

Ab Initio Study of Structural and Electronic Properties of Barium Chalcogenide Alloys

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ABSTRACT

First-principles calculations have been used to study the structural and electronic properties of $\text{BaS}_{1-x}\text{Se}_x$ ternary alloy using full-potential muffin-tin orbital's (FP-LMTO) method within density functional theory (DFT). In this approach, the local-density approximation (LDA) and generalized gradient approximation (GGA) are used for the exchange-correlation (XC) potential. The effect of composition on lattice parameter, bulk modulus, band gap and effective mass was investigated. The deviations of the lattice constant from Vegard's law and the bulk modulus from linear concentration dependence were observed for $\text{BaS}_{1-x}\text{Se}_x$ alloy. The microscopic origins of bowing parameter were explained using approach of Zunger and co-workers. Accordance is found from the comparison of our results with other experimental and theoretical calculations.

Keywords: Semiconductor; FP-LMTO; Effective Mass

1. Introduction

II-VI compounds have attracted great interest due to their potential applications in fields of light-emitting diodes (LEDs) and laser diodes (LDs) [1]. As important members of II-VI compounds, the Barium mono-chalcogenides; BaS and BaSe have already been systematically studied by both experiments and first-principles calculations [2,3] for many years, due to their interesting phase transition from the rocksalt crystal structure to the CsCl-crystal structure under pressure. The experimental [4,5] and theoretical [6] studies of BaX ($X = \text{S}, \text{Se}$) compounds have been made by many researchers. Most of available experimental results on the reflectivity and absorption of these compounds are limited to excitonic transitions [5-7]. From a theoretical point of view, the electronic properties of BaS, BaSe have been determined by Pourghazi and Dadsetani [8].

Recent works show that $\text{BaS}_{1-x}\text{Se}_x$ compounds have directed energy gaps, comparing with the indirect ones of BaS, BaSe. In this work, we report the structural and electronic calculations for $\text{BaS}_{1-x}\text{Se}_x$ ($x = 0, 0.25, 0.50, 0.75$ and 1) alloys using full potential muffin-tin orbital's (FP-LMTO) method. The physical origins of gap bowing are calculated following the approach of Zunger and workers [9], in this approach, the alloy was studied in an ordered structure (we used here a cubic super cell of eight atoms) designed

to reproduce the most important paircorrelation functions of random (disorder) alloy. In our calculations, we describe the method of calculation, results and discussion concerning structural, electronic, bowing parameters, effective masses and finally the conclusions.

2. Computational Methods

The calculations here were carried out using *ab initio* full-potential linear muffin-tin orbital (FP-LMTO) method [10, 11] as implemented in the Lmtart code [12]. The exchange and correlation potential was calculated using the local density approximation (LDA) [13] and the generalized approximation (GGA) [14]. This is an improved method compared to previous LMTO methods. 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

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MTS by spherical harmonics up to $l_{\max} = 6$. The integrals over the Brillouin zone are performed up to 64 special k -points for binary compounds and 47 special k -points for the alloys in the irreducible Brillouin zone (IBZ), using the Blöchl's modified tetrahedron method [15]. The self-consistent calculations are considered to be converged when the total energy of the system is stabled 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), used in our calculation are summarized in **Table 1**.

3. Results and Discussion

3.1. Structural Properties

We have computed the structural properties of the binary

compounds BaS and BaSe in the rocksalt structure. As for the semiconductor ternary alloy in the type $B_xA_{1-x}C$, we have started our FP-LMTO calculation of the structural properties with the rocksalt structure and let the calculation forces to move the atoms to their equilibrium positions. The $B_xA_{1-x}C$ alloy are modelled some selected composition with ordered structures described in terms of periodically repeated supercells with eight atoms per unit cell of the compositions $x = 0.25, 0.5$ and 0.75 . For the considered structures, we performed the structural optimization by calculating the total energies for different volumes around the equilibrium cell volume (V_0) for BaS and BaSe binary compounds and their alloys. The calculated total energy at many different volumes around equilibrium were fitted to the Murnaghan's equation of state [16] in order to obtain the equilibrium lattice constant and bulk modulus for the binary compounds and their alloys. The results of our calculations were summarized in **Table 2**, were com-

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 BaS, BaSe and their alloys in rocksalt (NaCl) structure.

x	PW		E _{cut} total (Ry)			RMT (a.u.)	
	LDA	GGA	LDA	GGA		LDA	GGA
0	2974	6566	57.3335	91.2113	Ba	3.227	3.331
					S	2.64	2.725
0.25	20478	44472	79.9877	127.1894	Ba	3.26	3.345
					S	2.687	2.757
					Se	2.72	2.791
0.50	20478	44472	78.7354	124.7552	Ba	3.277	3.397
					S	2.741	2.79
					Se	2.741	2.79
0.75	20478	44472	77.3465	122.6856	Ba	3.286	3.383
					S	2.765	2.814
					Se	2.774	2.832
1	2974	6566	53.31612	85.515	Ba	3.285	3.377
					Se	2.798	2.877

Table 2. Calculated lattice parameter (a_0), bulk modulus (B) and its pressure derivative (B') compared to experimental and theoretical values of BaS and BaSe and their alloys.

x	Lattice constant a_0 (Å)			Bulk modulus B (GPa)			B'		
	This work		Exp.	This work		Exp.	This work		
	LDA	GGA	Theo.	LDA	GGA	Theo.	LDA	GGA	
0	6.21	6.41	6.389 ^c	47.05	38.52	39.42 ^c	51.13 ^b	3.16	3.01
							6.273 ^b 6.444 ^b 6.196 ^a 6.407 ^c 6.276 ^c		
0.25	6.32	6.486	6.327 ^b 6.496 ^b 6.46 ^c	46.60	38.37		49.48 ^b 37.80 ^b	3.34	3.63
0.5	6.37	6.55	6.378 ^b 6.559 ^b	45.87	38.08		47.52 ^b 36.48 ^b	3.47	3.126
0.75	6.427	6.604	6.428 ^b 6.632 ^b 6.584 ^c	45	37.8		45.69 ^b 34.88 ^b	3.41	3.335
1	6.44	6.62	6.595 ^d	43.81	37.49	43.4 ^d	44.38 ^b 32.82 ^b 45.41 ^a 46.8 ^d	3.33	3.08
							6.477 ^b 6.677 ^b 6.42 ^a 6.640 ^c 6.477 ^c		

^aRef [3]; ^bRef [17]; ^cRef [18]; ^dRef [19]; ^eRef [20].

pared to other experimental and theoretical calculations. It is observed that our calculated lattice parameters are in agreement with experimental data and theoretical work. **Table 2** also indicates that GGA slightly overestimates while LDA underestimates the theoretical lattice parameter compared to the experimental results. As it can be seen that the calculated lattice parameter for BaS ($x = 0$) is smaller than those of BaSe ($x = 1$); a_0 (BaS) $<$ a_0 (BaSe). The calculated Bulk modulus, B as given in **Table 2**, agree with other experimental and theoretical calculations. It is observed that LDA gives bulk modulus closer to experiment while GGA approximation consistently tends to underestimate experiment. Furthermore, the values of the calculated bulk modulus using both approximations decreases from BaS to BaSe, suggesting that the compressibility increases from BaS to BaSe. The obtained pressure derivatives of bulk modulus are given in **Table 2**.

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 [21]:

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

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 [22] and theoretically [23]. 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 show the variation of the calculated equilibrium lattice constants and bulk modulus versus concentration x for $BaS_{1-x}Se_x$ alloy. The obtained results for the composition dependence of the calculated equilibrium lattice parameter show an excellent agreement to Vegard's law [21]. In going from BaS to BaSe; when the Se-content increases, the values of the lattice parameters of the $BaS_{1-x}Se_x$ alloy increases. Oppositely, one can see from **Figure 2** that the values of the bulk modulus decrease with increasing "Se" concentration. The values of the bowing parameters are determined by a polynomial fit. Using the LDA approximation, we obtained upward bowing parameters equal to -0.22 \AA and -1.84 GPa for the lattice constant and bulk modulus, respectively. While, the GGA approximation gave values of -0.15 \AA and -0.35 GPa for the bowing lattice parameter and the bulk modulus, respectively. The physical origin of this large deviation should be mainly due to the large mismatches of the lattice constants of BaS and BaSe compounds. But our results are relatively close to those of Ref. [17] obtained using the full potential-linear augmented plane wave (FP-LAPW) method.

3.2. Electronic Properties

The calculated band gap of binary compounds as well as their alloy using FP-LMTO method within LDA and GGA approximations gave a direct band gap at point Γ for $BaS_{1-x}Se_x$ with x varying between 0.25 and 0.75. For BaS and BaSe, the valence-band maximum (VBM) and the

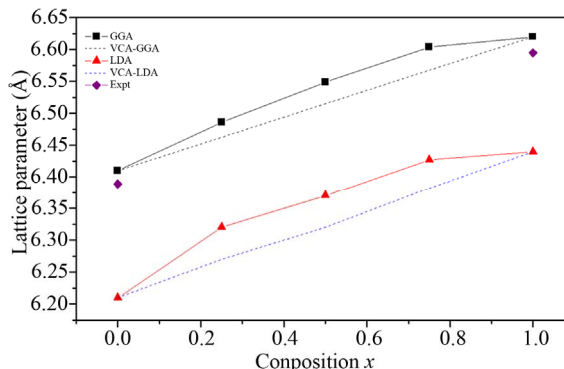


Figure 1. Composition dependence of the calculated lattice constants within LDA (solid circle) and GGA (solid triangle) of $BaS_{1-x}Se_x$ alloy compared with experimental (dotted line).

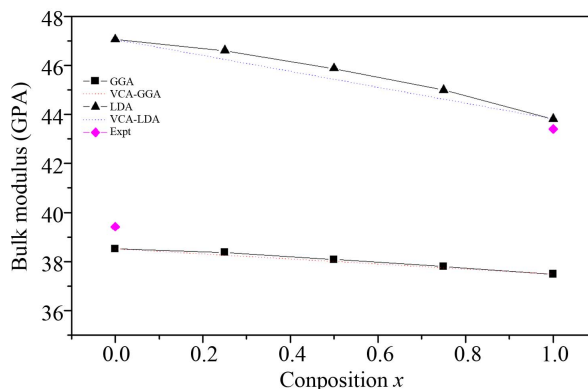


Figure 2. Composition dependence of the calculated bulk modulus within GGA (solid circle) and LDA (solid square) of $BaS_{1-x}Se_x$ alloy compared with experimental (dotted line).

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

x	Energy gap (eV) (Γ - Γ)		Energy gap (eV) (Γ -X)			
	This work	Theo.	This work	Exp.	Theo.	
	LDA	GGA	LDA	GGA		
0	3.72	3.68	3.72 ^g	1.74	2.08	3.88 ^e 1.94 ^b 2.26 ^b 3.07 ^b 1.83 ^d 3.90 ^f 2.17 ^d 2.30 ^e 3.88 ^d 3.90 ^f
0.25	1.75	2.08	2.17 ^a 2.92 ^a	2.42	2.81	
0.5	1.70	2.01	2.10 ^a 2.85 ^a	2.40	2.66	
0.75	1.67	1.97	2.02 ^a 2.75 ^a	2.31	2.55	
1	3.21	3.09		1.57	1.85	3.58 ^e 1.74 ^b 2.04 ^b 2.77 ^b 1.63 ^d 3.60 ^f 2.02 ^d 2.01 ^e 3.58 ^d 3.60 ^f

^aRef [24]; ^bRef [25]; ^cRef [3]; ^dRef [18]; ^eRef [26]; ^fRef [27]; ^gRef [28].

conduction-band minimum (CBM) occurs at the Γ - and X-point, respectively. The principal energy gaps are given in **Table 3**, as well as the theoretical and the experimental ones.

It is well known that the LDA and the GGA usually underestimate the energy gap [29,30]. This is mainly due to the fact that they have simple forms that are not sufficiently flexible for accurately reproducing both exchange-correlation energy and its charge derivative. It is important to note that the density-functional formalism is limited in its validity [31] and the band structure derived from it cannot be used directly for comparison with the GW method, which is known to give energy band gaps in excellent agreement with experiment.

The important applications of $\text{BaS}_{1-x}\text{Se}_x$ alloy in optical devices require the determination of the band gap nature (direct or indirect band gap). The results of direct and indirect band gaps are given in **Table 3**. It is clear that the band gap values given by the LDA and GGA, are in a good agreement with the other computational works, but lower than the experimental work.

The variation of the direct $E_{\Gamma-\Gamma}$ and indirect $E_{\Gamma-X}$ band gaps of the alloys is shown in **Figure 3**. The calculated band structure yields an indirect gap (Γ -X) for BaS and BaSe, while for $\text{Se}_{0.25}\text{S}_{0.75}\text{Ba}$, $\text{Se}_{0.5}\text{S}_{0.5}\text{Ba}$ and $\text{Se}_{0.75}\text{S}_{0.25}\text{Ba}$, a direct gap (Γ - Γ) has been determined. We calculated the total bowing parameter, by fitting the nonlinear variation,

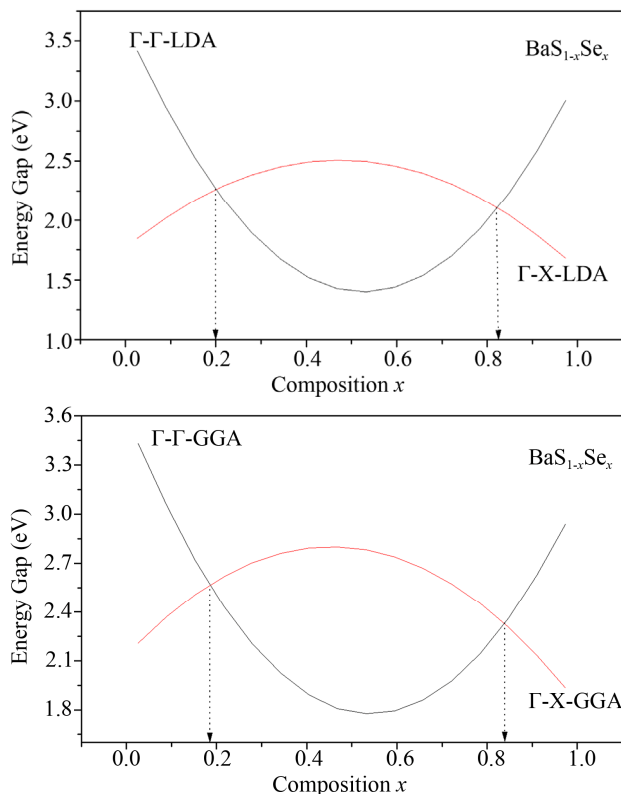


Figure 3. Energy band gap of $\text{BaS}_{1-x}\text{Se}_x$ alloy as a function of Se composition using LDA and GGA approximations.

with polynomial functions, of the calculated direct and indirect band gaps versus concentration. Using the LDA approximation, we could distinguish three regions: one direct band gap (Γ - Γ) for $(0.19 \leq x \leq 0.82)$ and two other indirect band gaps (Γ -X) for $(0 \leq x \leq 0.19 \text{ and } 0.82 \leq x \leq 1)$. The GGA approximation gave one direct band gap (Γ - Γ) for $(0.18 \leq x \leq 0.84)$ and two other indirect band gaps (Γ -X) for $(0 \leq x \leq 0.18 \text{ and } 0.84 \leq x \leq 1)$. It is clearly seen that our LDA values are in good agreement with the values found from the GGA.

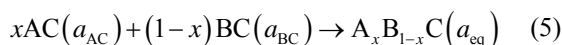
And obey the following variations:

$$\begin{cases} E_{\Gamma-\Gamma} = 3.63 - 8.49x + 8.06x^2 \\ E_{\Gamma-X} = 1.76 + 3.14x - 3.32x^2 \end{cases} \quad (\text{LDA}) \quad (3)$$

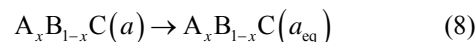
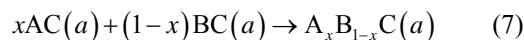
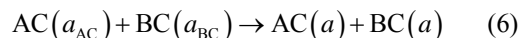
$\text{BaS}_{1-x}\text{Se}_x \rightarrow$

$$\begin{cases} E_{\Gamma-\Gamma} = 3.60 - 6.76x + 6.24x^2 \\ E_{\Gamma-X} = 2.13 + 2.93x - 3.23x^2 \end{cases} \quad (\text{GGA}) \quad (4)$$

In order to attain a better understanding of the physical origin of the bowing parameters in $\text{BaS}_{1-x}\text{Se}_x$ alloy, we followed the procedure of Bernard and Zunger [9] and decomposed the total bowing parameter b into physically distinct contributions. The overall bowing coefficient at each composition x measures the change in the band gap according to the formal reaction



where BaSe and BaS are the equilibrium lattice constant of the binary compounds and a_{eq} is the equilibrium lattice constant of the alloy with average composition x . Equation (5) is decomposed into three steps:



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 BaSe and BaS 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 bow-

ing 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 $E_{BaSe}(a_{BaSe})$, $E_{BaS}(a_{BaS})$, and the total bowing parameter b is given by

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

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 $BaS_{1-x}Se_x$ alloy are listed in **Table 4** using FP-LMTO method within LDA and GGA approximations. We note that the obtained bowing parameter for $x = 0.5$ is an excellent agreement with the others using EVGGA-FPLAPW method [24].

The small b_{CE} value of $BaS_{1-x}Se_x$ alloy is due to the weak ionicity mismatch of BaS and BaSe. The importance of b_{VD} can be correlated to the large mismatch of lattice constants of the corresponding binary compounds. Finally, it is clearly seen that our LDA values for total bowing parameters are better than the corresponding with in GGA in comparison with other. **Figure 4** shows the variation

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

x		This work		Other cal.
		LDA	GGA	
0.75	b_{VD}	0.038	0.0585	
	b_{CE}	-0.12	-0.2788	
	b_{SR}	-0.2278	-0.1258	
	b	-0.3098	-0.3261	
0.5	b_{VD}	0.0438	0.0709	0.06 ^b
	b_{CE}	0.012	-0.1515	0.04 ^b
	b_{SR}	-0.201	-0.0912	0.00 ^b
	b	-0.1452	-0.1718	0.1 ^b
0.25	b_{VD}	0.0130	0.0357	
	b_{CE}	-0.0074	-0.2432	
	b_{SR}	-0.279	-0.0834	
	b	-0.2734	-0.2909	

^bRef. [24].

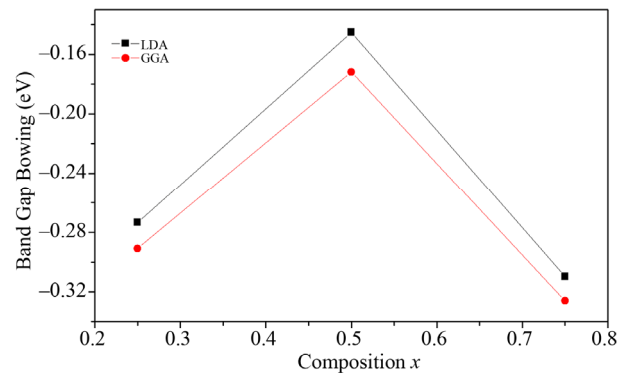


Figure 4. Calculated band gap bowing parameter as a function of Se concentration within GGA (solid square) and LDA (solid circle).

of the band gap bowing versus concentration. The bowing remains linear and varies slowly for $x = 0.5$, and beyond $x = 0.50$ it decreases rapidly.

3.3. Calculated Effective Masses

Knowledge of the electron and hole effective mass values is indispensable for the understanding of transport phenomena, exciton effects and electro-hole in semiconductors. Excitonic properties are of great interest for binary BaS, BaSe and their alloys; therefore, it is worthwhile to estimate the electron and hole effective mass values for these materials. Experimentally, the effective masses are usually determined by cyclotron resonance, electro reflectance measurements, analysis of transport data or transport measurements [32].

Theoretically, the effective masses can be estimated from the energy band curvatures. Generally, the effective mass is a tensor with nine components, however for the much idealized simple case, where the E-k diagram can be fitted by a parabola $E = \hbar^2 k^2 / 2m^*$, 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 BaS, BaSe 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 for $BaS_{1-x}Se_x$ at point Γ of the Brillouin zone at various compositions, except for $x = 0$ and $x = 1$, where we calculated electron effective mass at point X 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 holes are much heavier than electrons, for all concentrations in $BaS_{1-x}Se_x$ alloy, the carrier transport in this alloy should be dominated by electrons. It is clearly seen that our LDA values for hole effective masses are smaller than the those using GGA, but the electrons effective mass values given by LDA are in good agreement with those using GGA.

Table 5. Electron (m_e^*), light hole (m_{lh}^*) and heavy hole (m_{hh}^*) effective masses (in units of free electron mass m_0) at the Γ point of the Brillouin zone of the ternary alloys under investigation compared with the available experimental and theoretical predictions.

Alloy	(m_e^*)			(m_{lh}^*)			(m_{hh}^*)			
	This work		Exp	Other works	This work		Other works	This work		Other works
	LDA	GGA			LDA	GGA		LDA	GGA	
ZnS	0.195	0.205	0.341 ^a	0.205 ^b , 0.185 ^c 0.245 ^c , 0.150 ^d 0.185 ^e , 0.244 ^e	0.632	0.754	0.26 ^b , 1.174 ^c 1.283 ^c , 0.775 ^d 1.766 ^d , 2.755 ^d 1.163 ^e , 1.272 ^e	0.304	0.305	0.0651 ^b , 0.167 ^c 0.215 ^c , 0.224 ^d 0.188 ^d , 0.188 ^d 0.167 ^e , 0.214 ^e
O _{0.25} S _{0.75} Zn	0.229	0.224			2.344	2.891		1.060	1.316	
O _{0.5} S _{0.5} Zn	0.203	0.215			1.666	1.735		1.031	1.100	
O _{0.75} S _{0.25} Zn	0.192	0.196			1.254	2.946		1.254	1.477	
ZnO	0.112	0.129		0.110 ^d	0.68	0.834	0.390 ^d , 0.571 ^d 0.385 ^d	1.018	0.468	1.520 ^d , 1.10 ^d 1.330 ^d

^aRef. [29], ^bRef. [14], ^cRef. [13], ^dRef. [27], ^eRef. [15].

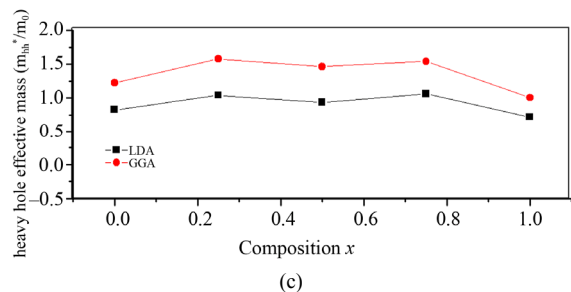
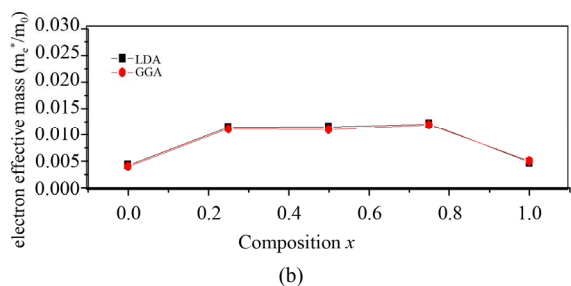
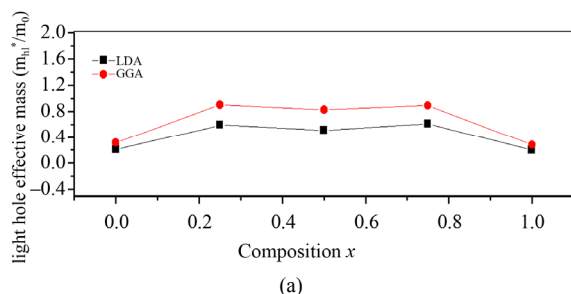


Figure 5. (a) Light hole effective mass at point Γ as function of Se composition within LDA and GGA; (b) Electron effective mass (in units of free electron mass m_0) of Se composition within LDA and GGA; (c) Heavy hole effective mass at point Γ as function of Se composition within LDA and GGA.

4. Conclusion

We have used the FP-LMTO method within LDA and ment with the experimental data for structural properties. We observed that GGA somewhat overestimates the ex-

perimental data while LDA underestimates. For electronic band structure, our results with LDA and GGA, although in good agreement with other computational work, are lower than the experimental results. This is due to a simpler form of the exchange-correlation functional. The deviations of the lattice constant from Vegard’s law and bulk modulus from linear concentration dependence were observed for BaS_{1-x}Se_x alloy. 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. To the best of knowledge .there are no earlier studies of the effective masses of electrons and holes of this compound; we feel that our calculations can be used to cover the lack of data for this compound.

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