

## **SIMULATION OF OPTICAL PROPERTIES OF ZnO SUPERCELL BASED ON DENSITY FUNCTIONAL THEORY.**

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### **ABSTRACT**

This work presents the optical properties of ZnO semiconductor calculated by full potential linearized augmented plane wave (FP-LAPW) method with the local density approximation (LSDA) and the modified Becke-Johnson (mBJ) potential. The scope of this work is to study some optical properties as (Dielectric function, Loss Function, Refractive index ...) of ZnO (1×1×1), (1×2×2) supercell in Zincblende (ZB) and Rocksalt (RS) phases. Our analysis revealed that the mBJ potential gives good results for the treatment of the d-orbitals.

**Keywords:** Dielectric function, Refractive index, ZnO, mBJ, Supercell, FP-LAPW.

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## **1. INTRODUCTION**

### **1.1. Theory and computational method**

This work is done by using the enhanced total potential linearized plane wave method implemented in the Wien2K [1] code to explore the optical properties of semiconductor oxides which are also widely used such as ZnO.

The determination of the structural properties is the first important step preceding the calculation of the physical properties of ZnO in Zincblende and Rocksalt phases. Nowadays, it is possible to calculate the total energy of the solids in a rather precise way by means of approximations such as those of the local density (LDA) [2].

## 1.2. Calculation details

In the manner of the calculation of optical properties in the spectral range makes an important role in the profound understanding of the character of this material. This new ledge provides a transparent photograph for the usage of this material in optoelectronic devices.

We can describe the optical properties by means of the dielectric function  $\varepsilon(w) = \varepsilon_1(w) + \varepsilon_2(w)$ . The imaginary part  $\varepsilon_2(w)$  is calculated from the momentum matrix elements between the occupied and unoccupied wave functions within the selection rules. The real part  $\varepsilon_1(w)$  of the complex dielectric function can be obtained using the Kramers-Krönig relationship [3].  $\varepsilon_1(w)$  and  $\varepsilon_2(w)$  are given by this relations:

$$\varepsilon_2(w) = \left( \frac{4\pi^2 e^2}{2w^2} \right) \sum_{i,j} \int_k \langle i|M|j \rangle^2 f_i(1-f_j) \times \delta(E_{i,j} - E_{i,k} - w) d^3k \quad (1)$$

$$\varepsilon_1(w) = 1 + \frac{2}{\pi} p \int_0^\infty \frac{w' \varepsilon_2(w') dw'}{(w'^2 - w^2)} \quad (2)$$

Were  $e$  : Charge of a free electron

$m$  : Mass of a free electron

$w$  : Frequency of incident photon

$M$  : Dipole matrix

$i, j$  : Initial and final states respectively

$f_i$  : Fermi distribution function for the  $i$ -th state

$E_i$  : Energy of electron in the  $i$ -th state

$p$  : Principal value of the integral

Other optical constants such as refractive index  $n(w)$ , extinction coefficient  $K(w)$  and absorption coefficient  $\alpha(w)$  can be calculated with the knowledge of the complex dielectric function, using the formulas as follows [4-6] :

$$n(w) = \frac{1}{\sqrt{2}} [(\varepsilon_1^2 + \varepsilon_2^2)^{1/2} + \varepsilon_1]^{1/2} \quad (3)$$

$$K(w) = \frac{1}{\sqrt{2}} [(\varepsilon_1^2 + \varepsilon_2^2)^{1/2} - \varepsilon_1]^{1/2} \quad (4)$$

$$\alpha(w) = \sqrt{2}w [(\varepsilon_1^2 + \varepsilon_2^2)^{1/2} - \varepsilon_1]^{1/2} \quad (5)$$

## 2. RESULTS AND DISCUSSION

For the present analysis, WIEN2k simulation package [1] code based on density functional theory (DFT) was used. The approach is based on Kohn-Sham equation [3] of the density functional theory. In the interstitial region, energy cut off  $k_{max} \cdot R_{mt} = 7$ , the  $R_{mt}$  were chosen for Zn and O as 1.5000 a.u , we used 125 kpoint ( $n_{div} = 8 \times 4 \times 4$ ) in the special irreducible Brillouin zone to obtain very good results for well convergence .

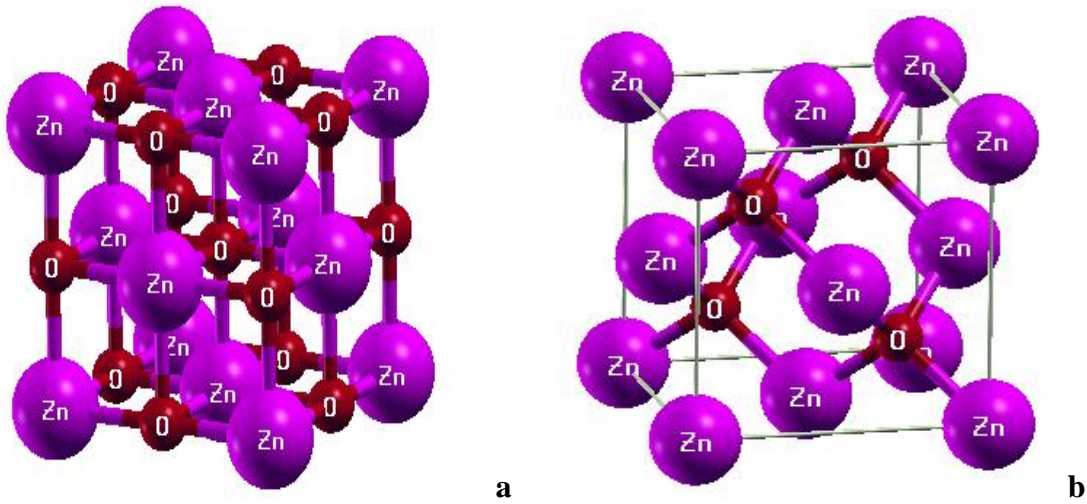
In our calculations, lattice parameter for Rocksalt structure is found to be  $a = 4.331 \text{ \AA}$  which shows a great consistency with the experimental value of  $4.271 \text{ \AA}$  [18] ; for Zincblende, the predicted lattice parameter  $a = 4.331 \text{ \AA}$  is also in good agreement with the experiment value of  $4.62 \text{ \AA}$  [17]. The same observation is valid for  $B_0$  and  $B'$  as well, as shown in table 1

**Table.1.** The lattice constants  $a(\text{ \AA})$ , Bulk modulus  $B_0$  (GPa) and its pressure derivative  $B'$  of ZnO in the RS and ZB in (1x1x1) structures.

<u>ZB structure</u>		This	
A	4.4836	4.52 <sup>a</sup> , 4.6329 <sup>b</sup>	4,62 <sup>c</sup>
$B_0$	167.1607	168 <sup>a</sup> , 139.32 <sup>b</sup>	
$B'$	4.8836	4.6 <sup>a</sup> , 3.7586 <sup>b</sup>	
<u>RS structure</u>			
A	4.331	4.223 <sup>a</sup> , 4.3379 <sup>b</sup>	4.271 <sup>d</sup>
$B_0$	201.98	209.6 <sup>a</sup> , 164.91 <sup>b</sup>	202 <sup>f</sup>
$B'$	4.2927	4.46 <sup>a</sup> , 4.5318 <sup>b</sup>	4 <sup>d</sup> , 3.54 <sup>f</sup>

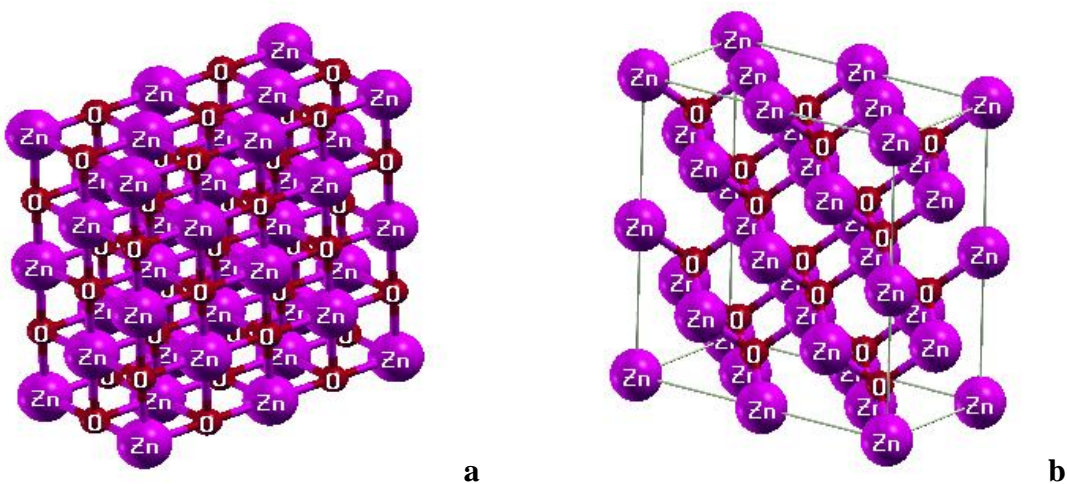
<sup>a</sup> Ref [7] <sup>b</sup> Ref [8] <sup>c</sup> Ref [9] <sup>d</sup> Ref [10] <sup>e</sup> Ref [11]

In fig.1, we present the schematic overview of structures of ZnO ( $1 \times 1 \times 1$ ) in Rocksalt (a) and Zinc blende (b) phases. The colors of Zn, O atoms are rose, red respectively .



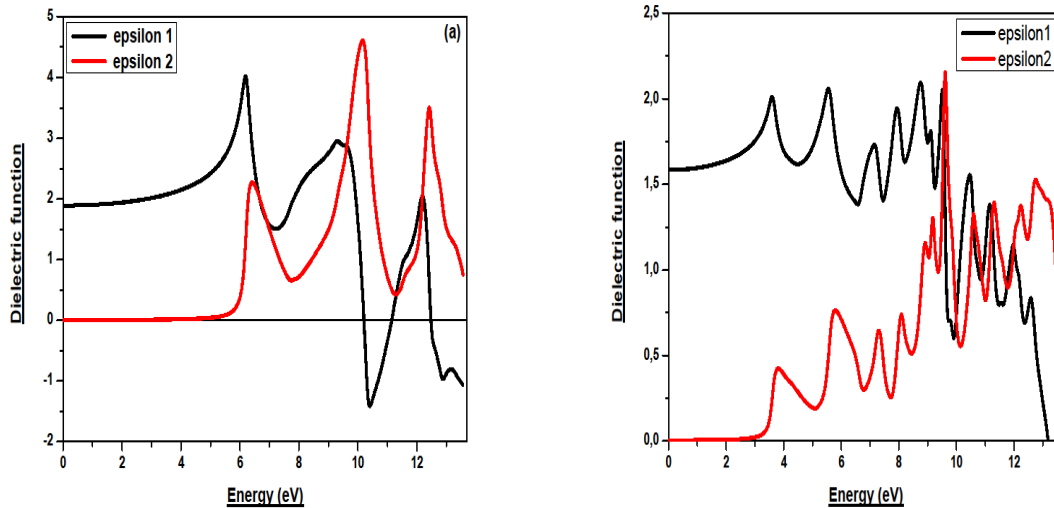
**Fig.1.** Structures of ZnO mono-crystal ( $1 \times 1 \times 1$ ) in Rocksalt phase (a) and Zinc blende phase (b). The colors of Zn, O atoms are rose and red respectively.

When we zoom the structure ( $1 \times 1 \times 1$ ) of ZnO in Rocksalt and Zincblende phases according to the axes Y and Z, we found a new structure called supercell of ZnO. Fig.2. presente Schematic overview of ZnO supercell structures ( $1 \times 2 \times 2$ ). The colors of Zn, O atoms are rose, and red respectively.



**Fig.2.** Structures of ZnO supercell structures ( $1 \times 2 \times 2$ ) in Rocksalt phase (a) and Zinc blende phase (b). The colors of Zn, O atoms are rose and red respectively.

Optical constants are calculated to study the optical properties of ZnO superlattices (1x2x2). The calculated of real and imaginary parts of the dielectric function of the ZnO superlattices in Rocksalt (a) and Zinc blende (b) phases are shown in Fig.3.

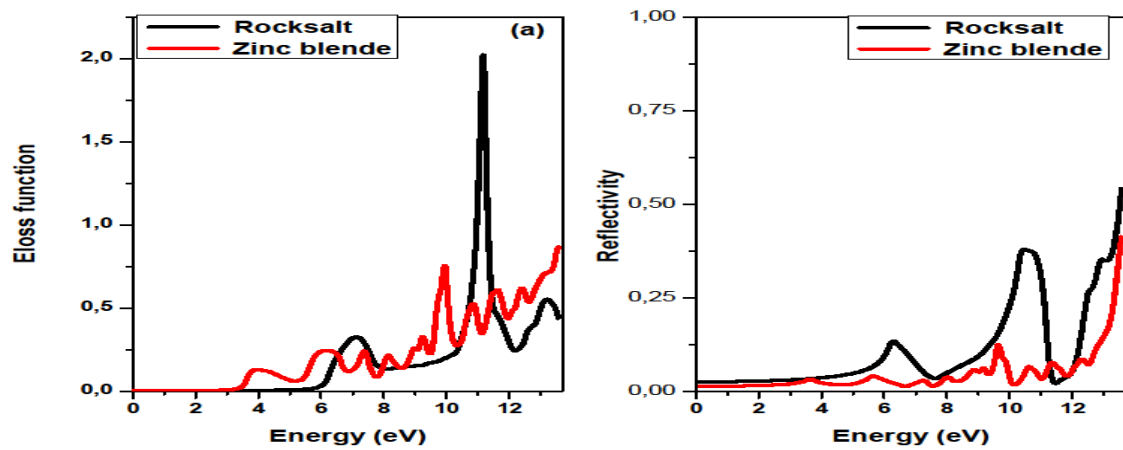


**Fig.3.** Real parts  $\epsilon_1(\omega)$  and imaginary  $\epsilon_2(\omega)$  of the dielectric function for ZnO (1x2x2 superlattice) in Rocksalt phase (a) and Zinc blende phase (b)

In fig.3, for the Rocksalt phase, the imaginary part consists of three peaks. The first peak between (6 - 8 eV) corresponds to the transition from 3d-Zn states to 2p-O states to the  $\Gamma$  point, while the second peak between (9, 11 eV) comes from the transition between states of 4s- Zn and 2p- O. For the Zinc blende phase, we observe that there are several peaks but we choose the most intense peaks, the first peak is between (5 - 7 eV) which corresponds to the transition of the 3d- Zn states with the 2p- O states at the  $\Gamma$  point, in the energy range between (9 - 10 eV), there is a transition between the 4s- Zn and 2p- O states.

For the real part, the static dielectric constants at the zero frequency limit of ZnO are (12 - 13 eV). A negative distribution appears in (10 – 12eV), it indicates that the ZnO in this phase shows a metallic behavior in this frequency region.

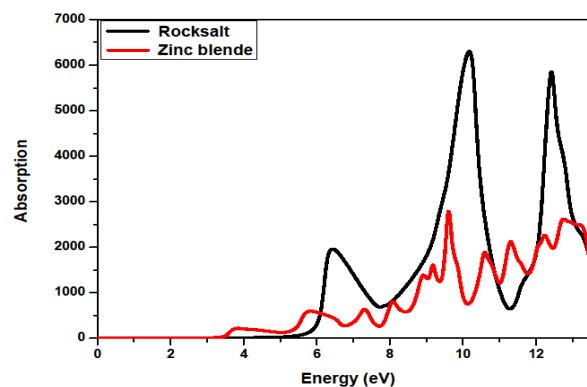
The calculated values of the energy loss function (Eloss function) and reflectivity of ZnO in two phases Rocksalt and Zinc blende are shown in the fig.4.



**Fig.4.** Eloss function (a) and Reflectivity (b) of ZnO supercell

The loss function describes a fast electron traveling in a material, the higher value in the spectra  $L(\omega)$  represents the characteristic associated with the plasma resonance, the loss of energy resonance is located about (9 - 10.5 eV) for the phase Zinc blende and between (10.5 - 11.5 eV) for Rocksalt phase. The reflectivity is about (10 - 11 eV) for the Rocksalt phase and between (9 - 10 eV) for the Zinc blende phase.

In fig.5. We present the curve of absorption, there are three intense peaks in the interval of (5.5 - 7 eV), (9 - 11 eV) and (12 - 13 eV) in Rocksalt phase, but in Zinc blende, there is one peak between (9 - 10 eV).



### 3. EXPERIMENTAL

This experimental section can be divided into subsections, the contents of which vary according to the subject matter of the article. It must contain all the information about the experimental procedure and materials used to carry out experiments.

### 4. CONCLUSION

The ZnO is a new material who has several properties of absorption and Eloss function , It have shown the best piezoelectric and photoelectric properties and great potential applications

### 5. ACKNOWLEDGEMENTS

To Prof f. Chemam, who provided help during this research .

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