A Comparative Theoretical Study of ZnO and BeO Oxides in Terms of Electronic Properties

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ZnO and BeO are attractive materials given their unique physical parameters, wide direct band gap of 3.37 eV and 10.6 eV for ZnO and BeO, respectively, and high exciton binding energy. These good parameters make them suitable for various applications, ultraviolet (UV) emission and detection, surface acoustic wave (SAW) devices, gas sensors, and transparent conducting electrodes. For these reasons, our work is focused on the investigation of the band structure and density of states of both ZnO and BeO semiconductors using the density functional theory (DFT) with two terms of exchange and correlation, generalized gradient approximation (GGA) and local density approximation (LDA). The structural parameters are calculated, the values of the average bond length are well compared with other data. The electronic properties such as band structures of both ZnO and BeO compounds are determined and compared with available values of energy gap and interpreted chemically.

Keywords: Density of states (DOS), ZnO, BeO, Structural properties, Band structures.

1. INTRODUCTION

Zinc and beryllium monoxides, ZnO and BeO, crystallized in the wurtzite phase with wide band-gap semiconductors with exciting characteristics such as electrical, optical, and mechanical. These properties are important and attracting for many applications in industries like electronics for the design of sensors, optical coatings, and scintillate. These materials are also used for the production of chemiluminescent, exoelectron emission, and EPR dosimeters of ionizing radiation [1-3]. They attract researchers and scientists to interpret and discuss different physical and chemical parameters via theoretical and experimental methods [4-8]. In particular, the properties of both ZnO and BeO compounds were obtained experimentally using films, ultrafine powders, various nanostructures, polycrystalline or ceramic samples from the moment of growing of ZnO and BeO single crystals [9, 10].

It is necessary to know more of the characteristics of these materials, such as electronic and optical properties, and to compare the two semiconductors to use very well the needed parameters of each compound. So, this present work is to compare them in terms of electronic and optical properties using the Siesta code within the density functional theory (DFT). The paper contains the following sections: section 2 presents the variables used in the calculations, section 3 shows the results obtained and their interpretation with a comparison of the studied compounds, finally the conclusion is given.

2. THEORETICAL METHOD OF CALCULATION

The present calculations are based on DFT [11] within the generalized gradient gpproximation (GGA), which is parameterized by Perdew, Burke and Ernzerhof (PBE) [12], and the local density approximation (LDA) [13], which is parameterized by exchange-correlation functions implemented in the SIESTA code. The calculation basis has a cutoff energy of 200 eV. We first optimize the bulk wurtzite structure of ZnO and BeO, yielding the following lattice parameters: $a = b = 3.284$ Å and $c = 5.33$ Å, $a = b = 5.304$ Å and $c = 7.905$ Å, respectively. These lattice parameters are in very good agreement with the experiment results. To prevent unphysical charge transfer between the top and bottom slab surfaces, pseudo hydrogens with fractional charges are used. A $6 \times 6 \times 1$ Monk Horst-Pack mesh is used for the Brillouin zone integration. Our total energy self-consistent-field (SCF) calculations were carried out with a convergence criterion of 5×10^{-4} eV, the optimized structures were obtained at atomic forces less than 0.005 eV/Å.

3. RESULTS AND DISCUSSION

3.1 Structural Parameters

Both compounds, ZnO and BeO, crystallize in the most stable form, according to the hexagonal structure, as shown in Fig. 1, with the length of the bond between Zn, O and Be atoms, which are shown in Table 1 and compared with the previous experimental and theoretical values. It is noticed from the results of Table 1 that the values of the average bond length are close to the previous theoretical results and are slightly far from the applied results. Using GGA gives better results than using LDA.
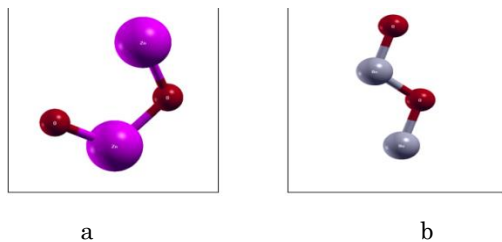
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Fig. 1 – (a) Structure of beryllium oxide (BeO), (b) structure of zinc oxide (ZnO)

Table 1 – Average bond length values for BeO and ZnO, according to GGA and LDA

Average bond length Å		Our work	Other works
ZnO	LDA	2.021	1.976[14]
	GGA	1.994	
BeO	LDA	1.431	1.483[15]
	GGA	1.414	

3.2 Electronic Property

The energy gap is an energy field in a solid in which no electrons can exist and is often expressed in electron volts (eV), and it represents the difference between the top of the valence band and the bottom of the conduction band. The energy gap property is prominent in insulators and semiconductors, where the gap value determines many of the optical and electrical properties of the solid body.

The energy band structure of two compounds, ZnO and BeO, obtained in the calculation program according to GGA and LDA is shown in Fig. 2 and Fig. 3, respectively. The energy gap values were derived from these two figures and recorded in Table 2.

From the results obtained through Fig. 2 and Fig. 3, which are recorded in Table 2, we can conclude that all calculated energy gap values for zinc oxide (ZnO) and beryllium oxide (BeO) for each of the two approximations are in the range of the previously obtained experimental values, and they are very close to the values obtained in the theoretical study [14]. They are closer than the results of previous studies, and in this case, it is more appropriate to know the energy gap in semiconductors compared to the case of using GGA.

The results also indicate that the ZnO compound is a semiconductor compound, and it can transfer electric current if it is affected by one of the influences such as temperature or pressure, etc. It is also deduced from these values that BeO is an insulating compound because it has a large energy gap.
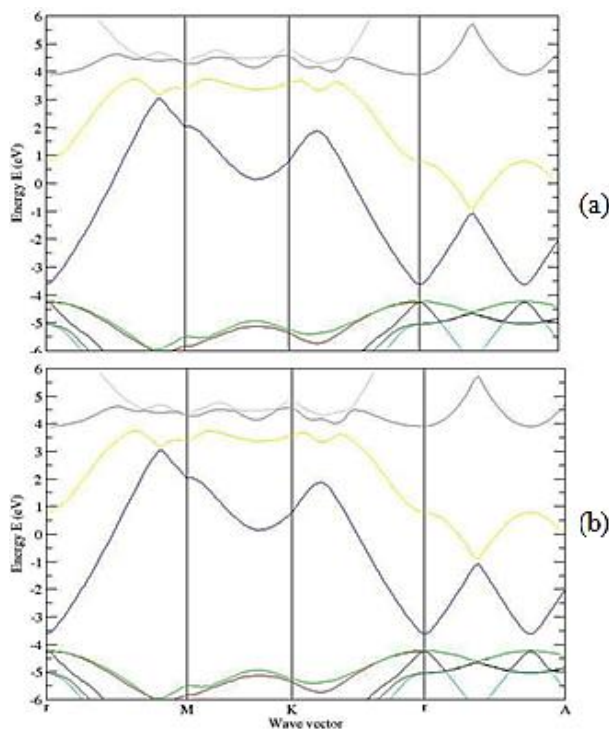

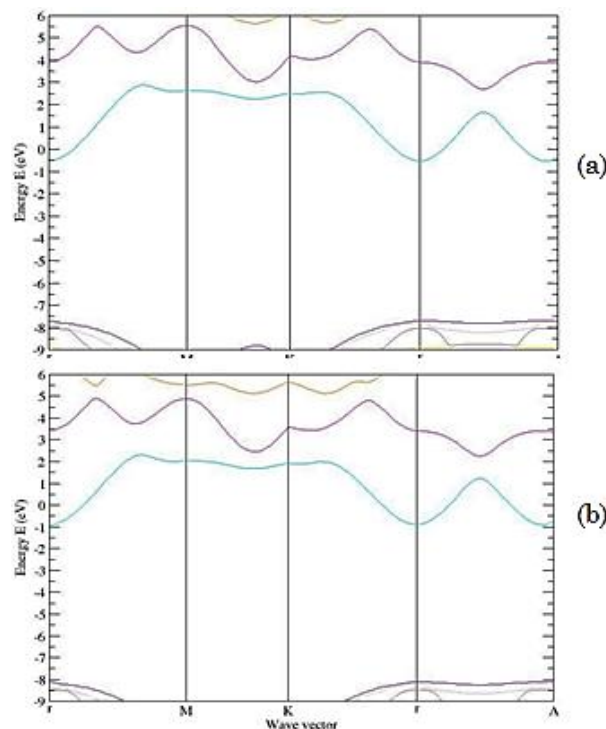**Fig. 2** – Energy band of ZnO in approximations: (a) GGA and (b) LDA

Fig. 3 – Energy band for BeO in approximations: (a) GGA and (b) LDA

Table 2 – Energy gap values and their comparison with theoretical and experimental results for ZnO and BeO using GGA and LDA

	Compounds	Other works [16]	Our works	Approximations	Experimental values
Energy gap (eV)	ZnO	0.7571	0.5983	GGA	0.15-3.5 [17]
		0.7965	0.7266	LDA	
	BeO	8.0470	7.1659	GGA	7-10 [18]
		8.3560	8.0312	LDA	

4. CONCLUSIONS

The aim of the work was to compare the structural and electronic properties of both ZnO and BeO compounds and bring them closer to the available results, using DFT with the help of GGA and LDA. We found that the values of the average bond length are close to the previous theoretical results and slightly far from the experimental results. From the band structures, it is indicated that the ZnO compound is a semiconductor compound and BeO is an insulating compound because it has a large energy gap. ZnO can transfer an electric current if it is affected by one of the influences such as temperature or pressure etc. The compound that has a density of electrons close to the Fermi level is the best qualified for chemical activity and reaction, while the one that records a low density of states at this level is then considered chemically stable.

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Порівняльне теоретичне дослідження оксидів ZnO та BeO з точки зору електронних властивостей

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ZnO та BeO є привабливими матеріалами з огляду на їх унікальні фізичні параметри, широку пряму заборонену зону, рівну 3,37 eV та 10,6 eV для ZnO та BeO відповідно та високу енергію зв'язку екситонів. Такі параметри роблять зазначені матеріали придатними для різних застосувань, ультрафіолетового (УФ) випромінювання та виявлення, пристроїв поверхневої акустичної хвилі (SAW), датчиків газу та прозорих провідних електродів. З цих причин наша робота зосереджена на дослідженні зонної структури та щільності станів обох напівпровідників ZnO і BeO з використанням теорії функціоналу щільності (DFT) з точки зору обміну та кореляції, наближення узагальненого градієнта (GGA) та наближення локальної щільності (LDA). Розраховані структурні параметри і значення середньої довжини зв'язку добре узгоджуються з іншими даними. Такі електронні властивості, як зонна структура сполук ZnO і BeO, визначені і порівняні з наявними значеннями енергетичної зони та інтерпретуються хімічно.

Ключові слова: Густина станів (DOS), ZnO, BeO, Структурні властивості, Зонні структури.