

First Principles Study of Structural and Electronic Properties of $O_xS_{1-x}Zn$ Ternary Alloy

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ABSTRACT

We perform self-consistent *ab-initio* calculations to study the structural and electronic properties of zinc blende ZnS, ZnO and their alloy. The full-potential muffin-tin orbitals (FP-LMTO) method was employed within density functional theory (DFT) based on local density Approximation (LDA), and generalized gradient approximation (GGA). We analyze composition effect on lattice constants, bulk modulus, band gap and effective mass of the electron. Using the approach of Zunger and coworkers, the microscopic origins of band gap bowing have been detailed and explained. Discussions will be given in comparison with results obtained with other available theoretical and experimental results.

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

1. Introduction

The II-VI compound semiconductors have recently received considerable interest a lot of experimental and theoretical work on this alloy's, they were promoted much interest because of their numerous applications in optoelectronic devices such as visual displays, high-density optical memories, transparent conductors, solid-state laser devices, photodetectors, solar cells, etc. for $O_xS_{1-x}Zn$ few studies that have been done on this alloy due the difficulty in the synthesis of this material, due to the large electronegativity differences between O and S [1]. From this the purpose of this paper is to illustrate such modifications by providing original *ab initio* structural and electronic properties for the zinc blende (ZB) $O_xS_{1-x}Zn$ alloy with different discrete compositions, namely $x = 0, 0.25, 0.50, 0.75, 1$ and compare them with ZB ZnS and ZnO. The calculations were carried out within the density functional theory (DFT) [2,3]. Therefore, the main aim of the present study was to investigate the electronic and structural properties of $O_xS_{1-x}Zn$ ternary alloy in cubic phase over a wide range of compositions $0 \leq x \leq 1$ by using the full-potential muffin-tin orbitals (FP-LMTO) method. Various quantities, including lattice parameters, bulk modulus, band gap, optical

bowing and effective masses, were obtained for these alloy.

The organization of this paper is as follows: we explain the FP-LMTO computational method in Section 2. In Section 3, the results and discussion for structural and electronic properties are presented. Finally, a conclusion is given in Section 4.

2. Computational Methods

The calculations reported in this work were carried out by FP-LMTO [4,5] within the density functional theory DFT based on local density Approximation LDA [6] and generalized gradient approximation GGA [7]. In this method the space is divided into an interstitial region (IR) and non-overlapping muffin-tin (MT) spheres centered at the atomic sites. In the IR region, the basis functions are represented by Fourier series. Inside the muffin-tin spheres, the basis sets is described by radial solutions of the one-particle Schrödinger equation (at fixed energy) and their energy derivatives multiplied by spherical harmonics. The valence wave functions inside the spheres are expanded up to $l_{\max} = 6$. The k integration over the Brillouin zone is performed using the tetrahedron method [8]. The values of the sphere radii (MTS) and the number of plane waves (NPLW) used in our calculation are listed in Table 1.

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3. Results and Discussion

3.1. Structural Properties

The calculations were firstly carried out to determine the structural properties of ZB binary compounds ZnS and ZnO and $O_xS_{1-x}Zn$ alloys. To model the $O_xS_{1-x}Zn$ ZB structure alloys, we applied a 8-atom supercell. For the considered structures and at different oxygen concentrations x ($x = 0, 0.25, 0.50, 0.75, 1$), the structural properties were obtained by a minimization of total energy as a function of the volume for ZnS, ZnO and $O_xS_{1-x}Zn$ in the ZB structure. The bulk modulus and their pressure derivatives were obtained by a non-linear fit of the total

energy versus volume according to the Birche-Murnaghan's equation of state [9]. In **Table 2**, we summarize the calculated modulus and their pressure derivatives) of ZnS, ZnO compounds and $O_xS_{1-x}Zn$ alloys. Considering the general trend that the GGA usually overestimates the lattice parameters while LDA is expected to underestimates them [10], It is clear that our results are in reasonable agreement with experimental values and theoretical results. 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 composition x according to the so-called Vegard's law [30].

Table 1. The plane wave number PW, energy cutoff (in Ry) and the muffin-tin radius (RMT) (in a.u.) used in calculation for binary ZnS and ZnO and their alloy in zinc blende (ZB) structure.

Alloy	PW		E_{cut} Total (Ryd)			RMT (u.a.)	
	LDA	GGA	LDA	GGA		This work	Other works
ZnS	5064	12050	111.249	188.482	Zn	LDA 2.144	GGA 2.197
					S	2.232	2.286
$O_{0.25}S_{0.75}Zn$	33400	65266	164.6126	242.7004	Zn	2.078	2.139
					S	2.162	2.226
					O	2.162	2.226
$O_{0.5}S_{0.5}Zn$	33400	65266	177.408	263.309	Zn	2.078	2.053
					S	2.16	2.137
					O	2.162	2.137
$O_{0.75}S_{0.25}Zn$	33400	65266	195.175	286.915	Zn	1.869	1.927
					S	2.02	2.088
					O	2.025	2.088
ZnO	5064	12050	156.454	263.159	Zn	1.993	2.049
					O	1.698	1.745

^aRef. [16], ^bRef. [20].

Table 2. Lattice constants a , bulk modulus B , and pressure derivative of bulk modulus B , for ZB ZnS, ZnO and $O_xS_{1-x}Zn$ solid solutions.

Alloy	Lattice constant a (Å)			Bulk modulus B (Gpa)		
	This work	Exp	Other works	This work	Exp	Other works
ZnS	LDA	GGA		LDA	GGA	
	5.349	5.479	5.409 ^a , 5.465 ^c , 5.338 ^d , 5.458 ^e , 5.336 ⁿ	90.424	79.543	76.9 ^a , 80.573 ^d , 69.353 ^e , 69.62 ^e , 81.2 ⁿ
$O_{0.25}S_{0.75}Zn$	5.182	5.335		86.16	68.369	
$O_{0.5}S_{0.5}Zn$	4.992	5.122		100.128	98.069	
$O_{0.75}S_{0.25}Zn$	4.759	4.907		120.124	94.099	
ZnO	4.511	4.637	4.62 ^b , 4.507 ^k , 4.512 ^f , 4.483 ^g , 4.616 ^h , 4.595 ^{l,m}	175.407	144.825	166 ^f , 157.28 ^g , 125.345 ^h , 156.2 ⁱ , 168 ^j
			4.506 ⁱ , 4.520 ^j			

^aRef. [11], ^bRef. [12], ^cRef. [13], ^dRef. [14], ^eRef. [15], ^fRef. [16], ^gRef. [17], ^hRef. [18], ⁱRef. [19], ^jRef. [20], ^kRef. [21], ^lRef. [22], ^mRef. [23], ⁿRef. [24].

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

where a_{AC} and a_{BC} are the equilibrium lattice constants of the binary compounds AC and BC. 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 constant and the bulk modulus versus concentration for $O_xS_{1-x}Zn$ alloy. A slight large deviation from Vegard's law [30] is clearly visible for the $O_xS_{1-x}Zn$ alloy. The bowing parameter determined by LDA, are obtained by fitting the calculated values respectively, $a(A_xB_{1-x}C)$ is the alloy lattice constant. With a polynomial function we found an upward and down-

ward bowing parameter equal to -0.2359 \AA and 142.9979 GPa for lattice and bulk modulus. The GGA results are -0.2887 \AA and 142.9981 GPa . The physical origin of this slight large deviation could be mainly due to the large size difference between the O and S atom and the mismatch of the lattice constants of ZnS and ZnO compound.

3.2. Electronic Properties

The calculations of the electronic band structure properties, magnitude of band-gap were carried out for ZnS, ZnO and $O_xS_{1-x}Zn$ in ZB structure at the equilibrium calculated lattice constants. The band-gaps calculated using the FP-LMTO method for ZB ZnS, ZnO and $O_xS_{1-x}Zn$ are listed in Table 3 for the high-symmetry

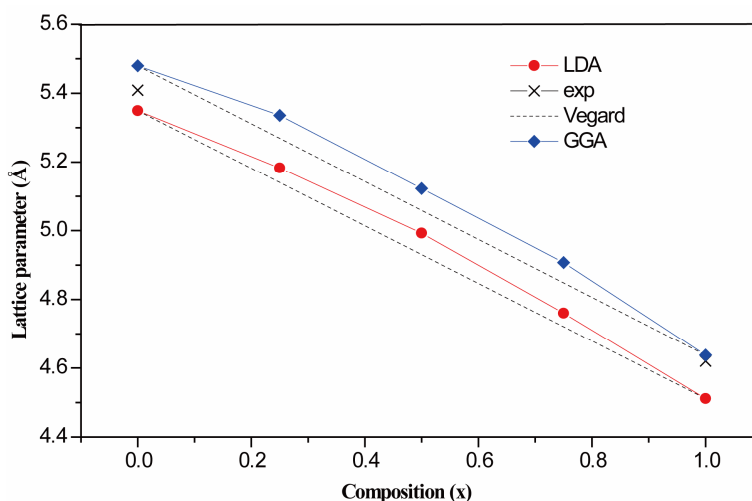


Figure 1. Composition dependence of the calculated lattice constants using the GGA (solid squares) and LDA (solid circles) for $O_xS_{1-x}Zn$ alloy compared with Vegard's law (dashed line).

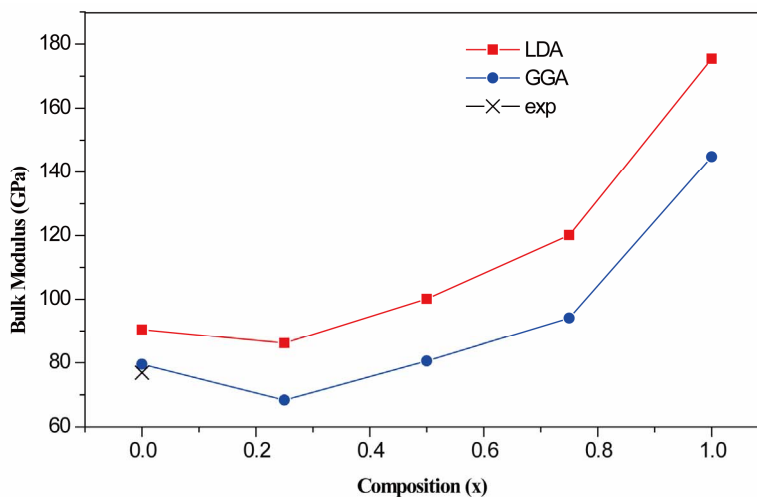


Figure 2. Composition dependence of the calculated bulk modulus using the LDA (solid squares) and GGA (solid circles) of $O_xS_{1-x}Zn$ alloy.

points Γ and X in the Brillouin zone. All energies are with reference to the top of the valence band at Γ point. The results show that ZnS and ZnO compound is a direct-gap semiconductor with the minimum of conduction band at Γ point. The calculated GGA (LDA) energy gaps of ZnS and ZnO E_g are 1.97(2.12) eV and 0.69(0.79) eV, respectively, which are in good agreement with the theoretical values as listed in **Table 3**. Focusing now on the electronic properties of the $O_xS_{1-x}Zn$ alloy system we obtained the direct band-gap at Γ point. **Figure 3** presents the variation of the direct and indirect band gap energies as functions of the composition x for the ternary alloys. We note direct (Γ - Γ) and indirect (Γ -X) band gap not intersect because the computed band structures of the alloys using both LDA and GGA schemes indicate a direct band gap at various concentrations.

Indeed it is a general trend to describe the bandgap of an alloy $A_xB_{1-x}C$ in terms of the pure compound energy gap E_{AC} and E_{BC} by the semi-empirical formula:

$$E_g(x) = xE_{AC} + (1-x)E_{BC} - bx(1-x) \quad (3)$$

where E_{AC} and E_{BC} corresponds to the gap of the ZnO and ZnS for the $O_xS_{1-x}Zn$ alloy. The calculated band gap versus concentration was fitted by a polynomial equation. The results are shown in **Figure 3** and are summarized as follows

$$\begin{aligned} O_xS_{1-x}Zn &\rightarrow \left\{ \begin{array}{l} E_{\Gamma\Gamma} = 2.053 - 1.512x + 0.317x^2 \\ E_{\Gamma X} = 3.353 + 1.832x - 0.148x^2 \end{array} \right\} \text{LDA} \\ O_xS_{1-x}Zn &\rightarrow \left\{ \begin{array}{l} E_{\Gamma\Gamma} = 1.92 - 1.244x + 0.065x^2 \\ E_{\Gamma X} = 3.625 + 0.308x - 1.211x^2 \end{array} \right\} \text{GGA} \end{aligned} \quad (4)$$

In order to better understand the physical origins of the large and composition-dependent bowing in $O_xS_{1-x}Zn$ alloy alloys, we follow the procedure of Bernard and Zunger [31] and decompose the total bowing parameter b into physically distinct contributions. The overall bowing

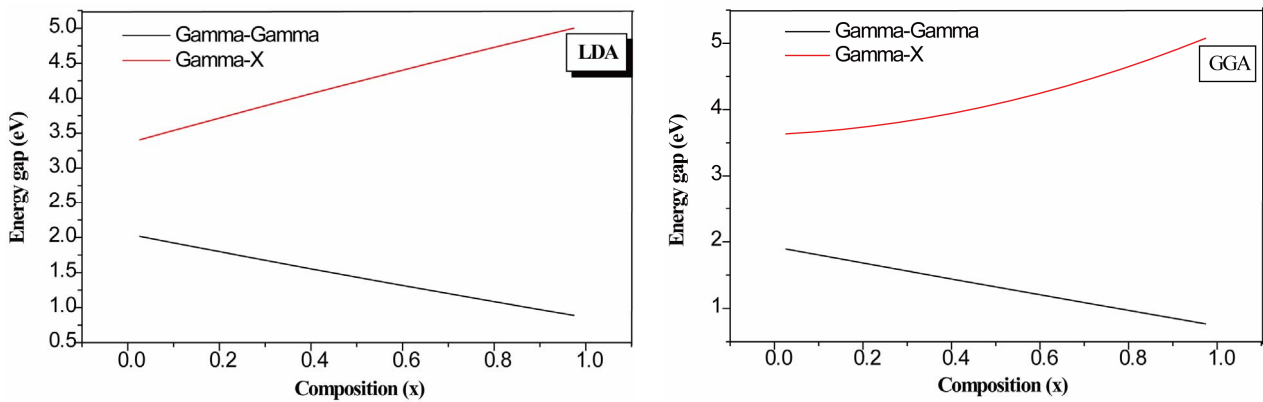


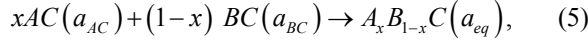
Figure 3. Direct and indirect band gap energies as a function of O composition using the LDA and GGA of $O_xS_{1-x}Zn$ alloy.

Table 3. Direct (Γ - Γ) and indirect (Γ -X) band gaps of ZnS and ZnO and their alloy at equilibrium volume (The energy is given in eV).

Alloy	$\Gamma \rightarrow \Gamma$			$\Gamma \rightarrow X$			
	This work		Exp	Other works	This work		Other works
	LDA	GGA			LDA	GGA	
ZnS	2.12	1.97	3.68 ^a	2.16 ^b , 1.96 ^c , 2.8 ^e 2.37 ^d , 2.792 ^f , 1.953 ^f 1.8745 ^h , 2.1134 ^h , 0.70 ⁱ	3.17	3.47	3.16 ^b , 3.47 ^c , 4.47 ^c
$O_{0.25}S_{0.75}Zn$	1.55	1.52			4.1	4	
$O_{0.5}S_{0.5}Zn$	1.38	1.33			4.44	4.35	
$O_{0.75}S_{0.25}Zn$	0.22	1.12			4.07	3.96	
ZnO	0.79	0.69		0.71 ^e , 0.55 ^e , 1.4 ^e 0.65 ^g , 0.58 ^g , 1.4 ^g 0.6409 ^h , 0.5732 ^h , 3.59 ^j	5.29	5.39	

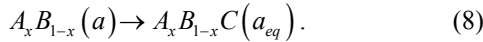
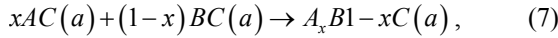
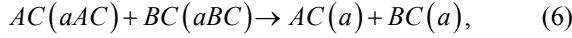
^aRef. [25], ^bRef. [14], ^cRef. [15], ^dRef. [26], ^eRef. [16], ^fRef. [13], ^gRef. [18], ^hRef. [27], ⁱRef. [19], ^jRef. [28].

coefficient at a given average composition x measures the change in band gap according to the formal reaction.



where a_{AC} and a_{BC} are the equilibrium lattice constants of the binary compounds, which a_{eq} is the equilibrium lattice constant of the alloy with the average composition x .

We decompose reaction into three step:



The first contribution, the volume deformation (b_{VD}) represents the relative response of the band structure of the binary compounds AC and BC to hydrostatic pressure. The second contribution, the charge-exchange (CE) contribution b_{CE} , reflects a charge-transfer effect that is due to the different (averaged) bonding behavior at the lattice constant a . The final step measures by b_{SR} , changes due to the structural relaxation (SR) in passing from the unrelaxed to the relaxed alloy. Consequently, the total gap 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 alloys in terms of binary compounds gaps of the, $E_{AC}(a_{AC})$ and $E_{BC}(a_{BC})$, and the total bowing parameter b is

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

where b_{VD} , b_{CE} and b_{SR} represents respectively the volume deformation (VD) effect, the charge exchange (CE) contribution and the structural relaxation (SR) of the alloy according to the following expressions:

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

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

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

The addition of the three contributions (11), (12), and (13) leads to the total bowing parameter b . The computed bowing coefficients b together with the three different contributions for the band gaps as a function of the molar fraction ($x = 0.25, 0.5$ and 0.75) are shown in the **Table 4**. The calculated band gap bowing parameter exhibits a strong composition dependence, as calculated within the GGA and LDA calculations, which show a weakly composition dependent bowing parameter. The variation of

the band gap bowing versus concentration shown in **Figure 4**. The bowing remains linear and Decreases rapidly from $x = 0.25$ to $x = 0.75$ in both approaches (GGA and LDA). The calculated GGA and LDA gap bowing for $O_xS_{1-x}Zn$ alloy ranges from 0.69 eV, 1.25 eV ($x = 0.25$) to -0.59 eV, -0.55 eV ($x = 0.75$), a negligible volume deformation term b_{VD} was registered for $O_xS_{1-x}Zn$ system can be correlated to the large mismatch of the lattice constants of the corresponding binary compounds between ZnS and ZnO . The charge transfer contribution b_{CE} has been found greater than b_{VD} . This contribution is due to the different electronegativities of the O and S or Zn atoms. Indeed, b_{CE} scales with the electronegativity mismatch. The contribution of the structural relaxation b_{SR} is small, the band gap bowing is due essentially charge exchange effect.

Table 4. Decomposition of optical bowing into VD, CE and SR contributions compared with other prediction.

Energy (eV)		This work	
Alloy		LDA	GGA
$O_{0.25}S_{0.75}Zn$	b_{VD}	-1.51	-1.34
	b_{CE}	2.61	1.55
	b_{SR}	0.15	0.47
	b	1.25	0.69
$O_{0.5}S_{0.5}Zn$	b_{VD}	-1.66	-29.51
	b_{CE}	1.71	29.19
	b_{SR}	0.25	0.39
	b	0.29	0.07
$O_{0.75}S_{0.25}Zn$	b_{VD}	-1.83	-165
	b_{CE}	1.02	0.67
	b_{SR}	0.253	0.39
	b	-0.55	-0.5

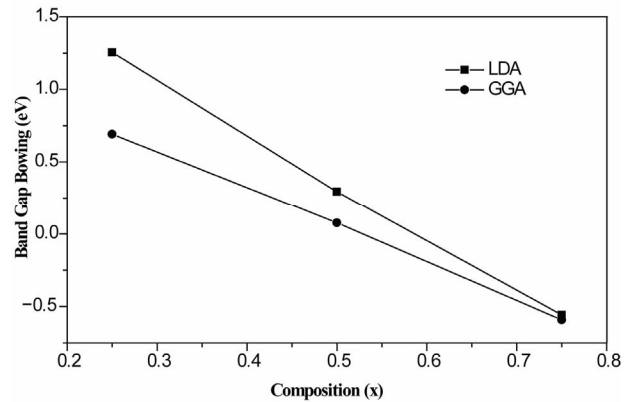


Figure 4. Composition dependence of the calculated band gap bowing parameter using LDA (Solid Square) and GGA (Solid Circle).

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_{hh}^*			m_{lh}^*			
	This work		Exp	Other work		This work	Other work			
	LDA	GGA		LDA	GGA	LDA	GGA			
	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 ^c , 1.272 ^c	0.304	0.305	0.0651 ^b , 0.164 ^c 0.215 ^c , 0.224 ^d 0.188 ^d , 0.188 ^d 0.164 ^c , 0.214 ^c
$O_{0.25}S_{0.75}Zn$	0.229	0.224			2.344	2.891		1.06	1.316	
$O_{0.5}S_{0.5}Zn$								1.031	1.1	
$O_{0.75}S_{0.25}Zn$								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].

3.3. Effective Masses

It is also interesting to discuss at the end of the band structure study the effective masses of electrons and holes, which are important for the excitonic compounds. We have calculated the effective masses of electrons and holes using both LDA and GGA schemes are mentioned in **Table 5**. A theoretical effective mass in general turns out to be a tensor with nine components. However, for a very idealized simple case where $E(k) = \hbar^2 k^2 / 2m^*$ is a parabola at $k = 0$ (high symmetry point Γ) the effective mass becomes a scalar.

4. Conclusion

In summary, we have studied the electronic, structural properties of $O_xS_{1-x}Zn$ alloys by using the FP-LMTO method. We found a slight large deviation from Vegard's law for the lattice constant of $O_xS_{1-x}Zn$. The physical origin of this effect should be mainly due to the significant mismatch between the lattice constants of ZnS and ZnO compounds. Particular attention has been paid to the gap bowing, which exhibits linear behaviour versus the concentration. In addition, we have computed the effective masses of the electron (hole), which increases with the composition x . Our results are compared to other theoretical and experiment values.

REFERENCES

- [1] K. Iwata, P. Fons, A. Yamada, H. Shibata, K. Matsubara, K. Nakahara, T. Takasu and S. Niki, "Bandgap Engineering of ZnO Using Se," *Physica Status Solidi (b)*, Vol. 229, No. 2, 2002, pp. 887-890.
- [2] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," *Physical Review*, Vol. 136, No. 3B, 1964, pp. B864-B871. [doi:10.1103/PhysRev.136.B864](https://doi.org/10.1103/PhysRev.136.B864)
- [3] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," *Physical Review A*, Vol. 140, No. 4A, 1965, pp. A1133-A1138.
- [4] S. Savrasov and D. Savrasov, "Full-Potential Linear-Muffin-Tin-Orbital Method for Calculating Total Energies and Forces," *Physical Review B*, Vol. 46, No. 19, 1992, pp. 12181-12195. [doi:10.1103/PhysRevB.46.12181](https://doi.org/10.1103/PhysRevB.46.12181)
- [5] S. Y. Savrasov, "Linear-Response Theory and Lattice Dynamics: A Muffin-Tin-Orbital Approach," *Physical Review B*, Vol. 54, No. 23, 1996, pp. 16470-16486. [doi:10.1103/PhysRevB.54.16470](https://doi.org/10.1103/PhysRevB.54.16470)
- [6] J. P. Perdew and Y. Wang, "Accurate and Simple Analytic Representation of the Electron-Gas Correlation Energy," *Physical Review B*, Vol. 45, No. 13, 1992, pp. 13244-13249. [doi:10.1103/PhysRevB.45.13244](https://doi.org/10.1103/PhysRevB.45.13244)
- [7] J. P. Perdew, S. Burke and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," *Physical Review Letters*, Vol. 77, No. 18, 1996, pp. 3865-3868. [doi:10.1103/PhysRevLett.77.3865](https://doi.org/10.1103/PhysRevLett.77.3865)
- [8] P. Blochl, O. Jepsen and O. K. Andersen, "Improved Tetrahedron Method for Brillouin-Zone Integrations," *Physical Review B*, Vol. 49, No. 23, 1994, pp. 16223-16233. [doi:10.1103/PhysRevB.49.16223](https://doi.org/10.1103/PhysRevB.49.16223)
- [9] F. D. Murnaghan, "The Compressibility of Media under Extreme Pressures," *Proceedings of the National Academy of Sciences USA*, Vol. 30, No. 9, 1944, pp. 244-247. [doi:10.1073/pnas.30.9.244](https://doi.org/10.1073/pnas.30.9.244)
- [10] A. Mokhtari and H. Akbarzadeh, "Electronic and Structural Properties of β -Be₃N₂," *Physica B: Condensed Matter*, Vol. 324, No. 1-4, 2002, pp. 305-311.

- [doi:10.1016/S0921-4526\(02\)01416-3](https://doi.org/10.1016/S0921-4526(02)01416-3)
- [11] O. Madelung, Ed., "Londolt-Bornstein," New Series III, Vol. 22, Springer, Berlin, 1987.
- [12] W. H. Bragg and J. A. Darbyshire, *Joint Management Entrance Test*, Vol. 6, 1954, p. 238.
- [13] Z. Charifi, F. El Haj Hassan, H. Baaziz, S. Khosravizadeh, S. J. Hashemifar and H. Akbarzadeh, "Structural and Electronic Properties of the Wide-Gap $Zn_{1-x}Mg_xS$, $Zn_{1-x}Mg_xSe$ and $Zn_{1-x}Mg_xTe$ Ternary Alloys," *Journal of Physics: Condensed Matter*, Vol. 17, No. 44, 2005, pp. 7077-7088. [doi:10.1088/0953-8984/17/44/001](https://doi.org/10.1088/0953-8984/17/44/001)
- [14] M. Ameri, D. Rached, M. Rabah, F. El Haj Hassan, R. Khenata and M. Doui-Aici, "First Principles Study of Structural and Electronic Properties of $Be_xZn_{1-x}S$ and $Be_xZn_{1-x}Te$ Alloys," *Physica Status Solidi (B)*, Vol. 245, No. 1, 2006, pp. 106-113. [doi:10.1002/pssb.200743128](https://doi.org/10.1002/pssb.200743128)
- [15] H. Baaziz, Z. Charifi, F. El Haj Hassan, S. J. Hashemifar, and H. Akbarzadeh, "FP-LAPW Investigations of $Zn_{1-x}Be_xS$, $Zn_{1-x}Be_xSe$ and $Zn_{1-x}Be_xTe$ Ternary Alloys," *Physica Status Solidi (B)*, Vol. 243, No. 6, 2006, p. 1296.
- [16] Y. Z. Zhu, G. D. Chen and H. G. Ye, "Electronic Structure and Phase Stability of MgO, ZnO, CdO, and Related Ternary Alloys," *Physical Review B*, Vol. 77, No. 24, 2008. [doi:10.1103/PhysRevB.77.245209](https://doi.org/10.1103/PhysRevB.77.245209)
- [17] D. Maouche, F. S. Saoud and L. Louail, "Dependence of Structural Properties of ZnO on High Pressure," *Materials Chemistry and Physics*, Vol. 106, No. 1, 2007, pp. 11-15. [doi:10.1016/j.matchemphys.2007.05.029](https://doi.org/10.1016/j.matchemphys.2007.05.029)
- [18] A. S. Mohammadi, S. M. Baizae and H. Salehi, "Density Functional Approach to Study Electronic Structure of ZnO Single Crystal," *World Applied Sciences Journal*, Vol. 14, No. 10, 2011, pp. 1530-1536.
- [19] H.-L. Shi and Y. Duan, "Band-Gap Bowing and P-Type Doping of (Zn, Mg, Be)O Wide-Gap Semiconductor Alloys: A First-Principles Study," *The European Physical Journal B*, Vol. 66, No. 4, 2008, pp. 439-444. [doi:10.1140/epjb/e2008-00448-6](https://doi.org/10.1140/epjb/e2008-00448-6)
- [20] B. Amrani, I. Chiboub, S. Hiadi, T. Benmessabih and N. Hamdadou, "Structural and Electronic Properties of ZnO under High Pressures," *Solid State Communications*, Vol. 137, No. 7, 2006, pp. 395-399. [doi:10.1016/j.ssc.2005.12.020](https://doi.org/10.1016/j.ssc.2005.12.020)
- [21] O. Madelung, "Semiconductor: Data Handbook," 3rd Edition, Springer, New York, 2003.
- [22] S.-K. Kim, S.-Y. Jeong and C.-R. Cho, "Structural Reconstruction of Hexagonal to Cubic ZnO Films on Pt/Ti/SiO₂/Si Substrate by Annealing," *Applied Physics Letters*, Vol. 82, No. 4, 2003, p. 562. [doi:10.1063/1.1536253](https://doi.org/10.1063/1.1536253)
- [23] A. Ashrafi and C. Jagadish, "Review of Zincblende ZnO: Stability of Metastable ZnO Phases," *Journal of Applied Physics*, Vol. 102, No. 7, 2007, p. 71101. [doi:10.1063/1.2787957](https://doi.org/10.1063/1.2787957)
- [24] H. Y. Wang, J. Cao, X. Y. Huang and J. M. Huang, "Pressure Dependence of Elastic and Dynamical Properties of Zinc-Blende ZnS and ZnSe from First Principle Calculation," *Condensed Matter Physics*, Vol. 15, No 1, 2012, pp. 1-10.
- [25] H. Okuyama, Y. Kishita and A. Ishibashi, "Quaternary Alloy $Zn_{1-x}Mg_xS_ySe_{1-y}$," *Physical Review B*, Vol. 57, No. 4, 1998, pp. 2257-2263. [doi:10.1103/PhysRevB.57.2257](https://doi.org/10.1103/PhysRevB.57.2257)
- [26] S.-G. Lee and K. J. Chang, "First-Principles Study of the Structural Properties of MgS-, MgSe-, ZnS-, and ZnSe-Based Superlattices," *Physical Review B*, Vol. 52, No. 3, 1995, pp. 1918-1925. [doi:10.1103/PhysRevB.52.1918](https://doi.org/10.1103/PhysRevB.52.1918)
- [27] S. Zh. Karazhanov, P. Ravindrana, A. Kjekhus, H. Fjellvag, U. Grossner and B. G. Svensson, "Electronic Structure and Band Parameters for ZnX ($X = O, S, Se, Te$)," *Journal of Crystal Growth*, Vol. 287, No. 1, 2006, pp. 162-168. [doi:10.1016/j.jcrysgro.2005.10.061](https://doi.org/10.1016/j.jcrysgro.2005.10.061)
- [28] M. Oshikiri and F. Aryasetiawan, "Band Gaps and Quasiparticle Energy Calculations on ZnO, ZnS, and ZnSe in the Zinc-Blende Structure by the GW Approximation," *Physical Review B*, Vol. 60, No. 15, 1999, pp. 10754-10757. [doi:10.1103/PhysRevB.60.10754](https://doi.org/10.1103/PhysRevB.60.10754)
- [29] H. Kukimoto, S. Shionoya, T. Koda and T. Hioki, "Infrared Absorption Due to Donor States in ZnS Crystals," *Journal of Physics and Chemistry of Solids*, Vol. 29, No. 6, 1968, pp. 935-944. [doi:10.1016/0022-3697\(68\)90228-X](https://doi.org/10.1016/0022-3697(68)90228-X)
- [30] L. Vegard, "Formation of Mixed Crystals by Solid-Phase Contact," *Journal of Physics*, Vol. 5, No. 5, 1921, pp. 393-395.
- [31] J. E. Bernard and A. Zunger, "Optical Bowing in Zinc Chalcogenide Semiconductor Alloys," *Physical Review B*, Vol. 34, No. 8, 1986, pp. 5992-5995. [doi:10.1103/PhysRevB.34.5992](https://doi.org/10.1103/PhysRevB.34.5992)