, ZnSe and their ternary alloys, the results of our calculations were investigated in **Table 5**, that shows the calculated electron and hole (heavy and light) effective masses from 0 to 1.0 for $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloys at point Γ of the Brillouin zone. Our results concerning the electrons, heavy holes and light hole effective mass are shown in **Figure 5**. From **Table 5**, we can outline that the calculated electron effective masses for the studied composition are much smaller, predicting a higher mobility of electrons, for all

concentrations in $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy, the carrier transport in this alloy should be dominated by electrons. Our calculated effective masses for ZnSe are found comparable by Baaziz *et al.* [72].

4. Conclusion

The (FP-LMTO) method is used to calculate the structural and electronic properties zinc-blende phase of CdSe, ZnSe and their $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy within LDA and GGA approximations. We observed that GGA somewhat overestimates the experimental data on the other side are underestimated with the LDA approximation. A small deviation of the lattice constant from Vegard's law was observed for $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$ alloy. The electronic band structure is in good agreement with the experimental and other

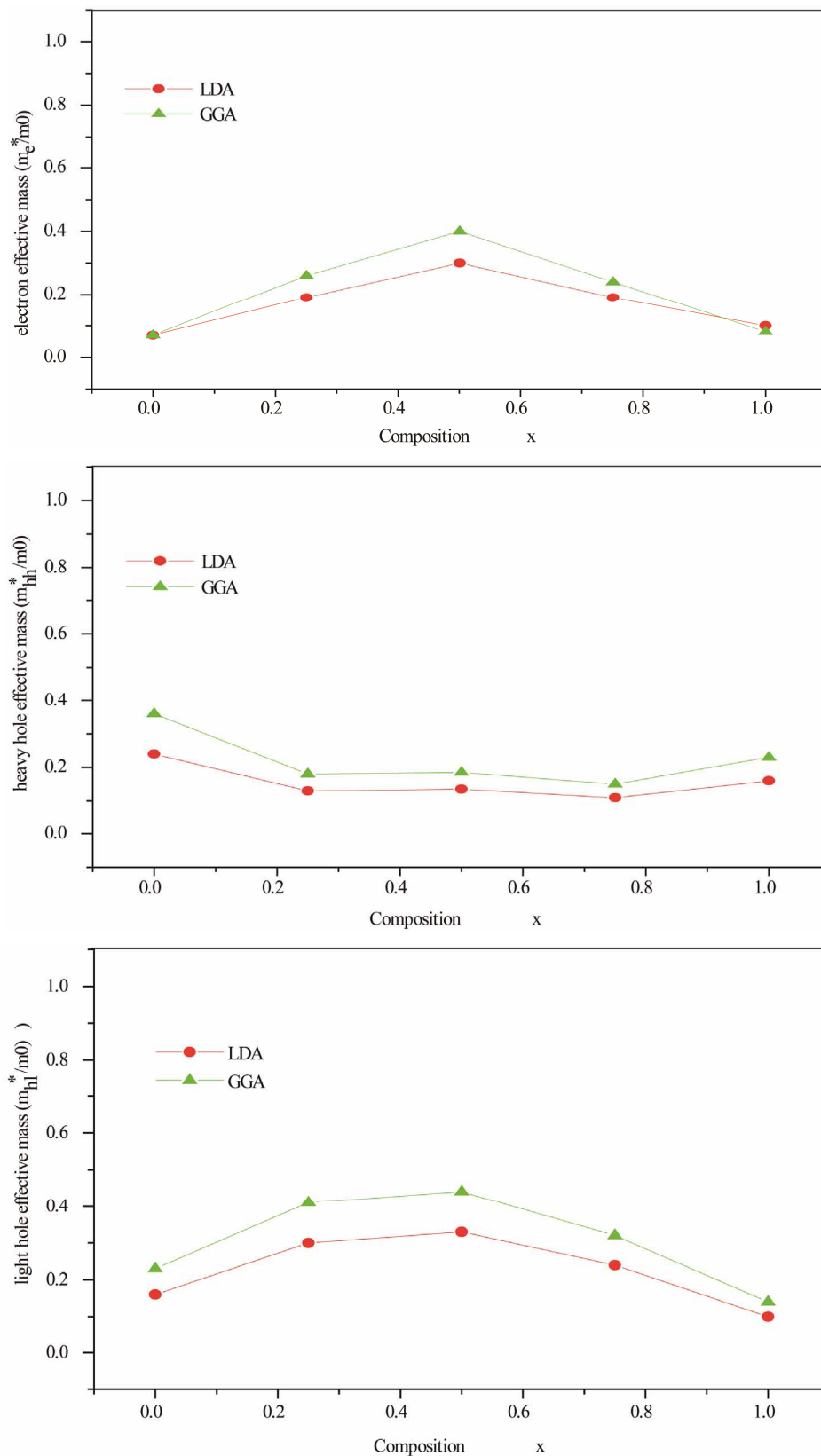


Figure 5. (a) Electron effective mass at point Γ as function of Se composition within LDA and GGA. (b) Heavy hole effective mass (in units of free electron mass m_0) of Se composition within LDA and GGA. (c) Light hole effective mass at point Γ as function of Se composition within LDA and GGA.

computational work. Our results show a strong dependence of the band gap bowing factor using Zunger approach on composition. The effective masses are investigated and showed good accordance using LDA and GGA especially for electron mass.

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