

STUDY OF MgO UNDER PRESSURE STRUCTURAL AND ELECTRONIC PROPERTIES[†]

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Received April 11, 2023; revised April 26, 2023; accepted April 29, 2023

In this study, the Density Function Theory (DFT), Generalized Gradient Approximation (GGA) and Local Density Approximation (LDA) were used, based on the Siesta code, in order to study the magnesium oxide compound (MgO) and focus on the (B4) Wurtzite phase. This is to find the primary cell constants and energy gap at 0 pressure, which are consistent with previous results. The effect of pressure on the energy gap and the size of the primary cell as well as the dielectric constant were studied. The study also revealed that the (B4) phase can move to the (B2) phase at the pressure of 45.86 GPa and from the h-MgO phase to the (B2) phase at 70 GPa.

Keywords: MgO; Siesta; Structural Properties; Electronic Properties; Pressure

PACS: 71.15.Mb, 73.61.Cw

1. INTRODUCTION

In recent years, the compound MgO has emerged as one of the most intriguing oxides. Several theoretical and practical studies have been conducted on it. The majority of phases on which it crystallizes are either B1, B3 or B4. Many researchers have attempted to conduct several laboratories experiments whose goal was to search for the formed crystal structures of MgO, resulting from their deposition on metal substrates [2–5]. The B1 phase is called the rocky structure; the B3 and B4 phases are called Zinc blend and Wurtzite respectively. MgO is a solid, white mineral that is found in the earth's crust. It belongs to group (II-VI), meaning that it consists of an oxygen atom with an ionic bond. It is one of a large group of industrially important materials due to its energy gap of 7.833 eV [6].

In the ordinary case, we find that MgO crystallizes in the B1 phase, with a space group (Fm3m), under ordinary conditions. Under the influence of pressure, we find that the phase (B1) moves to (B2), but experimentally speaking, the researchers were unable to confirm such a transition. MgO compound has been studied theoretically and experimentally in order to know its electronic structure and properties. This is what was highlighted by the works [7-12]. H. Abu-Farsakh et al. [7] investigated the structural and electrical characteristics of MgO in the B1 and B2 phases, using the DFT and the LDA and Jaffe et al. [8] using both LDA and GGA in studying the two compounds MgO and ZnO under high pressure, which results in a phase transition. Through the use of the linearized augmented plane wave (FP-LAPW) approach, Zhu et al [10], also discovered the general characteristics of MgO at the B1 phase.

The structure and optoelectronic properties of MgO were also researched and verified by Liu et al. [11]. Besides, to determine the characteristics of the MgO structure, Anderson and Andreatch [12] carried out experimental research, as it is one of the prominent components of the earth's layers, so its electronic structure will inevitably and significantly change under the earth, compared to its state under high pressure. Our study theoretically explains how these transitions occur, which in turn stresses the importance of knowing the way and conditions of the occurrence of transitions between some phases of MgO compound subject to different pressure values. In fact, we will focus on Wurtzite (B4), how is it transitioned and how does its energy gap change along with the pressure changing.

2. THEORETICAL CALCULATION METHOD

We have concentrated on magnesium oxide in the Wurtzite structure, which is an appropriate host for weakly attractive semiconductors. A Wurtzite structure has two zinc particles and two oxygen ions in its unit cell, and it has P6₃mc space group evenness. We utilized test estimates for our three gem boundaries, in particular $a = b = 3.283 \text{ \AA}$, $c = 5.095 \text{ \AA}$ and $u = 0.388 \text{ \AA}$ [13]. To profit from Bloch's hypothesis in intermittent designs, we made a $2 \times 2 \times 2$ super-cell of the unit cell that contains 24 particles. The estimations were acted in the structure of thickness utilitarian hypothesis in the free molecule guess utilizing Kohn and Sham [14,15] eigen states and eigen values. Was used the Generalized Gradient Approximation by Perdew-Burke-Ernzerh (PBE-GGA) [16] and of Local Density Approximation (LDA) by Ceperley and Alder [17] are employed in the exchange correlation effect calculation. The summed-up inclination estimate and the nearby thickness guess were utilized for the trade connection energy. Likewise, we utilized an equal simultaneous molecule approach in our computations, as executed in the Rest code. Central electrons that do not have a significant

[†] Cite as: Y. Benkrima, A. Achouri, D. Belfennache, R. Yekhle, and N. Hocine, East Eur. J. Phys. 2, 215 (2023), <https://doi.org/10.26565/2312-4334-2023-2-23>

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effect on chemical and electronic properties are replaced by effective Troullier-Martins pseudo-potentials in their fully separable form in the SIESTA code [18]. In this code, a set of pseudo-atomic orbitals (PAO's) for valence electrons has been used for wave function expansion. These orbitals are built by multiplying an angular function with defined quantum values m and l , which are used to indicate the size of the orbitals, by a numerical radius function. Among the three basic set types of the code, DZP was chosen. There are two parameters of the SIESAT that need to be optimized [19]. These parameters, which correspond to the Kgrid-cutoff and Mesh-cutoff energy values, were optimized by bringing the total energy to 20, and 350 eV respectively. The convergence criterion – the total energy – is set at 10^{-4} .

3. RESULTS AND DISCUSSION

3.1. Structural Properties

Over a decade of research, the lattice constants of MgO have been confirmed numerous times [20]. The P63mc group and the lattice constants estimated to be: $a=b=3.283\text{\AA}$, $c=5.095\text{\AA}$, $\alpha = 90.03^\circ$, $\beta = 90.037^\circ$, and $\gamma = 119.90^\circ$ [13] characterize the stable main cell structure of MgO, which is (B4) Wurtzite. Each primary cell of MgO consists of four atoms, each two atoms of Mg occupy the following positions (0, 0, 0), (1/3.2/3.1/2). As far as O atoms are concerned, they occupy the following implantation positions (0, 0, μ), (1/3.2/3. μ), whereas μ is the internal variable of the Wurtzite structure, which determines the length of the bonds between Mg and O atoms. The variable μ is given as the following: $\mu = (1/4 + (c/(3.a^2)))$. The Siesta software, which was used to determine the primary cell constant constants of MgO, is a factor in the computations in this paper. The primary cell constants of MgO were calculated using the following results. The Table 1 contains the results.

Table 1. Comparison of primary cell constants of MgO with theoretical and practical results

	a (Å)	c (Å)	μ (Å)	c/a	
Present work	3.327	5.025	1.0117	1.5103	
	GGA	3.288	5.004	1.2205	
	LDA				
Theoretical works	3.281 [21]	5.1360 [21]	0.3930 [21]	/	
	GGA	3.3105 [22]	5.12363 [22]	0.3915 [22]	
	/	/	/	1.547 [21] 1.530 [13]	
Theoretical works	3.322 [20]	/	0.3916 [20]	/	
	LDA	3.249 [22]	5.277 [22]	0.3917 [22]	1.546 [20]
	3.320 [13]	5.056 [13]	0.386 [13]	1.547 [22]	
	3.322 [23]	/	0.392 [23]	1.565 [13]	
	3.169 [24]	5.175 [24]	0.3750 [24]	/	
	/	/	0.3935 [25]	1.536 [24]	
	[26] 3.278	/	/	1.506 [25]	
Experimental work	3.283 [13]	5.062 [26]	0.388 [13]	1.552 [13]	

We were able to compute the primary cell constants using the Density Function Theory (DFT) and the Siesta software, and we subsequently discovered the values of 3.327\AA for constant a and 5.025\AA for constant c . It should be noticed that these findings substantially agree with the conclusions of applied theory included in Table 1 results of previous theoretical and experimental work [13, 21-26]. Additionally, the percentage of error in the obtained values has been calculated. Assuming that they are compared to the experimental values that were used as a reference, we discovered that the error value was estimated at 1.34 percent for the constant a and 1.37 percent for the constant c with GGA. With LDA, it was calculated to be 0.15% for constant a and 1.79% for constant c . This suggests that the determined error results are likely to be minor and that the calculation's procedure was logical and reasonable.

The selected Brillion region is the primary structure to study electronic properties of the matter. The Figure 1 shows the Brillion region related to the hexagon.

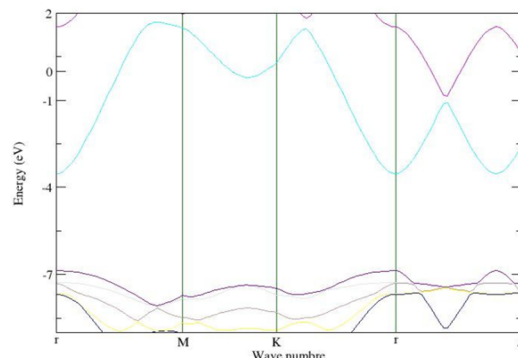


Figure 1. Energy band structure of the Wurtzite phase MgO

It is worth noting that the study of properties on this region can be generalized later to MgO. DFT and GGA were used to determine the energy gap of MgO. This method has also been relied upon because it is among the best suitable methods for studying the electronic structures of materials. The energy bands structure of MgO was calculated for the previously obtained lattice constants ($a = 3.327\text{\AA}$, $c = 5.025\text{\AA}$, $\beta = 90.037^\circ$, $\alpha = 90.03^\circ$, $\gamma = 119.90^\circ$). The structure of energy bands of MgO was calculated as shown in Figure 1.

It is noticeable in the previous figure that the highest peak of the valence band and the lowest peak of the conduction band are on the same line, passing through the point. This explains that MgO has a direct gap estimated at: 3.27 eV. The following values concern the energy gap, calculated with GGA and LDA and compared to other theoretical results, as shown in Table 2.

Table 2. The energy gap E_g (eV)

Used method	Energy gap E_g (eV)	
	GGA	LDA
Our results	3.27	/
Otherresults	4.408 [27]	/
	4.431 [28]	968.4 [28]
	4.450 [29]	5.05 [30]
	EV-GGA 5.419 [28]	
	MBJ-GGA 7.2 [28]	
Experimentalresults	7.833 [6]	
	3.48 [21]	
Proportionaleerror (%)	15.96	

We note that the value of the energy gap obtained by this theory was close to the theoretical results listed in Table 2. Our calculated results for the structure of the energy bands by GGA method are smaller than the experimental ones. This indicates that it does not provide very precise results. Unfortunately, we found that the value of the energy gap calculated by GGA is smaller compared to the experimental results. Even if we use LDA, the value of the energy band will also be less than the experimental value as well. It is well known that the GGA reduces the calculated forbidden band value compared to the experimental value, so the calculated values remain as a lower estimate of the true values of the energy gap [31].

3.3. Characteristics of MgO by changing the pressure

In a previous study, we fixed the pressure value at 0 GPa, now we will change it from 0 GPa to 100 GPa, then we study the new structural and electronic properties.

a) Variation of the dielectric constant

The value of the dielectric constant of MgO is calculated by GGA and LDA. The results are shown in Figure 2.

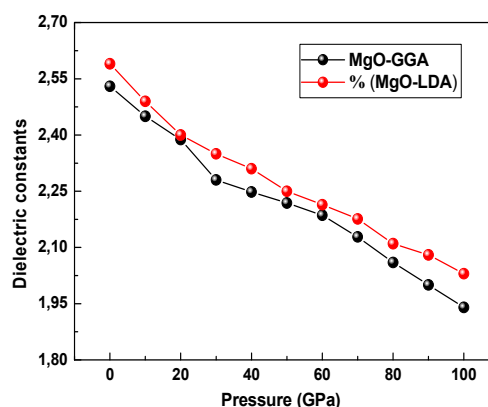


Figure 2. Variations of the dielectric constant with GGA and LDA in terms of pressure

Figure 2 displays the changes of the dielectric constant values in terms of the change of the pressure value exerted on MgO compound using GGA and LDA. We notice that the values of the dielectric constant are decreasing the more the value of the pressure exerted on the primary cell is increasing. Besides, the two curves of variations of the dielectric constant value with GGA and LDA are the same. This is consistent with the work of S. Labidi et al. [28]. The results of the values of the dielectric constant at a 0 GPa pressure value with GGA and LDA, are shown in the Table 3.

Table 3. Values of the dielectric constant at 0 GP pressure

	Our results	Theoretical results	Experimental results
Value of the dielectric constant at 0 GP (pressure)	GGA (2.53)	2.840 [28]	2.95 [32]
	LDA (2.59)	3.12 [29]	

The table shows that the values of the dielectric constant with GGA and LDA are close. Actually, the value of the dielectric constant at 0 GPa is very close to the theoretical work [28,29], and to the practical one [32].

b) Energy Gap Variation

The energy gap was calculated in terms of the pressure change of MgO by GGA and LDA, as shown in the Figure 3.

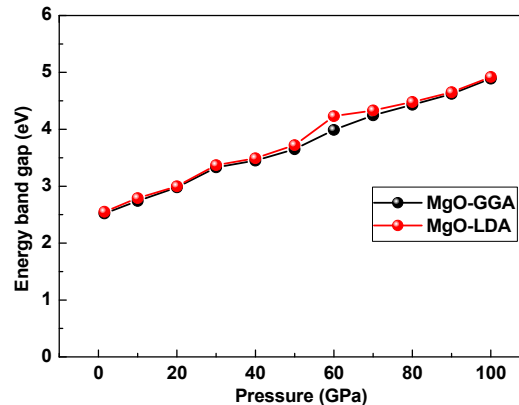


Figure 3. Energy gap by GGA and LDA in terms of pressure

The diagram shows that the greater the value of the pressure exerted on the primary cell, the higher the value of the energy gap for both curves by GGA and LDA. This is consistent with the work of S. Labidi et al [28].

c) Change in Enthalpy Energy

The changes in enthalpy energy value of MgO were calculated for the transition from B4 to B2 phase and from h-MgO phase to B2 using GGA. In order to study the possibility of structural optimization and to know the value of the pressure transition P_T of MgO from B4 to B2 phase and from h-MgO to B2 phase, we used the GGA, where an increasing pressure was applied to the MgO compound to study the phase transition from B4 to B2 structure, as well as from h-MgO to B2 structure. We performed the enthalpy calculations in the case of B2 and B4 phases, we got the curve of the Figure 4a, and in the case of B2 and h-MgO phases, we got the curve of the Figure 4b.

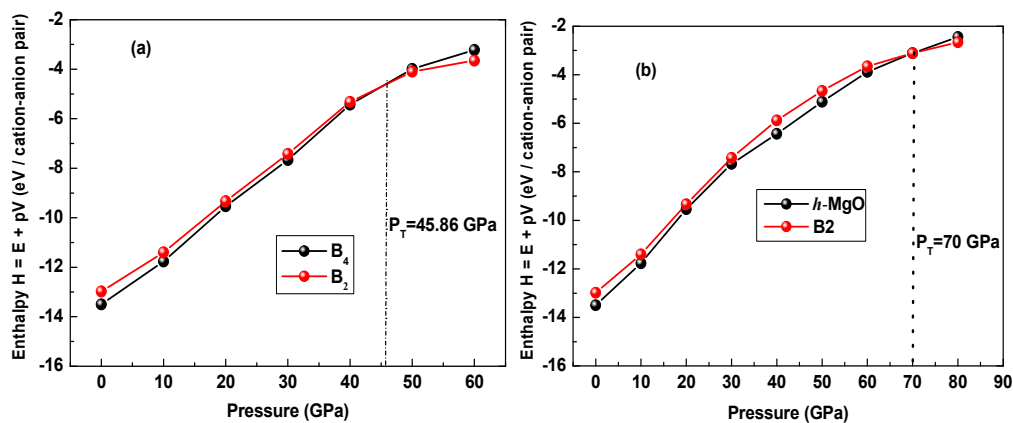


Figure 4. Enthalpy H as a function of transition pressure from: (a) – B4 to B2 phase, (b) – h-MgO to B2 phase

Studying the curves, we notice that the Figure 4. Enthalpy H as a function of transition pressure from: (a) B4 to B2 phase, (b) h-MgO to B2 phase enthalpy value of B4 phase is the lowest compared to B2 phase. In Figure b, the enthalpy value of h-MgO phase is the lowest compared to B2 phase, considering the pressure value applied to this phase from (0 GPa to 44 GPa), (0 GPa to 70 GPa), respectively. This area was characterized by the fact that each of the phases B4, h-MgO is the most stable compared to B2 phase for both curves, at the pressure value 45.86 GPa, it was observed that the enthalpy value of the phases B4 and h-MgO is exactly equal to the enthalpy value of B2 phase. For both curves, respectively, this point is the value between the phase transition from B4 or h-MgO to B2 phase. For the values from 46 GPa to 60 GPa and from 70 GPa to 80 GPa, we see that B2 structure has become the one having lower enthalpy in both Figures 4a and 4b, respectively, and therefore higher stability. This is largely consistent with the results of K.B. Joshi et al [33].

d) Size Changes

Changes in the values of the size of MgO in terms of pressure have been recorded using both GGA and LDA. Figure 5 shows those findings.

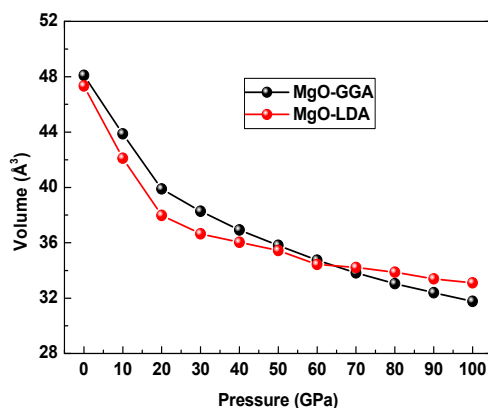


Figure 5. The size of MgO in terms of pressure using GGA and LDA

Through the curve of Figure 5, we see that whenever the value of the pressure exerted on the primary cell of the compound MgO is raised by GGA and LDA, the cell size decreases. It was also observed that the cell size in (0-62) GPa scope calculated by the GGA is larger than in the LDA, while the opposite is recorded after the pressure value reaching 63 GPa. Our results are consistent with the work of Jackson et al. [34], the Figure 3 shows that.

4. CONCLUSION

In this paper, we searched for the structural and electronic properties of the compound MgO with phase (B4) Wurtzite. The primary cell constants and the energy gap value were calculated by DFT, using GGA and LDA, with the help of Siesta program. Our results were very close with the available theoretical and experimental results. The calculations were carried out under the ordinary pressure value and other different values. The conclusions reached as summarized as follows:

- The ground state properties of the wurtzite structure such as the primary cell constants and the energy gap were found under ordinary conditions of temperature and pressure, which are consistent with previous theoretical and experimental results.
- The study also showed that the increase in the pressure value increases the energy gap value.
- The size of the primary cell is subject to change. If the structure is subjected to the influence of increasing pressure, there will be a decrease in its size.
- Calculations of the aliasing values predict the phase transition from: B4 → B2 and from: h-Mgo→B2. This is at the following pressure values: 45.86 GPa and 70 GPa, respectively.

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ДОСЛІДЖЕННЯ СТРУКТУРНИХ ТА ЕЛЕКТРОННИХ ВЛАСТИВОСТЕЙ MgO ПІД ТИСКОМ

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У цьому дослідженні використовувалися теорія функції густини (DFT), узагальнена градієнтна апроксимація (GGA) і локальна апроксимація густини (LDA) на основі коду Siesta для вивчення сполуки оксиду магнію (MgO) і зосередження на (B4) фазі Вюрцита. Це зроблено для визначення констант первинної комірки та енергетичного розриву при тиску 0, що відповідає попереднім результатам. Досліджено вплив тиску на ширину забороненої зони, розмір первинної комірки та діелектричну проникність. Дослідження також показало, що фаза (B4) може переходити у фазу (B2) при тиску 45,86 ГПа та з фази h-MgO у фазу (B2) при 70 ГПа.

Ключові слова: MgO; Siesta; структурні властивості; електронні властивості; тиск