

Density Functional Approach to Study Electronic Structure of ZnO Single Crystal

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Abstract: In this paper, we have performed first-principles calculations of electronic and structural properties of ZnO in rocksalt (B1), zincblende (B3) and wurtzite (B4) phases. The results for the electronic density of states (DOS) show that the lower part of the valence band is dominated by the O-2s orbital and the upper part by the O-2p orbital in ZnO. Also it is shown that the local-density approximation underestimates the band gap and misplaces the energy levels of the Zn-3d states. We have used the Engel-Vosko GGA formalism, which optimized the corresponding potential for band structure calculation of B1 and B3 phases. Typical errors in calculated band gaps originate from strong coulomb correlations, which are found to be highly significant in B4 phase. The LDA+U approach is found to correct the strong correlation of the Zn-3d electrons. The GGA+U approach is applied to Zn-3d and O-2p orbitals that cause to improve the band gap and correct the location of Zn-3d levels. Calculation of electron density in three phases of ZnO in (110) plane is shown that this compound has ionic and covalent bond simultaneously. The calculations are in good agreement with the theoretical and experimental values.

Key words: Band structure • FP-LAPW • GGA+U • WIEN2K • ZnO

INTRODUCTION

Most of the group II–VI binary compound semiconductors crystallize in either cubic zincblende or hexagonal wurtzite structure where each anion is surrounded by four cations at the corners of a tetrahedron and vice versa [1]. This tetrahedral coordination is typical of sp^3 covalent bonding nature, but these materials also have a substantial ionic character that tends to increase the bandgap further one expected from the covalent bonding. So, it is a semiconductor whose ionicity exists at the borderline between the covalent and ionic semiconductors [2]. ZnO has a band gap 3.44 eV [3] and bulk exciton-binding energy 60 meV [4], which is larger than the room temperature thermal energy. ZnO can be used in visible and ultraviolet light emitters, high-density optical memories, solid-state laser devices, sensors, solar cells etc [5-7]. At ambient conditions, ZnO has the wurtzite structure. Upon compression above 9.0 GPa, a phase transition to rocksalt structure. Zn-3d and O-2p can hybridize with together due to their close energy. The position of the Zn-3d levels is important. The hybridization of Zn-3d with O-2p levels pushes up the valence band level. In LDA [8] and GGA [9] the position of the Zn-3d levels is too high. Few works have ever been

reported about the electronic structure of ZnO and their main focus was the energy locality of Zn-3d states. Powell *et al.* carried out the ultraviolet photoemission spectroscopy of ZnO and found that locality of Zn-3d core level was at round 7.5 eV below Fermi energy [10, 11]. Rossler calculated the locality of Zn-3d states by using Green function method, but their predicted positions were far from satisfactory [12].

Recent researches based on LDA and GGA underestimated the band gap of ZnO and gave the energy of Zn-3d states too close to the VBM [13-15]. Although the calculated band gap with GW approximation method have good correlation with experimental results, it is unable to calculate the correct position of d states [16]. The results of Vogel *et al.* in study electronic structure by the LDA+SIC method were in good agreement with experimental value for gap and the bandwidth but the d states were 1 eV lower than the experimental one [17]. Zhou *et al.* calculated band gap equal to 1.8 eV using LDA+U method with consideration of $U_{\text{eff}}=8.5$ eV and found that the main peak of 3d states spans the energy from -6 eV to -7.8 eV [18]. Tula *et al.* by adding $U_s=43.54$ eV to $U_d=6.37$ eV found that this shifts the Zn-3d bands down to -7.41 eV, which is much closer to experimental position of -7.5 eV [19].

In this article, first, we calculate structure parameters. Next step in this research is calculation of the electronic structures by the energy of bands. Also we show that the LSDA+U [20] approach can be applied not only to the Zn-3d but also to the O-2p orbitals. In the next part we calculate electron density in (110) plane. Finally, a summary of the main results are given.

MATERIALS AND METHODS

Method of Calculation: The first-principles calculations are performed based on the density functional theory (DFT). The total energies were calculated within the full potential linearized augmented plane wave (FP-LAPW) method, by WIEN2K package [21]. Racksalt phase of ZnO has a cubic structure of NaCl with space group Fm3m and lattice parameter 4.271 Å [22]. The experimental lattice constant for zincblende structure of ZnO with space group F43m is $a=4.62$ Å [23]. In our calculations, we used lattice parameters of $a=3.258$, $c=5.220$ and $u=0.382$ [24] for wurtzite phase with space group F63m. In calculations, the convergence parameter, $R_{MT}K_{max}$, was set to 7.0. The maximum angular momentum quantum number as a cutoff for expanding the Kohn–Sham wave functions in terms of lattice harmonics inside the muffin-tin spheres was confined to $L_{max} = 10$. Self-consistency is obtained using 91, 56 and 147 special k-points in the irreducible wedge of the irreducible Brillouin zone (IBZ) for B1, B3 and B4 phases, respectively. All these values have been chosen so as to ensure the total energy converged to better than 0.0001 Ry. The cut-off energy, which defines the separation between the core and valence states, was set to -6.0 Ry.

For structural properties, the exchange–correlation potential was calculated using both the local-density approximation (LDA) [8] and the generalized-gradient (GGA) in the form suggested by Perdew *et al.* [9]. For electronic properties, we also applied the Engel-Vosko (EV-GGA) scheme [25]. The Zn-3d and O-2p bands are well separated in experiment, while they partly overlap in the LDA, GGA and EV-GGA. We use GGA+U and LDA+U approach [20] to correct the energy position of Zn-3d states. The optimized U_{eff} is 11.97 eV in this paper which is close to the values used in other previous work [18, 26, 27]. In order to improve band gap, we added both U_d (11.97 eV) and U_p (13.6) within the LSDA(GGA)+U approach.

RESULT AND DISCUSSION

Structural Properties: We are calculated the total energy as a function of volume within LDA, GGA and EV-GGA approach for ZnO in B1, B3 and B4 phases. In this calculations, we are used the experimental lattice parameter as the starting point and fitted the results with a Murnaghan equation of states (EOS) [28]. The calculated equilibrium lattice constants, bulk modulus B (GPa) and its pressure derivative B' for B1, B3 and B4 phases of ZnO crystal, are summarized in Table 1 that contains results of the previous theoretical calculations in addition to the experimental data for comparison. The present results agree well with the previous experimental and theoretical reports. Better theoretical results are obtained with the GGA, where in EV-GGA method the quantities that depend on an accurate description of exchange energy E_x , such as equilibrium volumes, are in poor agreement with experiment. In Table 1 it is obviously seen that in these phases the B1 structure has the highest bulk modulus value. Therefore, we can expect that this phase should show higher hardness than B3 and B4 structures.

Electronic Properties: The partial and total density of states (DOS) are calculated by tetrahedron method [29]. We have calculated the total densities of states and band structure using LDA, GGA and EV-GGA schemes for the three phases B1, B3 and B4 of ZnO. The partial and total density of states are presented in Figure 1. The GGA functionals have simple forms that are not sufficiently flexible to accurately reproduce both the exchange–correlation energy and its charge derivative. Engel and Vosko [25] by considering this shortcoming, constructed a new functional form of the GGA which is better able to reproduce the exchange potential at the expense of less agreement in the exchange energy. This approach, which is called the EV-GGA, gives a better band splitting and some other properties which mainly depend on the accuracy of the exchange correlation potential [30]. Total density of states figures suggested that the lower part of the valence band is dominated by the O-2s orbital and the upper part by the O-2p orbital in ZnO. The lower part of the conduction band is dominated by the Zn-2s orbital. From Fig. 2, we found that ZnO in B3 and B4 phases is a semiconductor with a direct gap of 0.6 eV and 0.75 eV and an indirect gap of 0.98 eV for B1 phase in the GGA, in agreement with [31, 32], but these band gaps are

Table 1: Lattice parameter, bulk modulus B and its pressure derivation for rocksalt, zincblende and wurtzite structures of ZnO with GGA approximation

Phase	Lattice parameter		B(GPa)	B'	Reference
Wurtzite	a(Å)	c(Å)			
	3.281	5.256	135.05	4.9	This work
	3.258	5.220	181.0	4.0	Exp. [24]
	3.283	5.309	131.5	4.2	Theor. [36]
	3.250	5.204	183	4	Exp. [22]
	3.238	5.232	154	4.3	Theor. [24]
	3.292	5.292	133.7	3.8	Theor. [15]
	3.198	5.167	159.5	4.5	Theor. [37]
	3.183	5.124	162	-	Theor. [38]
Zincblende	a(Å)				
	4.616		125.345	3.44	This work
	4.62		-	-	Exp. [23]
	4.627		131.6	3.3	Theor. [36]
	4.633		133.73	4.79	Theor. [31]
	4.633		135.3	3.7	Theor. [15]
Rocksalt	a(Å)				
	4.334		170.86	4.18	This work
	4.271		228	4	Exp. [22]
	4.334		167.8	5.3	Theor. [36]
	4.337		161.45	4.66	Theor. [31]
	4.345		172.7	3.7	Theor. [15]
	4.316		175	5.4	Theor. [40]
	4.225		209.1	2.7	Theor. [39]
	4.213		210.0	-	Theor. [38]

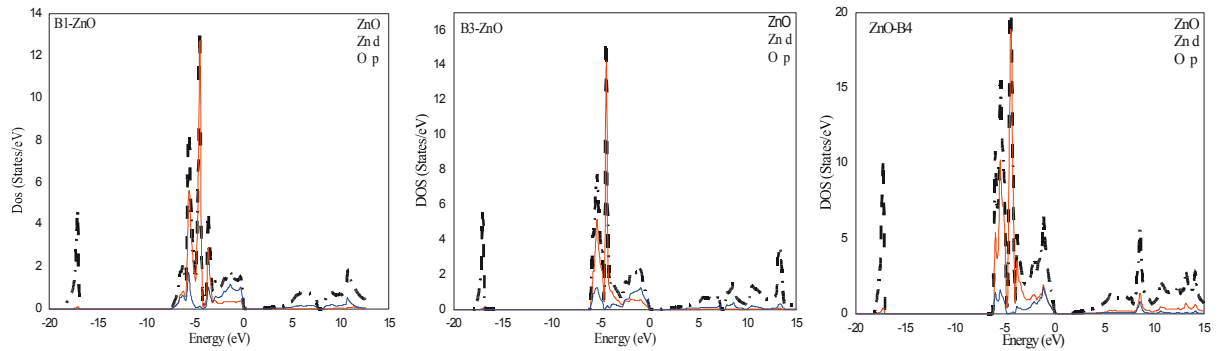


Fig. 1: The total DOS and the partial DOS for the Zn-3d and O-2p orbitals are computed in the GGA for three phases of ZnO

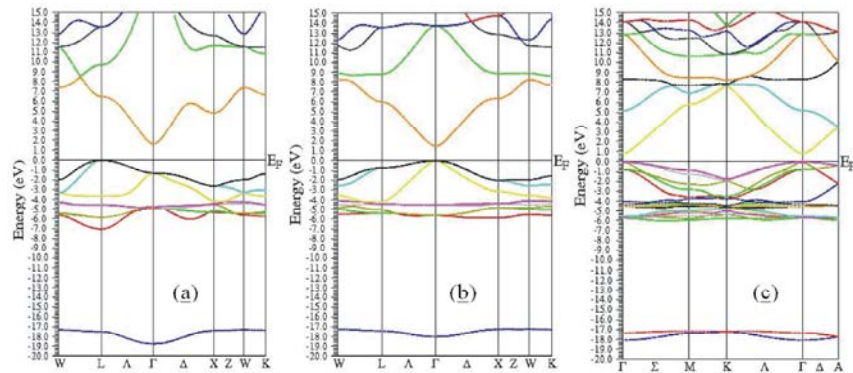


Fig. 2: Band structures for (a) B1, (b) B3 and (c) B4 phases of ZnO in EV-GGA approach

Table 2: Calculated bandgap with different approximations in the wurtzite, zincblende and rocksalt structures for ZnO compared with experimental and other theoretical results (all values are given in eV)

Present Work						Others	
Phase	LDA	GGA	GGA+SP	GGA+SOC	EVGGA	Exp.	Theor.
B1	0.97	0.98	0.95	0.94	1.62	2.45 ^b	0.75 ^a , 1.47 ^a , 1.1 ^b , 1.29 ^c , 4.2 ^d
B3	0.55	0.60	0.65	0.58	1.4	-	0.65 ^a , 1.46 ^a , 3.75 ^d , 3.59 ^e , 1.48 ^f , 0.87 ^g
B4	0.68	0.75	0.76	0.73	0.55	3.44	0.76 ^a , 1.57 ^a , 0.88 ^b , 3.5 ⁱ , 11.7 ^j , 2.26 ^k , 1.8 ^l , 1.98 ^f , 3.3 ^m
Phase	LSDA+U	GGA+U	LSDA+U _p +U _d	GGA+U _p +U _d	Exp.		
B4	1.53	1.61	2.11	2.22	3.44 ⁿ		

^aRef. [31]. ^bRef. [33]. ^cRef. [41]. ^dRef. [42]. ^eRef. [43]. ^fRef. [44]. ^gRef. [2]. ^hRef. [45]. ⁱRef. [17]. ^jRef. [46]. ^kRef. [14]. ^lRef. [18]. ^mRef. [19]. ⁿRef. [3].

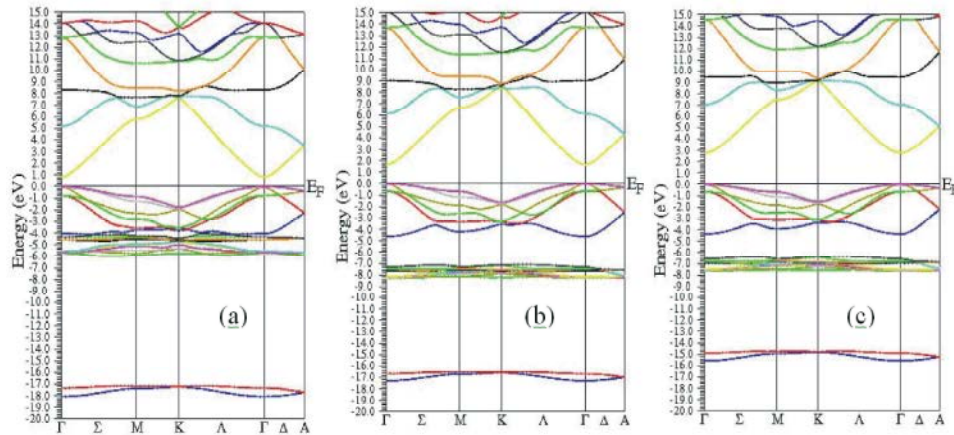
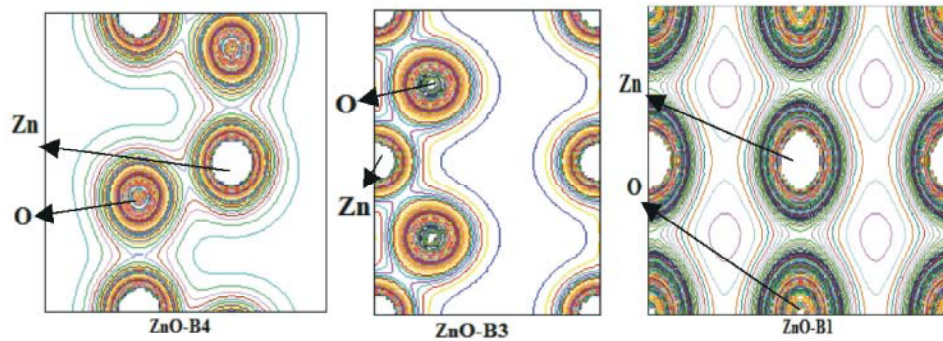
Fig. 3: Band structures for B4 phase of ZnO in (a) GGA, (b) GGA+U_d and (c) GGA+U_d+U_p formalisms

Fig. 4: Contour plot of the electron density in the (110) plane for three phases of ZnO

much smaller than the experimental value (3.44 eV for B4 and 2.45 eV for B1) [3, 33]. The calculated band gap are summarized in Table 2.

It is well known that DFT calculations within LDA and GGA locate the Zn-3d band inappropriately close to the topmost VB, hybridizing with the O-2p band, misrepresent the band dispersion and reduces the band gap. We use LDA(GGA)+U method to lower the Zn-3d energy levels derived from the simple LDA and give better agreement with the findings from X-ray emission spectra [26]. For B4 phase of ZnO, we use an effective U_{eff} which is considered a fitting parameter instead of separate U and J. Varying the value of U_{eff}, the Dos peaks of Zn-d shift.

When the position of the Zn-d peak is in good conformity with that of experiment [19] the U_{eff} is obtained. In this paper, the optimized U_{eff} is 11.97 eV which is close to the values used in other previous work [18, 26, 27]. By increasing U from 0 eV to 11.97 eV, one found that band gap improve to 1.61 eV. If we add only the U_d=4.0 eV, the center of the 3d-Zn orbital set at -6.15 eV. By increasing U_d to 11.97 eV it is shifted down to -7.58 eV which is similar to its position in experimental [26]. Compared to the GGA where the gap is only 0.75 eV, the gap with GGA+U becomes 1.61 eV. we add both U_d (11.97eV) and U_p (13.6 eV) within the LSDA(GGA)+U approach. The gap is adjusted to 2.22 eV, close to the experimental value of

3.4 eV. Simultaneously, we see that this also shifts the Zn-3d bands further down to -7.13 eV, which is much closer to experimental position of photoemission measurements [34]. As seen from Fig.3, calculations within the LDA+U approach somewhat correct the location of the energy levels of the Zn-3d electrons. The explanation of the eigenvalue problem and the order of states at the topmost VB from LDA, GGA and LDA+U calculations are discussed in Refs. [26, 35] will not be repeated here.

Electron Density: Electron density denotes the nature of the bond character. We have calculated electron density of ZnO in (110) plane for B1, B3 and B4 phases and displayed in Fig. 4. It is showed that there is the large difference of the electronegativity between Zn and O that is cause of charge transfer from Zn to O atoms. The calculated electron density shows that charge density lines are almost spherical in B1 structure that is sign of existence ionic bond between Zn and O atoms. In B3 and B4 structures Zn and O atoms shared electron more than B1 structure that causes the strong covalent interaction of the Zn-O bonds in ZnO. Hence ZnO has ionic and covalent bond simultaneously.

CONCLUSIONS

The structural and electronic properties of ZnO in three phases have been investigated using the FP-LAPW method. The equilibrium lattice parameters, bulk modulus and its pressure derivative are calculated using GGA approach are in better agreement with the experimental values. A density of states analysis showed that the lower part of the valence band is dominated by the O-2s orbital and the upper part by the O-2p orbital in ZnO. The lower part of the conduction band is dominated by the Zn-2s orbital. The results showed the effect of the spin polarized and spin-orbit coupling is negligible for band gap calculations. From the band structures, we found that ZnO is a wide band gap semiconductor with a indirect gap of 1.62 eV in B1 phase and B3 phase of ZnO has direct gap of 1.4 eV, calculated with EV-GGA formalism. In this paper, we found that the results obtained for B1 and B3 phases of ZnO, from the EV-GGA method, are generally in better agreement with the experimental value than other theoretical calculations. It is found that EV-GGA underestimates the band gap of B4 phase and the Zn-3d band hybridizing with the O-2p band. In this research, value of band gap for B4 phase was 1.61 eV with decreasing hybridization between 3d orbital of Zn atom

and 2p orbital of O atom by applying $U_d=11.97$ eV. Also, we added both U_d (11.97eV) and U_p (13.6 eV) within the GGA+U approach that the gap is adjusted to 2.22 eV, close to the experimental value of 3.4 eV.

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