JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **14** No 1, 01034(4pp) (2022)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **14** № 1, 01034(4cc) (2022)

Ab Initio Study of the Electronic and Optical Properties of ZnO and BeO: First Principles Calculations

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(Received 11 January 2022; revised manuscript received 25 February 2022; published online 28 February 2022)

The ab initio pseudopotential method is based on Density Functional Theory (DFT), in which the Generalized Gradient Approximation (GGA) according to the scheme described by Perdew-Burke-Ernzerhof (PBE) and the Local Density Approximation (LDA) according to the scheme described by Ceperly-Alder (CA) are used. The method is realized utilizing the Siesta program to study the structural and electronic properties of the wurtzite phase of zinc oxide (ZnO) and beryllium oxide (BeO) compounds. Indeed, it is a useful method to predict the crystal structures of ZnO and BeO. Actually, the calculated structural parameters of these compounds are consistent with the available experimental data, so these results can be considered as a good prediction. Both the lattice constants and band gaps at zero pressure are found to be consistent with previous theoretical and experimental results. In addition, the bond length is verified and compared with that of the previous work. The band structure results calculated by GGA are compared with those obtained using LDA, where the approximated values turn out to be the most accurate. The electronic properties, especially the total density of states (TDOS), show the process of electron density distribution in the region close to the Fermi level for both compounds. Comparison of the calculated lattice parameters and all electronic properties with the available experimental values reveals their compatibility. These results are in good agreement with the theoretical results.

Keywords: Density functional theory (DFT), ZnO and BeO, Density of states (DOS), Optical properties.

DOI: 10.21272/jnep.14(1).01034 PACS numbers: 71.20. – b, 78.66.Hf

1. INTRODUCTION

Recently, it has become possible to calculate and predict with great accuracy a significant number of electronic and optical parameters of materials such as semiconductors by the first-principles calculations. This type of development of simulation methods has allowed to explain and predict the properties of solids that were previously difficult to obtain empirically [1]. Wurtzite semiconductors ZnO and BeO are very important wide bandgap materials due to their applications as visible and ultraviolet light emitters, transparent field effect transistors, sensors and piezoelectric devices [2]. ZnO and BeO have taken a perfect place directly in different devices such as optical and photonic, or as a substrate for growing other semiconductors like GaN and SiC [3].

These materials, called alkaline earth oxides, play a very important role in catalysis as well. [4] From this family of compounds, we can isolate hexagonal wurtzite BeO. Studies of this semiconductor show that the Be–O chemical bond is not completely ionic but has only a somewhat covalent nature. BeO with a band gap of about 10 eV is a nonmagnetic insulator.

This work is focused on the electronic and optical properties of ZnO and BeO semiconductors using density functional theory (DFT). Many studies of these materials are carried out by both methods, theoretically and experimentally. In particular, electronic properties depend on electrical properties such as electrical conductivity and dielectric response, and on optical properties such as refractive index, damping constant, absorption, etc., which explain the response of the material to electromagnetic radiation. Also, the dielectric function explains the linear response of the system [5]. The rest of the paper is organized as follows: calculation details, results obtained by the Siesta code with their discussion and final conclusions.

2. THEORETICAL CALCULATION METHOD

The calculation method relies on the wurtzite ZnO and BeO structural and electronic properties. Actually, it is necessary to use the Full Potential Linearized Augmented Plane Wave (henceforth FP-LAPW) method for the results to be precise. The latter is then applied on the basis of DFT [6] followed by the Siesta code [7]. Ceperly-Alder (CA) of the Local Density Approximation (LDA) [8] and Perdew-Burke-Ernzerhof of the Generalized Gradient Approximation (PBE-GGA) [9] are used to calculate the exchange correlation effect. In our study, the kinetic cut-off energy for plane waves of 270 eV and k-point mesh parameters 9×9×3 were used in accordance with the Monkhorst-Pack. The total energy was converged to less than 5×10^{-6} eV per atom, while the maximum ionic Hellmann-Feynman force per atom was approximately less than 0.04 eV/A.

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3. RESULTS AND DISCUSSION

3.1 Structural Parameters

Both compounds, ZnO and BeO, crystallize in the most stable form in a hexagonal structure, as shown in Fig. 1, with the bond length between Zn, O and Be atoms, which are given in Table 1 and compared with previous experimental and theoretical values.

It is seen from the data in Table 1 that the values of the average bond length are close to the previous theoretical results and somewhat far from the applied results. Using LDA gives better results than using GGA.

Table 1– Comparison of the average bond lengths for BeO and ZnO according to GGA and LDA

Average bond length (Å)		Other works	Our works
Zn–O	GGA	2.021	1.976 [10]
	LDA	1.994	
Be–O	GGA	1.431	1.443 [11]
	LDA	1.414	

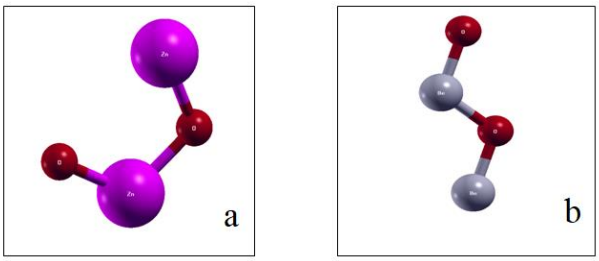

Fig. 1 – Structure of BeO (a) and ZnO (b)

As can be seen from Table 1, the calculated bond length between the oxygen and zinc atoms in ZnO compound is close in both approximations used and shows a great similarity with the theoretical results obtained earlier. The same observation is made for the distance obtained in the initial structure of BeO compound, when we find that the distance is estimated at about 1.6681 Å for LDA, while a value of 1.6602 Å is recorded for GGA.

3.2 Electronic Property

Electronic density of states (DOS) represents the number of electronic states available in the energy unit [12]. It is a function that depends only on energy, and it is a very important criterion for calculating and determining various physical properties such as electronic, optical, and material properties [13]. Fig. 2 shows the calculated DOS and related to the most stable structure obtained for each of the two compounds ZnO and BeO according to GGA, while Fig. 3 shows the calculated DOS for each of ZnO and BeO compounds according to LDA. The Fermi level is shown in the figures, it was placed at the 0 eV point by shifting all DOS relative to its value. The results obtained are very close to the results of previous studies [14, 15].

Where we see a large peak for ZnO compound followed by a smaller peak for BeO compound, in this case BeO compound is the most stable compared to ZnO compound. From a chemical point of view, a compound that has DOS close to the Fermi level is the most suitable for chemical activity and reaction, while a compound that has a low DOS at this level is considered to be chemically stable.

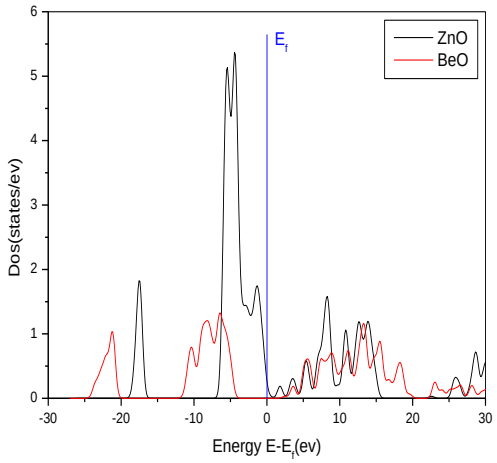

Fig. 2 – DOS for ZnO and BeO using GGA

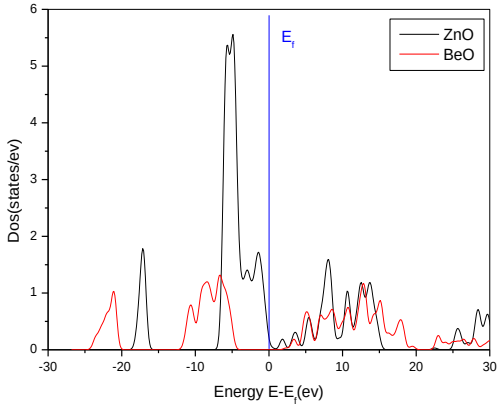

Fig. 3 – DOS for ZnO and BeO using LDA

As seen from the general form of the DOS curves of the two compounds ZnO and BeO, the presence of high peaks is detected for ZnO compound in the observed energy field, while very low peaks are recorded for BeO compound. In this case, it can be said that BeO compound is the most stable compared to ZnO compound.

From Fig. 2 and Fig. 3, we note that ZnO compound has DOS close to the Fermi level, meaning that it is more reactive from a chemical point of view, while we note that BeO compound exhibits a sharp decrease in DOS in this region, and thus it can be considered chemically stable. From the figures, we notice that ZnO and BeO compounds generally maintained DOS when using GGA and LDA, indicating that the type of approximation used in this study does not make a clear difference in the results of the calculated DOS.

We were able to extract the absorbance curve of the two compounds ZnO and BeO and compare them with previous experimental results.

From Fig. 4, we notice that ZnO has a higher light absorbance than BeO. The absorption field of ZnO is approximately within the range of 1-110 eV, that is, in the range of 11.2-1240 nm, and the largest value of its absorption is approximately within the energy limits of

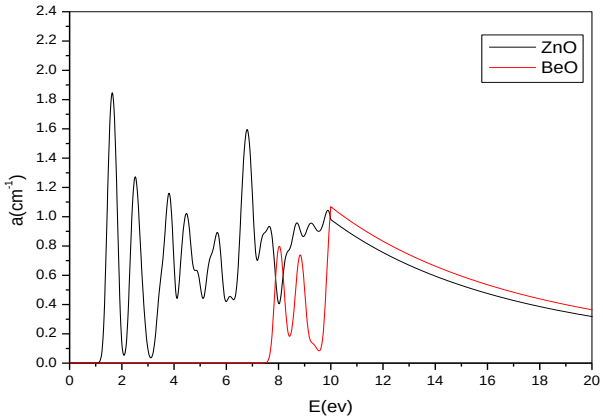

Fig. 4 – Absorbance curve for ZnO and BeO with GGA

1.5 eV, i.e., equivalent to the wavelength estimated at 826.6 nm, which is fairly close to the results of previous studies [16]. The absorption range of BeO is approximately 7-120 eV, i.e., in the range of 10.33-165.33 nm, and its largest absorbance value is approximately at an energy of 10.2 eV, i.e., at a wavelength of 121.56 nm, and these results are very close to what has been previously achieved [17].

4. CONCLUSIONS

Our work is based on the use of the Siesta code to calculate DOS and optical property of both monoxide compounds ZnO and BeO within two approximations, LDA and GGA, with their comparison with previous works. First, the average bond lengths agree well with previous theoretical results and are somewhat far from applied results. A compound having DOS close to the Fermi level is the most appropriate for chemical activity and reaction, whereas the one that has a small DOS at this level is considered to be chemically stable. BeO compound is more stable compared to ZnO compound. The absorption of the studied compounds is calculated and compared with other studies.

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Ab Initio дослідження електронних та оптичних властивостей ZnO та BeO: розрахунки з перших принципів

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Ab initio метод псевдопотенціалу заснований на теорії функціоналу щільності (DFT), в якій використовуються наближення узагальненого градієнта (GGA) за схемою, описаною Perdew-Burke-Ernzerhof (PBE), і наближення локальної щільності (LDA) за схемою, описаною Ceperly-Alder (CA). Метод реалізовано за допомогою програми Siesta для дослідження структурних та електронних властивостей фази вюрциту сполук оксиду цинку (ZnO) та оксиду берилію (BeO). Дійсно, це корисний метод для прогнозування кристалічної структури ZnO та BeO. Фактично розраховані структурні параметри цих сполук узгоджуються з наявними експериментальними даними, тому отримані результати можна вважати хорошим прогнозом. Виявлено, що як параметри решітки, так і ширина забороненої зони при нульовому тиску узгоджуються з попередніми теоретичними та експериментальними ре-

зультатами. Крім того, отримана довжина зв'язку порівнюється з результатами попередньої роботи. Результати зонної структури, розраховані за допомогою GGA, порівнюються з результатами, отриманими з використанням LDA, де наближені значення виявляються найбільш точними. Електронні властивості, особливо загальна густина станів (TDOS), показують процес розподілу електронної густини в області, близькій до рівня Фермі, для обох сполук. Порівняння розрахованих параметрів решітки та всіх електронних властивостей з наявними експериментальними значеннями виявляє узгодженість між ними. Ці результати в цілому узгоджуються з теоретичними результатами.

Ключові слова: Теорія функціоналу щільності (DFT), ZnO та BeO, Густина станів (DOS), Оптичні властивості.