

Accurate, Calculated Electronic and Related Properties of Zinc Blende ZnSe

Moussa Diawara¹, Yacouba Issa Diakite¹, Yuriy Malozovsky², Diola Bagayoko^{2*}

¹Department of Physics, College of Sciences and Techniques, University of Sciences, Techniques, and Technologies of Bamako (USTTB), Bamako, Mali

²Department of Mathematics and Physics, Southern University and A & M College in Baton Rouge (SUBR), Baton Rouge, Louisiana, USA

Email: *bagayoko@aol.com

How to cite this paper: Diawara, M., Diakite, Y.I., Malozovsky, Y. and Bagayoko, D. (2026) Accurate, Calculated Electronic and Related Properties of Zinc Blende ZnSe.

Journal of Modern Physics, 17, 1229-1244.

<https://doi.org/10.4236/jmp.2026.1710054>

Received: July 14, 2026

Accepted: October 5, 2026

Published: October 8, 2026

Copyright © 2026 by author(s) and

Scientific Research Publishing Inc.

This work is licensed under the Creative

Commons Attribution International

License (CC BY 4.0).

<http://creativecommons.org/licenses/by/4.0/>



Open Access

Abstract

Presently known technological applications of ZnSe-based devices partly motivated this study which illustrates how one can perform accurate calculations of properties of semiconductors in the framework of density functional theory (DFT). Unlike numerous, previous DFT results, ours for ZnSe are in agreement with available, corresponding experimental findings. In particular, our calculated band gap of 2.65 eV is in excellent agreement with experiment. In addition to the band structure, we also report the calculated eigenvalues at high symmetry points, the total and partial densities of states, and the curve of the total energy versus the lattice constant. We employed a local density functional approximation (LDA) potential and the linear combination of Gaussian orbitals. As explained below, the use of successively augmented basis sets, starting with the minimum basis set or one slightly larger, to perform self-consistent calculations leads to a generalized minimization of the energy content of the Hamiltonian down to the absolute minima of the occupied energies, *i.e.*, the ground state. This process guarantees that our calculations strictly adhere to the two DFT theorems and produce results that possess the full physical content of DFT and agree with experiment.

Keywords

BZW-EF Method, Self-Consistent, Ground State, Basis Sets

1. Introduction

ZnSe (zinc selenide) is a II - VI binary semiconductor that crystallizes predominantly in the cubic zinc-blende structure [1]-[4]. It is characterized by a direct band gap located at the Γ point of the Brillouin zone. It has a wide band gap and

remarkable optoelectronic properties. The measured room-temperature band gap of ZnSe is 2.60 - 2.72 eV [5]-[7], while the low-temperature value is reported to be 2.82 eV [8]. ZnSe has attracted considerable attention for applications in blue and near-ultraviolet light-emitting diodes (LEDs), semiconductor lasers, photodetectors, and photovoltaic devices [6] [7]. The importance of its technological applications makes it an extensively studied semiconductor, both theoretically and experimentally [9]-[12].

A thorough understanding of the electronic properties of ZnSe is essential for optimizing its performance in technological applications. Fundamental parameters such as the electronic band structure, density of states (DOS), the magnitude and nature of the energy gap, and the orbital contributions to the valence and conduction bands play a crucial role in determining its optical and electrical properties [10] [13]-[16].

Several sources have reported results of experimental studies of ZnSe as indicated in **Table 1**.

Table 1. Experimental measurements of the band gap of ZnSe.

Experimental works	Eg (eV)
Optical absorption/PL (RBS); (XRD) and (SEM)	2.6 - 2.72 [13] [14] [16] at (300 K)
Optical absorption/spectroscopy (TEM); UV-Vis-NIR and FT-IR	2.58 [15] at (300 K)
Transmission Spectroscopy measurements	2.763 [17] at (273 K)
Wavelength-modulated spectra	2.70 [8] at (295 K)
Extrapolated Model-Solid Approach [delete if for hexagonal]	2.82 [18] at (low T)

Theis [17] focused on the electronic band structure and critical optical transitions in II - VI semiconductors, emphasizing the effect of spin-orbit coupling on the valence bands and providing a theoretical basis for interpreting the fine optical properties of ZnSe. He observed a direct gap of 2.76 eV. Venkatachalam *et al.* [13] deposited ZnSe thin films via vacuum evaporation. X-ray diffraction confirmed a polycrystalline zinc-blende structure and optical measurements indicated a direct gap of 2.6 - 2.72 eV. Electrical measurements revealed thermally activated semiconductor behavior. Furthermore, Thirumavalavan *et al.* [14] extended the analysis using chemical bath deposition (CBD) and also examined morphological and dielectric properties. The measured direct gap was 2.65 eV, slightly lower than the one for evaporated films. Differences in film thickness and microstructure likely explain the small variations of the gap.

Ebina *et al.* [16] measured the E_0 and $E_0 + \Delta_0$ transitions as a function of x and

observed band-gap bowing, *i.e.*, a nonlinear dependence of the gap on composition. Homann *et al.* [10] combined optical measurements and simulations to confirm the band gap bowing, providing a predictive model for designing semiconductors with tailored gaps.

From the content of the table, we conclude that zinc blende ZnSe exhibits a large direct band gap of 2.60 to 2.76 eV, depending on film thickness, deposition method, and microstructure.

In addition to the experimental works reported above, numerous theoretical studies of ZnSe have been performed. Some of them utilized ab-initio LDA or GGA potentials in first-principles calculations. Unlike the above experiments, the ab-initio calculations report different band gaps which woefully underestimate the measured ones. We do not elaborate on theoretical results obtained with ad hoc potentials, *i.e.*, those not resulting from the functional derivative of an exchange-correlation energy. In addition to the hybrid ones, these ad hoc potentials include those obtained by adding or subtracting Hubbard's U or other quantities to ab-initio LDA or GGA potentials.

Ghaleb *et al.* [19] studied the structural, electronic, and optical properties of cubic ZnSe in the sphalerite phase using density functional theory (DFT). They used an ab-initio LDA potential and the calculated band gap of ZnSe was 1.33 eV. Optical properties derived from the dielectric function indicate strong absorption in the ultraviolet region, highlighting the suitability of ZnSe for optoelectronic applications. Asadi *et al.* [20] employed the full-potential linearized augmented plane wave (FP-LAPW) formalism and reached a band gap value of 1.17 eV. Jafarova *et al.* [11] utilized the local spin density approximation (LSDA) and found 1.57 eV for the band gap of ZnSe. Calculations employing ad-hoc DFT potentials do not have predictive capability; their results vary with the number and nature of the adjustable parameters employed in the construction of the ad-hoc potential.

Other results obtained with generalized gradient approximation (GGA) potentials, as shown in **Table 2**, are either underestimates or overestimates of the band gap of ZnSe. The full potential linearized augmented plane wave plus local orbitals approach (FP-LAPW + lo) that obtained a gap of less 2 eV [21] [28] employed an additional potential besides that of Perdew-Burke-Ernzerhof (PBE). The use of the ab-initio PBE plus the Hubbard (PBE + U) produced a band gap of 2.5 eV [25]. While this value is close to the experimental one of 2.65 eV, PBE + U is an ad-hoc potential with no fully predictive capability. The Heyd-Scuseria-Ernzerhof 2006 (HSE06) hybrid functional is a DFT approach that includes a fraction of the exact Hartree-Fock exchange; it leads to an improved accuracy of band gap calculations compared to the mainstream ones that employed LDA or GGA functionals. The calculations with hybrid potentials obtained gaps of 2.0 - 2.85 eV [13] [19] [20], with the upper limit in agreement with the low-temperature experimental value of 2.82 eV [8]. Like PBE + U ones, hybrid potentials are essentially ad-hoc, with limited predictive capability due to the dependence of the output on the construction of the potential.

Table 2. Previous, calculated band gaps (Eg in eV) of ZnSe reported in the literature.

Computational Formalism	Potentials (DFT and Other)	Eg (eV)
Plane-wave pseudopotential	LDA	1.33 [19]
Full-Potential Linear Augmented Plane Wave (FP-LAPW)	LDA	1.17 [20]
Atomistix ToolKit code	LSDA	1.57 [11]
Plane-wave pseudopotential	GGA	<2.00 [21]
Full Potential Linearized Augmented Plane Wave plus Local Orbitals approach (FP-APW + LO)	GGA	<2.00 [22]
Plane-wave pseudopotential	GGA	1.22 [23]
Plane-wave pseudopotential	GGA	1.34 [19]
Full-Potential Linear Augmented Plane Wave (FP-LAPW)	GGA	<2 [24]
Projected augmented wave	PBE	2.56 [25]
Hybrid-functional and quasi-particle	PBE, PBE + U, and Hybrid HSE	1.70 [24]
Projector augmented plane wave (PAW)	GGA-GW	2.23 [26]
	PBE-PBE + U	2.0 - 2.85 [24]
	GGA + U	1.37 [23]
Plane-wave pseudopotential	Potential Variation Mixed Basis (PVMB)	1.45 [26]
Atomistix ToolKit code		2.7 [11]
Empirical pseudopotential method	LSDA + U	2.77 - 3.0 [15]
		[27]

For this reason, these results, while very useful, do not resolve the fundamental question of the serious band-gap underestimation by most mainstream DFT calculations using ab initio LDA or GGA potentials. With several fitting parameters, the empirical pseudopotential calculations shown in **Table 2** led to the correct room-temperature experimental band gap of ZnSe.

The above overview of the literature points to the need for our work. Indeed, numerous, calculated values of the band gap disagree with corresponding, experimental ones. The disagreement between sets of calculated band gaps, as evident above and in **Table 2**, adds to our motivation for this work. At the outset, we must answer the question of why our LDA calculations are expected to yield an accurate description of the electronic and related properties of ZnSe. Past, accurate descriptions and predictions [28] of semiconductor properties, using the distinctive features of our calculations, portend the same for ZnSe. This distinctive feature, the

Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), strictly adheres to the conditions of validity of DFT as elucidated by Bagayoko [29].

We are aware of some explanations of the failures of many previous calculations to lead to correct values of the band gaps of semiconductors or insulators. Prominent among them are the self-interaction [30] and the derivative discontinuity [31]-[33] of the exchange correlation energy. Bagayoko [29], using strictly DFT theorems and the Rayleigh theorem for eigenvalues, demonstrated that self-consistent calculations that do not adhere to well-defined, intrinsic features of DFT cannot claim to produce eigenvalues and other quantities that possess the full, physical content of DFT. Hence, disagreements between their results and experiment may arise mostly from the fact that their findings do not fully possess the physical content of DFT. Our perusal of the articles that reported the results in **Table 2** did not lead to any indication that these calculations adhered totally to these features of DFT: Specifically, we could not find any calculation that methodically searched for and verifiably attained the absolute minima of the occupied energies, using increasingly larger basis sets [29] [34] [35], *i.e.*, basis sets such that, except for the first, smaller one, each basis set is entirely included in the one immediately following it. The point here is that popular explanations of band gap underestimation by DFT calculations notwithstanding, our distinctive computational method is likely to describe ZnSe accurately. The rest of this paper is organized as follows.

This section, devoted to the introduction, is followed by a fuller description of our computational method, in Section 2. We subsequently present our results in Section 3 and discuss them in Section 4. Section 5 provides a short conclusion.

2. Method and Computational Details

More details about our computational approach are available in previous articles [29] [36]-[43]. We used the Ceperley and Alder LDA potential [44] with the parameterization of Vosko and his group [45], the linear combination of atomic orbitals (LCAO), and the BZW method, as enhanced by Ekuma and Franklin (BZW-EF) [46]. Both the BZW and BZW-EF employ successive augmentation of the initial, small basis set, by one orbital at a time, to execute several self-consistent calculations. The difference between the BZW and BZW-EF methods follows. In the BZW method, the basis set is augmented by adding orbitals in the order of increasing, unoccupied energies (in atomic or ionic species). As explained by Bagayoko [29], in systems with two or more atoms, the polarization orbitals p , d and f has primacy over the spherical symmetry of s orbitals, for the valence electrons; In the BZW-EF method, a basis set is augmented in such a way that, for any principal quantum number n , the p , d , and f orbitals, when applicable, are added in that order before the corresponding s orbital of that quantum number. An orbital is applicable if it is occupied by at least one electron in one of the atomic or ionic species.

We used a computer program developed at the US Department of Energy's Ames Laboratory in Iowa to perform non-relativistic calculations. We first performed the self-consistent calculations of the electronic energies for the atomic or ionic species in the material being investigated. These species are Zn^{2+} and Se^{2-} . Our choice was based on the results of preliminary calculations for ZnSe using neutral atoms. The preliminary results showed a transfer of approximately two electrons from Zn to Se. We subsequently performed ab-initio, self-consistent calculations to determine the atomic basis sets to be used in the solid-state calculations for ZnSe.

If two consecutive calculations lead to the same occupied energies, these energies belong, at least, to a local minimum. If the next, consecutive calculations reproduces the same occupied energies, then the absolute minimum energies, *i.e.*, the ground state, have been reached. Otherwise, the augmentation and calculations continue. The necessary and sufficient criterion for stopping the computation is to have three consecutive calculations that produce identical, occupied energies.

In accordance with the above, our calculations necessarily begin with a small basis set which accommodate all the electrons of the system under study. Calculation II follows, with a basis set comprising that of Calculation I plus an orbital representing an excited state. We compare the occupied energies of the two self-consistent calculations: invariably, some occupied energies from calculation II are lower than their corresponding values from calculation I. We augment the basis set of calculation II, with an orbital, to perform calculation III. We compare the occupied energies from calculations II and III. We continue this process until three consecutive calculations produce the same occupied energies, indicating that we reached the ground state. Among these last three (3) consecutive calculations, only the first, which has the smallest of the three basis sets, provides the DFT description of the ground state of the material [37]-[43]. The basis set for this calculation is the optimal one. The *optimal basis* set, once self-consistency is achieved, leads to the ground state charge density of the material. The use of basis sets which are larger than the optimal one, and which contain the optimal one, lead to the ground state energies and to the ground state charge density upon reaching self-consistency. As explained by our group in the publications referenced above and others, the use of these larger basis sets also lowers some unoccupied energies: these lowered unoccupied energies are not due to a physical interaction in the Hamiltonian which does not change from its value obtained with the optimal basis set. Incidentally, since the occupied energies do not change once, we reach the optimal basis set, the further lowering of some unoccupied energies because of the use of larger basis sets containing the optimum is one plausible explanation of the almost universal underestimation of band gaps and energy gaps by mainstream calculations [29] [36]-[43]. Indeed, these calculations, to date, have used a single basis set which was deliberately chosen to be large in order to ensure completeness. Some of these basis sets were likely over-complete for the

description of the ground state [29]. In the absence of a verifiable attainment of the ground state, many of these single basis sets were likely incomplete. The central point in LCAO calculations using ab-initio DFT potentials is the following. Any reasonable basis set can produce self-consistent results for the accurate description of stationary states. There exists an infinite number of such states. So, unless a DFT calculation verifiably attains the ground state, as described above, its results cannot possess the full, physical content of DFT.

The key computational details necessary for reproducing this work are provided below. Gaussian functions are in the radial parts of atomic wave functions. We employed a set of even-tempered Gaussian exponents, with a minimum of 0.148 and a maximum of 0.93061×10^5 in atomic units, for Zn^{2+} . Nineteen (21) Gaussian functions were used for s and p orbitals, and 20 for d orbitals. Likewise, to describe Se^{2-} , the exponents in Gaussian functions ranged from 0.125 to a maximum of 0.8×10^5 . The numbers of Gaussian functions for s and p orbitals are 21 and that of the d orbitals is 20. A mesh of 60 k -points, with appropriate weights in the irreducible Brillouin zone, was used in the iterations for self-consistency. The error in calculating the valence charge was -0.0027647 for 44 electrons, or -6.28×10^{-5} per electron. The convergence criterion of the iterations is to have a difference not greater than 10^{-5} between the values of the potentials for two consecutive iterations. The number of iterations for this convergence was around 60. With the method described above and the associated calculation details, we studied ZnSe as presented below.

3. Results and Discussions

We show the basis sets for the successive calculations in **Table 3**. Columns 1, 2 and 3 of the table indicate respectively the number of a calculation, the valence state orbitals for Zn^{2+} and the valence state orbitals for Se^{2-} . Columns 4 and 5 show the total number of valence functions and the direct band gap calculated at the Γ point, respectively. In this table, the occupied energies from calculations III, IV, V, and VI are identical. Therefore, Calculation III provides the DFT description of ZnSe, in accordance with the above description of our method.

Table 3. The successive, self-consistent calculations of the BZW-EF method for ZnSe.

Calculation number	Trial functions for valence states of Zn^{2+}	Trial functions for valence states of Se^{2-}	No of Valence functions	Band Gap at Γ (in eV)
I	$3s^23p^63d^{10}4s^1$	$3s^23p^63d^{10}4s^24p^5$	46	2.0417
II	$3s^23p^63d^{10}4s^14p^0$	$3s^23p^63d^{10}4s^24p^5$	52	2.6493
III	$3s^23p^63d^{10}4s^14p^0$	$3s^23p^63d^{10}4s^24p^54d^0$	62	2.6504
IV	$3s^23p^63d^{10}4s^14p^04d^0$	$3s^23p^63d^{10}4s^24p^54d^0$	72	2.6365
V	$3s^23p^63d^{10}4s^14p^04d^0$	$3s^23p^63d^{10}4s^24p^54d^05p^0$	78	2.6311
VI	$3s^23p^63d^{10}4s^14p^04d^05p^0$	$3s^23p^63d^{10}4s^24p^54d^05p^0$	84	2.6409

In particular, the occupied energies from this calculation are those for the ground state of the material. The resulting charge density is that of the ground state of ZnSe.

The total number of valence functions and the resulting band gaps at the Γ point, for each calculation, are also listed. As per the BZW-EF method, in going from one calculation to the next, one orbital is added to the basis set of the former. We see the progressive increase in the size of the basis set from one calculation to the next.

The generalized minimization of the occupied energies requires the described successive calculations with augmented basis sets. The calculations stopped at VI because Calculations III, IV, V, and VI produced identical occupied energies, *i.e.*, the ground state. **Figure 1** illustrates the overall lowering of the occupied energies as the size of the basis set is augmented. **Figure 2** shows that Calculation III and VI produced the same occupied energies. Calculation VI and V led to the same occupied energies as Calculation III, establishing that the occupied energies from Calculation III represent the ground state of the system.

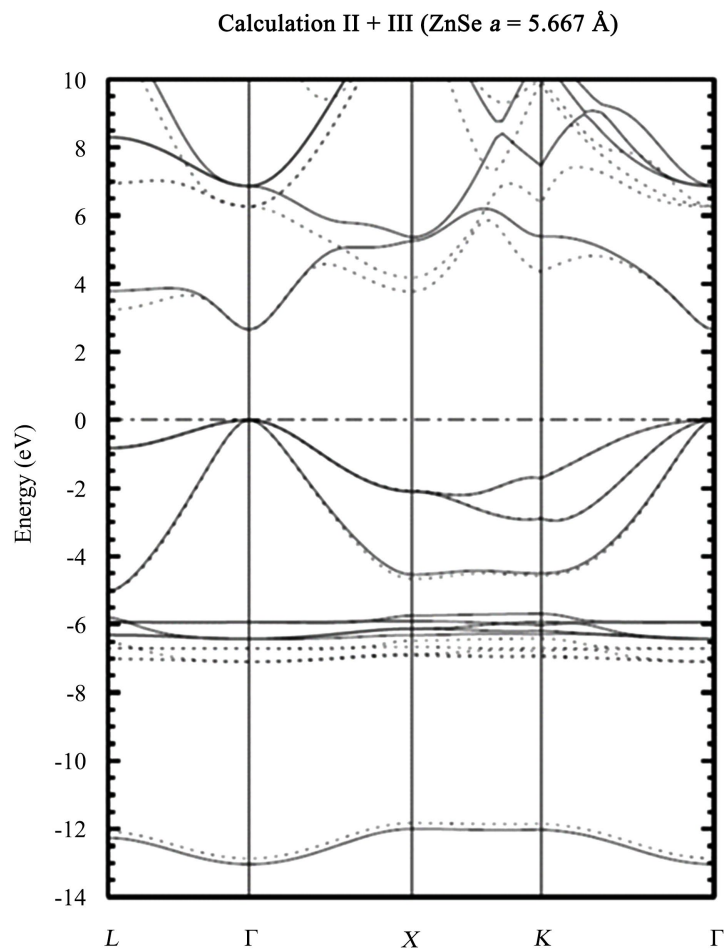


Figure 1. Electronic energy bands of cubic ZnSe from Calculation II (solid Lines) and Calculation III (dashed lines), upon setting the Fermi level to zero; this level is indicated by the horizontal dashed-dotted line.

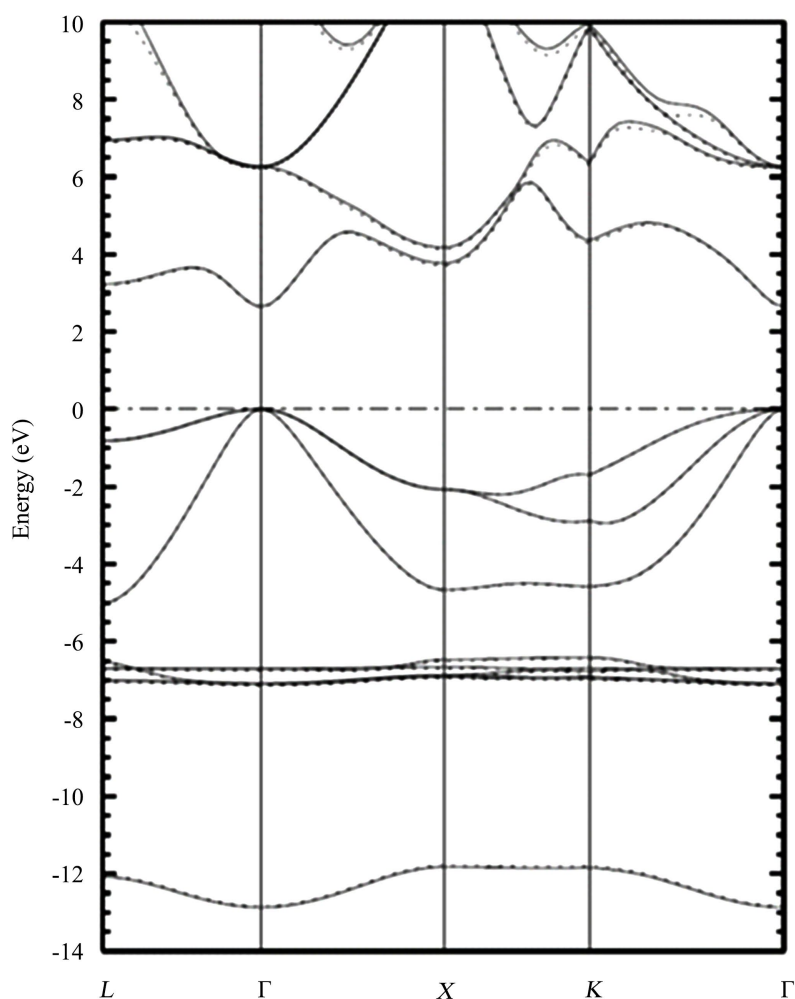
Calculation III + IV (ZnSe $a = 5.667 \text{ \AA}$)

Figure 2. Electronic energy bands of cubic ZnSe from Calculations III (solid lines) and IV (dashed lines), upon setting the Fermi level to zero; this level is indicated by the horizontal dashed-dotted line.

For all the six calculations (I - VI), the valence band maximum and the conduction band minimum are located at the same Γ point, as expected for a cubic crystal structure. Consequently, ZnSe is a direct band gap material. As illustrated above in **Figure 1** and **Figure 2**. The calculated band gap, from Calculation III, is 2.65 eV; this value is in excellent agreement with the experimental ones of 2.60 - 2.70 eV, at room temperature [10]-[12].

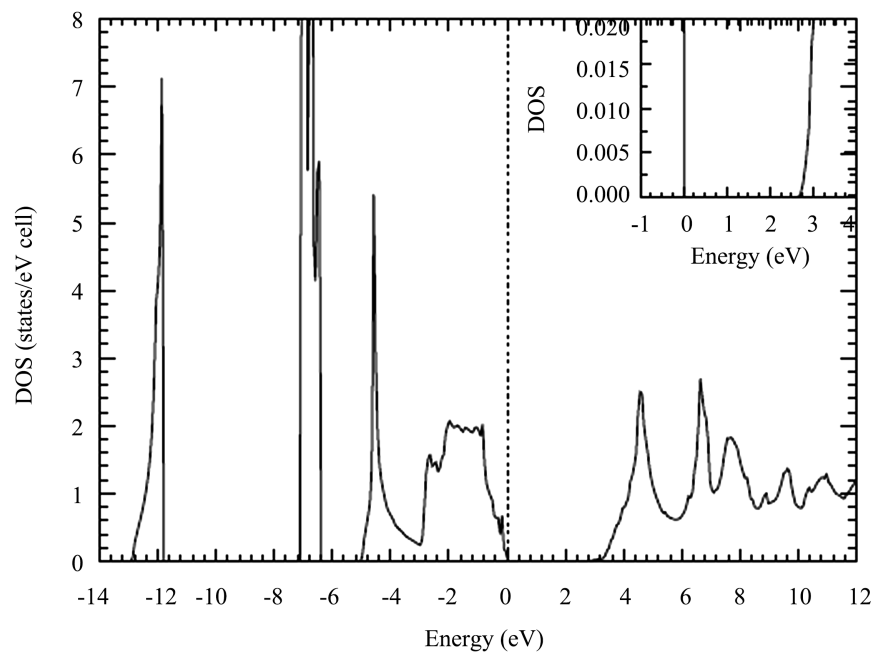
The basis set for Calculation III is the *optimal basis* set, *i.e.*, the smallest basis set that leads to the ground state charge density upon reaching self-consistency.

Table 4 exhibits the calculated eigenvalues at high symmetry points in the Brillouin zone. They permit detailed comparisons with features of X-ray and ultra-violet spectroscopy findings relative to the width of a band, inter-band transition energies, and the dominant states at the Fermi level or at the minimum of the conduction band.

Table 4. Calculated eigenvalues (in electron volts-eV) for zinc blende Zinc Selenide at high symmetry points in the Brillouin zone.

<i>L</i> -point	Γ -point	<i>X</i> -point	<i>K</i> -point
13.7067	12.1151	12.3450	10.5828
11.3028	6.2665	12.0196	9.9474
6.9430	6.2665	12.0196	9.8658
6.9430	6.2665	4.1791	6.3590
3.2305	2.6504	3.7666	4.3530
-0.8198	0.0000	-2.0757	-1.6985
-0.8198	0.0000	-2.0757	-2.8825
-5.0072	0.0000	-4.6643	-4.5810
-6.5356	-6.7052	-6.4733	-6.4143
-6.6932	-6.7052	-6.6575	-6.6834
-6.6932	-7.0935	-6.8769	-6.7805
-7.0099	-7.0935	-6.8769	-6.9101
-7.0099	-7.0935	-6.9245	-6.9582
-12.090	-12.8699	-11.8277	-11.8479

We show the total (DOS) and partial (PDOS) densities of states in **Figure 3** and **Figure 4**, respectively. We subsequently report the total energy curve, the equilibrium lattice constant, and the bulk modulus. The total density of state (DOS) and the partial ones (pDOS) were obtained using the bands from Calculation III.

**Figure 3.** Total density of states (DOS) of ZnSe, as derived from the bands from Calculation III. The vertical dashed indicates the position of the Fermi level. The insert panel is the magnified DOS near the band gap.

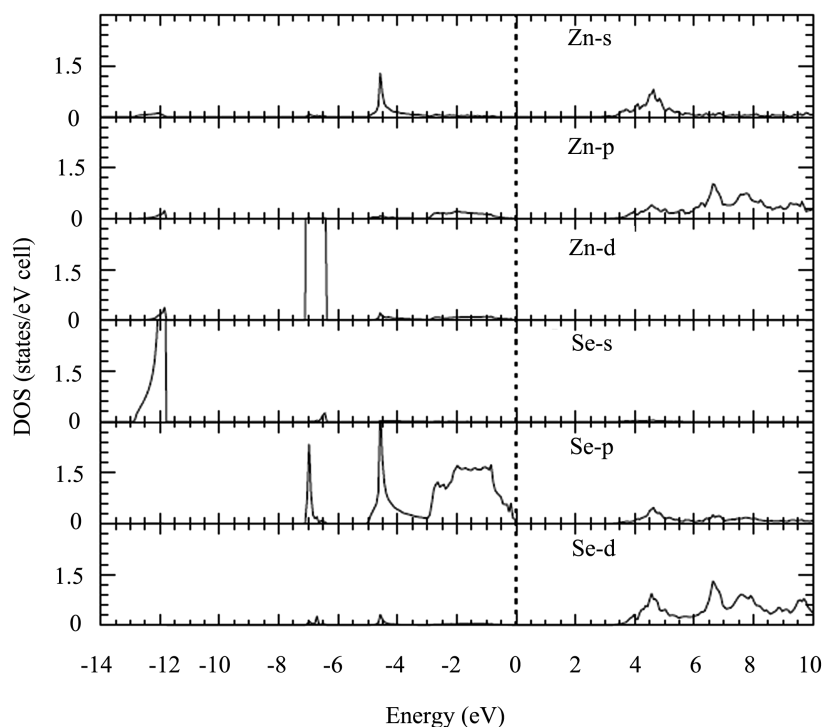


Figure 4. Partial densities of states (PDOS) of ZnSe, as derived from ground state band structure from Calculation III. The vertical dashed line indicates the position of the Fermi level.

The inset in **Figure 3** shows an enlarged view of the DOS near the absorption edge, with a magnification factor of 26.

Figure 4 shows the partial densities of states (PDOS) for the s, p, and d states of Zn and the s, p, and d states of Se, respectively. According to the content of **Figure 4**, the valence band of ZnSe is mainly dominated by the Se-p states near the Fermi level. The structure in the energy range from -13 to -11 eV is mainly due to the Se-s state, with relatively tiny contributions from Zn s, p, and d states. The upper group of valence bands is formed predominantly by hybridization of Se-p states with much weaker contributions from Zn orbitals. The minimum of the conduction band is mainly made up of 4s states of the Zn cation.

The total energy as a function of the lattice parameter is shown in **Figure 5**. The minimum total energy is obtained for a lattice parameter of $5.47 \text{ \AA}$, which corresponds to the calculated equilibrium lattice constant. The range of lattice parameters over which the total energy values were calculated extends from $5.37 \text{ \AA}$ to $5.57 \text{ \AA}$. To determine the bulk modulus, the first step consisted of obtaining a least-square fit of the total energy curve in the vicinity of its minimum. The bulk modulus is then obtained from the second derivative of this fitted curve at the equilibrium lattice constant. It is generally determined from the fitting of the energy-volume curve using an equation of state according to $B = V \frac{\partial^2 E}{\partial V^2}$. The bulk modulus is a physical quantity that characterizes the resistance of a material

to uniform compression. Our calculated value is 59.20 GPa. This value is not far from the experimental result we found of 62.4 GPa [47]-[49]; it is slightly higher than a previous, theoretical value of 57.30 GPa [28].

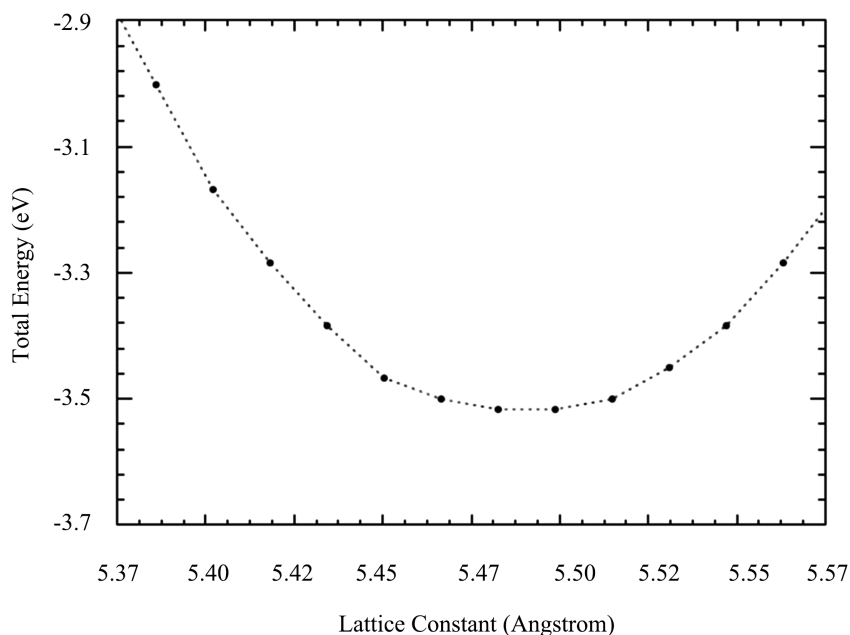


Figure 5. The total energy versus the lattice constant for the zinc blende ZnSe, obtained from calculations employing the optimal basis set.

4. Conclusion

We have presented electronic and related properties of ZnSe, obtained with an abinitio density functional theory (DFT) potential. ZnSe is among Important semiconductors with a multitude of applications. Unlike previous DFT calculations that led to underestimating the measured band gap, our results fully agreed with experiment without invoking a correction for self-interaction or derivative discontinuity of the exchange-correlation energy. This feat is credited to the strict adherence of our calculations to the two foundational theorems of DFT. In particular, we kept the total number of particles constant, and we successively augmented the initial, small basis set to lower the occupied energies down to the ground state.

Acknowledgements

The authors gratefully acknowledge the financial and institutional support provided by the U.S. Fulbright Fellowship Program (Program #G-10005 PS00383052), the Malian Ministry of Higher Education and Scientific Research, and the U.S. National Science Foundation (NSF Award No. HRD-2009765). The computational resources used in this work were provided by the Louisiana Optical Network Initiative (LONI). The authors also thank Southern University and A & M College and Louisiana Space Grant Consortium (LaSPACE) for their valuable support in

conducting this research.

Author Contributions

The respective contributions of the authors follow. Dr. Moussa Diawara performed the calculations and drafting the manuscript. Dr. Malozovsky guided Dr. Diawara in the running of our program package and assisted Dr. Diawara with some graphs. Dr. DIAKITE conducted a thorough search of the literature to provide most of the references cited in the manuscript. He also contributed to the finalization of the manuscript and to its submission to JMP. Dr. Bagayoko guided the overall effort and the editing of the draft manuscript. He is the director of the High-Performance Computer Laboratory where the calculations were done. He also handles the payment of the publication cost for the accepted manuscript.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- [1] Shobana, M. and Meher, S.R. (2018) Experimental and *Ab-Initio* Study of the Structural, Electronic and Vibrational Properties of ZnTe. *Journal of Alloys and Compounds*, **762**, 260-271. <https://doi.org/10.1016/j.jallcom.2018.05.208>
- [2] Taoufiq, M., Soussi, A., Brahim, I.A., Ou-khouya, A., boutagount, S., Elfanaoui, A., et al. (2025) Optical, Electronic, Morphological, and Structural Properties of Zn_{1-x}Cu_xSe Thin Films Deposited by Electrodeposition: A Combined DFT Calculation and Experimental Study. *Materials Science and Engineering: B*, **321**, Article ID: 118549. <https://doi.org/10.1016/j.mseb.2025.118549>
- [3] Zuo, H., Zhang, Y., Du, G., Ding, C. and Feng, G. (2025) First Principles Study of Structural and Electronic Properties of Single and Double-Walled ZnSe Nanotubes, toward the Photocatalyst Application. *Physical Chemistry Chemical Physics*, **27**, 11119-11128. <https://doi.org/10.1039/d5cp00704f>
- [4] Khurshid, N., Chaudhary, K., Imran, M., Tariq, M., Haider, Z. and Ashfaq Ahmad, M. (2026) Enhanced Quantum Capacitance and Metallic Transition in Mn-Doped ZnSe: A Route to High-Performance Electrodes. *Optical and Quantum Electronics*, **58**, Article No. 386. <https://doi.org/10.1007/s11082-026-08985-z>
- [5] Kleider, J. (2012) Band Lineup Theories and the Determination of Band Offsets from Electrical Measurements. In: Sark, W.G.J.H.M., et al., Eds., *Physics and Technology of Amorphous-Crystalline Heterostructure Silicon Solar Cells*, Springer, 405-444. https://doi.org/10.1007/978-3-642-22275-7_12
- [6] Srivastava, V., Chauhan, R.K., Pandey, A., Mishra, V.L., Mitharwal, C., Bajpai, R.S., et al. (2025) Enhanced Sensitivity of Photodetectors with ZnSe as Electron Transport Layer and Cz-Pyr as Hole Transport Layer. *Journal of Physics and Chemistry of Solids*, **203**, Article ID: 112712. <https://doi.org/10.1016/j.jpcs.2025.112712>
- [7] Yin, J. and Zhang, X. (2021) The Investigation of Sn Heavily Doped ZnSe for Promising Intermediate Band Materials. *Journal of Physics and Chemistry of Solids*, **152**, Article ID: 109951. <https://doi.org/10.1016/j.jpcs.2021.109951>
- [8] Van de Walle, C.G. (1989) Band Lineups and Deformation Potentials in the Model-Solid Theory. *Physical Review B*, **39**, 1871-1883. <https://doi.org/10.1103/physrevb.39.1871>

- [9] Jafarova, V.N., Rzayeva, S., Abdurahmanova, U., Aliyev, M.E., Scurtu, I., Popa, C., et al. (2026) Spintronic Potential of ZnSe Doped with 3d Transition Metals: Insights from First-Principles Calculations. *Indian Journal of Physics*, **100**, 509-523. <https://doi.org/10.1007/s12648-025-03794-8>
- [10] Homann, T., Hotje, U., Binnewies, M., Börger, A., Becker, K. and Bredow, T. (2006) Composition-Dependent Band Gap in $\text{ZnS}_x\text{Se}_{1-x}$: A Combined Experimental and Theoretical Study. *Solid State Sciences*, **8**, 44-49. <https://doi.org/10.1016/j.solidstatesciences.2005.08.015>
- [11] Jafarova, V., Eminova, V. and Hashimova, N. (2025) First-Principles Study of Electronic and Magnetic Properties of Cr-, Fe-, and Ni-Doped ZnSe Supercells. *Gazi University Journal of Science*, **38**, 1388-1402. <https://doi.org/10.35378/gujs.1553238>
- [12] Jafarova, V.N. and Musaev, M.A. (2023) First-Principles Study of Structural and Electronic Properties of ZnSe with Wurtzite Structure. *Technium: Romanian Journal of Applied Sciences and Technology*, **6**, 42-46. <https://doi.org/10.47577/technium.v6i.8487>
- [13] Venkatachalam, S., Mangalaraj, D., Narayandass, S.K., Kim, K. and Yi, J. (2005) Structure, Optical and Electrical Properties of ZnSe Thin Films. *Physica B: Condensed Matter*, **358**, 27-35. <https://doi.org/10.1016/j.physb.2004.12.022>
- [14] Thirumavalavan, S., Mani, K. and Sagadevan, S. (2016) A Study of Structural, Morphological, Optical and Electrical Properties of Zinc Selenide (ZnSe) Thin Film. *Materials Today: Proceedings*, **3**, 2305-2314. <https://doi.org/10.1016/j.matpr.2016.04.141>
- [15] Liang, W.Y. and Yoffe, A.D. (1968) Transmission Spectra of ZnO Single Crystals. *Physical Review Letters*, **20**, 59-62. <https://doi.org/10.1103/physrevlett.20.59>
- [16] Ebina, A., Fukunaga, E. and Takahashi, T. (1974) Variation with Composition of the E_0 and $E_0 + \Delta_0$ Gaps in $\text{ZnS}_x\text{Se}_{1-x}$ Alloys. *Physical Review B*, **10**, 2495-2500.
- [17] Schmidt, M. (1977) Acceptor Ground States in Nearly Cubic Semiconductors. *Physica Status Solidi (b)*, **79**, 533-538. <https://doi.org/10.1002/pssb.2220790217>
- [18] Huang, M. and Ching, W.Y. (1993) Calculation of Optical Excitations in Cubic Semiconductors. II. Second-Harmonic Generation. *Physical Review B*, **47**, 9464-9478. <https://doi.org/10.1103/physrevb.47.9464>
- [19] Ghaleb, A.M., Benkrima, Y., Ahmed, A.Q. and Ghaleb, Z.T. (2024) Structural, Electronic, and Optical Properties Investigation of ZnSe Cubic Sphalerite Compounds Using Density Functional Theory (DFT). *Problems of Atomic Science and Technology*, No. 1, 103-109. <https://doi.org/10.46813/2024-149-103>
- [20] Asadi, Y. and Nourbakhsh, Z. (2019) First Principle Study of the Structural, Electronic, Vibrational, Thermodynamic, Linear and Nonlinear Optical Properties of Zinc-Blende ZnSe and ZnTe Semiconductors. *Computational Condensed Matter*, **19**, e00372. <https://doi.org/10.1016/j.cocom.2019.e00372>
- [21] Adetunji, B.I., Adebambo, P.O. and Adebayo, G.A. (2012) First Principles Studies of Band Structure and Electronic Properties of ZnSe. *Journal of Alloys and Compounds*, **513**, 294-299. <https://doi.org/10.1016/j.jallcom.2011.10.039>
- [22] Saini, P.K., Singh, D. and Ahlawat, D.S. (2014) Calculations of the Structural, Elastic and Optical Properties of ZnSe at Ambient and High Pressure. *Chalcogenide Letters*, **11**, 405-414.
- [23] Habura, K.H., Afrassa, M.A. and Hone, F.G. (2023) Density Functional Theory Study of $\text{Zn}_{(1-x)}\text{Fe}_x\text{Se}$: Electronic Structure, Phonon, and Magnetic Properties. *AIP Advances*, **13**, Article ID: 035102. <https://doi.org/10.1063/5.0133408>

- [24] Flores, E.M., Moreira, M.L. and Piotrowski, M.J. (2020) Structural and Electronic Properties of Bulk ZnX (X = O, S, Se, Te), ZnF₂, and ZnO/ZnF₂: A DFT Investigation within PBE, PBE + *U*, and Hybrid HSE Functionals. *The Journal of Physical Chemistry A*, **124**, 3778-3785. <https://doi.org/10.1021/acs.jpca.9b11415>
- [25] Ray, S. and Tarafder, K. (2023) Investigation of CdSe and ZnSe as Potential Back Surface Field Layers for CdTe-Based Solar Cells: A Study from First Principles Calculations. *Advanced Theory and Simulations*, **6**, Article ID: 2200718. <https://doi.org/10.1002/adts.202200718>
- [26] Bernard, J.E. and Zunger, A. (1987) Electronic Structure of ZnS, ZnSe, ZnTe, and Their Pseudobinary Alloys. *Physical Review B*, **36**, 3199-3228. <https://doi.org/10.1103/physrevb.36.3199>
- [27] Rachidi, A., Atmani, E.H., Fazouan, N. and Boujnah, M. (2016) A Study by *Ab-Initio* Calculation of Structural and Electronic Properties of Semiconductor Nanostructures Based on ZnSe. *Materials Sciences and Applications*, **7**, 562-573. <https://doi.org/10.4236/msa.2016.79047>
- [28] Ferahtia, S., Saib, S. and Bouarissa, N. (2019) Computational Studies of Mono-Chalcogenides ZnS and ZnSe at High-Pressures. *Results in Physics*, **15**, Article ID: 102626. <https://doi.org/10.1016/j.rinp.2019.102626>
- [29] Bagayoko, D. (2014) Understanding Density Functional Theory (DFT) and Completing It in Practice. *AIP Advances*, **4**, Article ID: 127104. <https://doi.org/10.1063/1.4903408>
- [30] Perdew, J.P. and Zunger, A. (1981) Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems. *Physical Review B*, **23**, 5048-5079. <https://doi.org/10.1103/physrevb.23.5048>
- [31] Perdew, J.P. and Levy, M. (1983) Physical Content of the Exact Kohn-Sham Orbital Energies: Band Gaps and Derivative Discontinuities. *Physical Review Letters*, **51**, 1884-1887. <https://doi.org/10.1103/physrevlett.51.1884>
- [32] Sham, L.J. and Schlüter, M. (1983) Density-Functional Theory of the Energy Gap. *Physical Review Letters*, **51**, 1888-1891. <https://doi.org/10.1103/physrevlett.51.1888>
- [33] Sham, L.J. and Schlüter, M. (1985) Density-Functional Theory of the Band Gap. *Physical Review B*, **32**, 3883-3889. <https://doi.org/10.1103/physrevb.32.3883>
- [34] Bagayoko, D., Diakite, Y.I., Dioum, A. and Malozovsky, Y. (2025) The Completed Density Functional Theory (cDFT) for Accurate Description and Prediction of Properties of Materials. *Annals of Computational Physics and Material Science*, **2**, 1-5.
- [35] Bagayoko, D. and Diakité, Y.I. (2023) Realizing the Potentials of Density Functional Theory (DFT) and of the Materials Genome Initiative (MGI). *MRS Advances*, **8**, 619-625. <https://doi.org/10.1557/s43580-023-00562-w>
- [36] Bagayoko, D., Zhao, G.L., Fan, J.D. and Wang, J.T. (1998) *Ab Initio* Calculations of the Electronic Structure and Optical Properties of Ferroelectric Tetragonal. *Journal of Physics: Condensed Matter*, **10**, 5645-5655. <https://doi.org/10.1088/0953-8984/10/25/014>
- [37] Nwigboji, I.H., Malozovsky, Y., Franklin, L. and Bagayoko, D. (2016) Calculated Electronic, Transport, and Related Properties of Zinc Blende Boron Arsenide (zb-BAs). *Journal of Applied Physics*, **120**, Article ID: 145701. <https://doi.org/10.1063/1.4964421>
- [38] Bamba, C.O., Inakpenu, R., Diakite, Y.I., Franklin, L., Malozovsky, Y., Stewart, A.D., et al. (2017) Accurate Electronic, Transport, and Related Properties of Wurtzite Beryllium Oxide (w-BeO). *Journal of Modern Physics*, **8**, 1938-1949. <https://doi.org/10.4236/jmp.2017.812116>

- [39] Diakite, Y.I., Traore, S.D., Malozovsky, Y., Khamala, B., Franklin, L. and Bagayoko, D. (2017) Accurate Electronic, Transport, and Bulk Properties of Zinc Blende Gallium Arsenide (Zb-GaAs). *Journal of Modern Physics*, **8**, 531-546. <https://doi.org/10.4236/jmp.2017.84035>
- [40] Diakite, Y.I., Traore, S.D., Malozovsky, Y.M., Khamala, B., Franklin, L. and Bagayoko, D. (2015) Calculated Electronic and Related Properties of Wurtzite and Zinc Blende Gallium Nitride (GaN). *The African Review of Physics*, **10**, 0039. <http://lamp.ictp.it/index.php/aphysrev/article/viewArticle/1117>
- [41] Diakite, Y.I., Malozovsky, Y., Bamba, C.O., Franklin, L. and Bagayoko, D. (2022) *Ab Initio* Calculation of Accurate Electronic and Transport Properties of Zinc Blende Gallium Antimonide (zb-GaSb). *Journal of Modern Physics*, **13**, 414-431. <https://doi.org/10.4236/jmp.2022.134029>
- [42] Diakite, Y.I., Malozovsky, Y., Bamba, C.O., Franklin, L. and Bagayoko, D. (2022) First Principle Calculation of Accurate Electronic and Related Properties of Zinc Blende Indium Arsenide (zb-InAs). *Materials*, **15**, Article No. 3690. <https://doi.org/10.3390/ma15103690>
- [43] Dioum, A., Diakité, Y.I., Malozovsky, Y., Ayirizia, B.A., Beye, A.C. and Bagayoko, D. (2023) First-Principles Investigation of Electronic and Related Properties of Cubic Magnesium Silicide (Mg₂Si). *Computation*, **11**, Article No. 40. <https://doi.org/10.3390/computation11020040>
- [44] Ceperley, D.M. and Alder, B.J. (1980) Ground State of the Electron Gas by a Stochastic Method. *Physical Review Letters*, **45**, 566-569. <https://doi.org/10.1103/physrevlett.45.566>
- [45] Vosko, S.H., Wilk, L. and Nusair, M. (1980) Accurate Spin-Dependent Electron Liquid Correlation Energies for Local Spin Density Calculations: A Critical Analysis. *Canadian Journal of Physics*, **58**, 1200-1211. <https://doi.org/10.1139/p80-159>
- [46] Ekuma, C.E., Jarrell, M., Moreno, J., Franklin, L., Zhao, G.L., Wang, J.T., et al. (2012) First Principle Local Density Approximation Description of the Electronic Properties of Ferroelectric Sodium Nitrite. *Materials Chemistry and Physics*, **136**, 1137-1142. <https://doi.org/10.1016/j.matchemphys.2012.08.066>
- [47] Madelung, O. (ed.) (1991) Semiconductors: Group IV Elements and III-V Compounds. Springer-Verlag.
- [48] Madelung, O. (2004) Semiconductors Data Handbook. Springer.
- [49] Schlesinger, R. (2017) Fundamentals. In: Schlesinger, R., Ed., *Energy-Level Control at Hybrid Inorganic/Organic Semiconductor Interfaces*, Springer International Publishing, 7-45. https://doi.org/10.1007/978-3-319-46624-8_2