

## Structure, electronic properties of AlAs using first-principles calculations

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**Abstract.** Density functional theory has been used to study the structural and electronic properties of AlAs using generalized gradient approximation implemented through the WIEN2k code by the local density (LDA), generalized gradient approximations (GGAPBE), and generalized gradient approximation is given by Perdew-Burke-Ernzerhof (GGAPBE Sol) methods. The AlAs's cubic structure is mechanically stable in the Fd-3m space group and exhibits semi-conducteur behavior with a 2.259 eV indirect energy band gap ( $E_G$ ) along the  $\Gamma$ -X. The optimized lattice is constant ( $a_0=5,6605\text{\AA}$ ). The properties suggest that the material is also suitable for use as a photoconductor such as diodes, laser diode, optoelectronic devices, and such as light emitting diodes.

### Introduction

Knowing the structural properties in the physics of materials is important especially if it is related to simulation because it gives us information about the microstructure of the material. In order to study the physical properties of the material (electronic, elastic, compressive...) it is necessary to go through the structural properties. In this work, we will study the physical properties of AlAs using DFT and its approximations (LDA, GGA PBE, GGA PBE SOL) and using the FP-LAPW method included in the Wien2K program that we used in our study.

We mention that the aim of this study is not to study the matter as much as a comparative study of the validity of the derivatives of the density function theory in the study of the properties of the material, so we chose a binary alloy with a cubic structure.

Semiconductors are materials that are classified between conductors and insulators in terms of electrical conductivity.

The bands, which are the transport band and the valence band between them are a forbidden band. Semiconductors are affected by temperature, light, and magnetic field [1]. They are binary materials based on aluminum, AlX, which are in group III-V. They are specific to semiconductors, i.e. they are the family found in columns III and V of the periodic table of elements. They have been studied. It has become the subject of many experimental and theoretical studies, both under normal conditions and at high pressure, because it is widely used in electronic devices and optoelectronic devices.

The III-V elements have less electronic properties compared to the I-VII and II-VI elements. Most compounds similar in composition to semiconductors take the role of insulators, and from it can be said that the forbidden band is relatively small. As for the III-V compounds, they are among the best examples of the elements that it is characterized by partially ionic or partially covalent bonds [2].



These alloys are in normal (normal) conditions (of the zinc blende structure) case B3; symmetry group F43m ( $N^{\circ}=216$ ) knowing that the zinc blende network has a face-centered cubic structure (cfc) consisting of two atoms Al and X that are centered in the positions [3]:

Al : (0,0, 0) ; (1/2,1/2,0) ; (1/2, 0,1/2) ; (0,1/2,1/2).

X : (1/4,1/4,1/4) ; (3/4,3/4,1/4) ; (3/4,1/4,3/4) ; (1/4,3/4,3/4).

### Computational Details

In this paper, we present the structural, electronic, magnetic properties of a AlAs. The calculations were carried out on the basis of density functional theory. The semi-conducteur properties have been calculated by the procedure followed in the WIEN2k [4] code based on the full potential linearized augmented plane wave (FP-LAPW) method [5].

The generalized gradient approximation given by Perdew-Burke-Ernzerhof (PBE-GGA) has been treated within the exchange and correlation operations [6,7]. R MT  $\times$  K Max was set to be 7 in the plane wave augmentation. G Max, which is the optimal magnitude in Fourier expanded density of charge, was taken to be 12 a.u.<sup>-1</sup>. The order of energy was set to 0.00001 Ry for convergence. 500 k mesh points were used for integration in the Brillouin zone.

### Results and Discussion

#### Structural Properties

The aim of studying the structural properties of these compounds is to find the crystal lattice constant, and in order to study the structural properties, we decided to calculate the lattice constant and compressibility coefficient. By using the data recorded in the table

Table 1. Structure, special group and experimental crystal lattice constant of AlAs.

/	Structure, special group	experimental crystal lattice constant a(Å)
AlAs	Fd-3m 216 Al (0, 0, 0) As (1/4,1/4,1/4)	5,6605[1]

In general, this compound crystallizes into a coherent and stable cubic structure, so the microstructure of the alloy is according to the Fig. 1

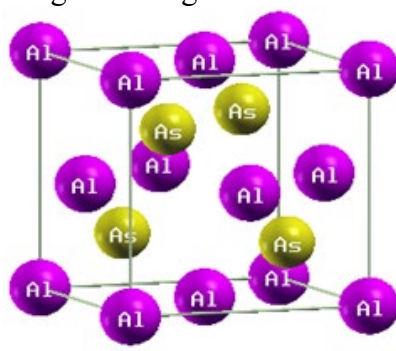


Fig. 1: Lattice view of AlAs.

The crystal structure of the AlAs, which is a semi-conducteur, is shown in Fig. 1, where the results of our calculations are given. In this structure

Al : (0,0, 0) ; (1/2,1/2,0) ; (1/2, 0,1/2) ; (0,1/2,1/2).

X : (1/4,1/4,1/4) ; (3/4,3/4,1/4) ; (3/4,1/4,3/4) ; (1/4,3/4,3/4).

In order to calculate the structural properties in the equilibrium state, experimental values of the crystal lattice constant should be established. By calculating the total energy for different values of the crystal lattice constants  $a$  (Å) next to the value of  $a_0$ , then drawing the curve of the energy values in terms of volume  $a^3$  then adapting them to the different state equations.

The results are presented in the form of four equations of state which are mentioned below and are listed in the table.

*state equations*

Define The **Murnaghan** equation given below has been used for volume optimization.

$$E(V) = E_0 + \frac{B_0 V}{B} \left[ (V/V_0)^{-B} \frac{1}{B-1} + 1 \right] - \frac{B_0 V_0}{B-1} \quad (1)$$

$B_0$  and  $B'$  compressibility modulus and the first derivative of the compressibility modulus at equilibrium

$V_0$  is the volume at equilibrium

The coefficient that expresses  $B$  is defined by the following expression:

$$B = V \frac{\delta^2 E}{\delta V^2}$$

The **Birch-Murnaghan** equation given below has been used for volume optimization

$$E(V) = E_0 + \frac{9\beta_0 V_0}{16} \left\{ \left[ \left( \frac{V}{V_0} \right)^{-2/3} - 1 \right]^3 \beta' + \left[ \left( \frac{V}{V_0} \right)^{-2/3} - 1 \right]^2 \left[ 6 - 4 \left( \frac{V}{V_0} \right)^{-2/3} \right] \right\} \quad (2)$$

The **Vinet-Rose** equation given below has been used for volume optimization

$$E(V) = E_0 + \frac{4B_0 V_0}{(\beta-1)^2} \left\{ 1 - \left[ \frac{3}{2} \left\{ 1 - \left( \frac{V}{V_0} \right)^{1/3} \right\} (\beta - 1) \right] \cdot \exp \left[ 1 - \left[ \frac{3}{2} \left\{ 1 - \left( \frac{V}{V_0} \right)^{1/3} \right\} (\beta - 1) \right] \right] \right\} \quad (3)$$

The **Poirier-Tarantola** equation given below has been used for volume optimization

$$E = E_0 + (B/14703.6) * (V_0/2) * (\ln(\eta))^{**2} + (B/14703.6) * (V_0/6) * (Bp-2) * (\ln(\eta))^{**3} \quad (4)$$

We calculated the crystal lattice constant  $a$ (Å), the compressibility modulus  $\beta$  and the first derivative of the compressibility modulus  $\beta'$

So we get the results according to the table:

*Table 1. Structure, special group and experimental crystal lattice constant of AlAs.*

	LDA			GGAPBE			GGAPBESol		
	a(Å)	$\beta$	$\beta'$	a(Å)	$\beta$	$\beta'$	a(Å)	$\beta$	$\beta'$
AlAs	5.6338 <sup>(1)</sup>	75.5430	4.5553	5.7332 <sup>(1)</sup>	71.8550	4.3825	5.6790 <sup>(1)</sup>	71.8558	4.3825
	5.6339 <sup>(2)</sup>	75.8273	4.5159	5.7330 <sup>(2)</sup>	72.0910	4.4511	5.6789 <sup>(2)</sup>	72.0910	4.4511
	5.6339 <sup>(3)</sup>	75.9565	4.4983	5.7329 <sup>(3)</sup>	72.2046	4.4841	5.6788 <sup>(3)</sup>	72.2046	4.4841
	5.6340 <sup>(4)</sup>	76.1201	4.4561	5.7328 <sup>(4)</sup>	72.3747	4.5113	5.6788 <sup>(4)</sup>	72.3747	4.5113

<sup>(1)</sup> The Murnaghan equation

<sup>(3)</sup> The Vinet-Rose equation

<sup>(2)</sup> The Birch-Murnaghan equation

<sup>(4)</sup> The Poirier-Tarantola equation

The selection of the Murnaghan, Birch-Murnaghan, Vinet-Rose, and Poirier-Tarantola equations was not important because of the convergence of the results, as most of the results obtained with the four equations were convergent on the order of  $10^{-3}$ .

Therefore, we compared the values obtained by the Murnaghan state equation for various approximations of the state density function with the experimental values, and we summarized the

results in Table 2, and drew the curve that represents the total energy changes in terms of volume for the element AlAs

We completed the calculation with three approximations (LDA), (GGA-PBE), (GGA-PBEsol) (and represented the energy curve in terms of volume as shown in documents No. IV.1, where we noticed that the energy changes curve decreases to a lower value and then increases) i.e. there is a limit value Lower Emin corresponds to a specific volume (this value corresponds to the value of the particle's ground state density since all physical properties are related to this state

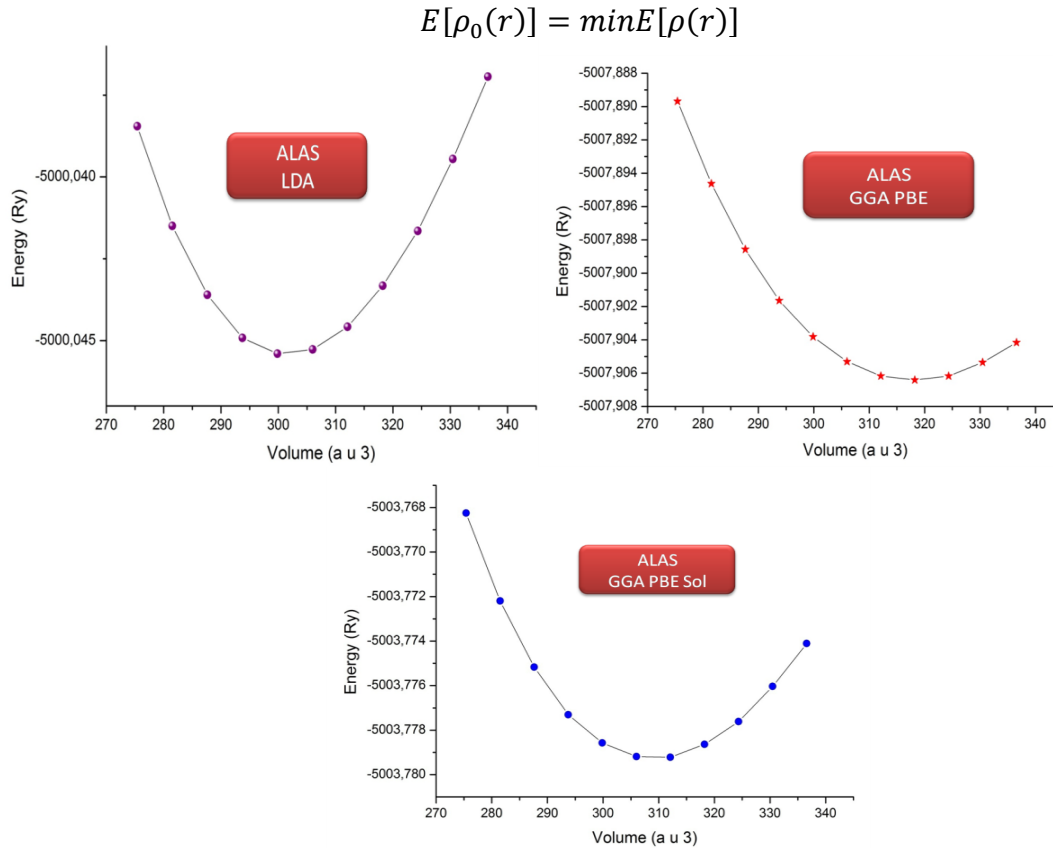


Fig. 2: Total energy changes as a function of volume for AlAs by the LDA, GGAPBE, and GGAPBE Sol methods.

We compared the results of the crystal lattice constant computationally obtained by the methods, (LDA) (GGA-PBE) and (GGA-PBEsol) (AlAs). With the experimental results, we chose to compare the corresponding results of the Murnaghan equation (Table IV.5) and recorded the following observations:

- Most of the values of the crystal lattice constant are close to the experimental results.
- The calculated values of the compressibility coefficient and the derivative of the compressibility coefficient by different methods were good and close to the theoretical values available in the references.

Table 3. Results of the crystal lattice constant by methods (LDA), (GGA-PBE), (GGA-PBEsol).

the theoretical values		GGA PBE Sol			GGA PBE			LDA			
$\beta$ $\beta'$	a(Å)	$\beta'$	$\beta$	a(Å)	$\beta'$	B	a(Å)	$\beta'$	B	a(Å)	
74±4 [8] 5.01± 1 [8]	5.6605 [1]	4.3825	71.8558	5.6790	4.3825	71.8550	5.7332	4.5553	75.5430	5.6338	AlAs

Table 4. The error ratio of the crystal lattice constant by (LDA), (GGA-PBE), (GGA-PBEsol) methods.

AlAs			/
5.6605			ao(Å)
GGA-PBEsol	GGA-PBE	LDA	method
5.6790	5.7332	5.6338	a(Å)
0.33	1.28	0.47	The error ratio %

### Electronic Properties

The importance of the electronic properties of solid materials is reflected in determining the quality of the studied material, knowing the nature of the different bonds between its atoms, these properties are explained by the structure of the bands and the state density. We used the method of linear plane waves and the full potential (FP-LAPW) in order to calculate the energy bands of the material (AlAs). ) using some DFT derivatives represented in (LDA) (GGA-PBE), and (GGA-PBEsol).

In solid physics, the theory of energy bands is the formation of energy by taking the internal electrons, from the diffusion equation  $E(K)$  and from this equation important values can be found, the most important of which are the energy ( $E_g$ , the energy gap or the energy gap), the effective mass, the valence band width, electron transmission, etc. ....

Using the value of the energy interval,  $E_g$ , it is possible to know the quality of the material, whether it is an insulator, a metal, a semi-conductor, or a semi-metal.... and justify it by studying the density of the state.

It is possible to know the quality of the materials, whether they are insulators, metals, semi-conductors, or semi-metals, and justify them by studying the density of the state.

The energy bands of AlAs are represented in Fig. 3 from the energy field boundaries [-12,14] eV.

In the case of LDA, the bands are grouped into two separate groups that share a point, the first group being in the [-12, 0] energy field.

The second group is confined from the Fermi level up to 12 eV What we notice well is the presence of an overlap between the energy band and the valence band.

As for (GGA-PBE), (GGA-PBEsol), we notice that the bands were collected in two separate groups separated by an energy barrier:

The first group in the energy field [-12, 0]

The second group is in the energy range from 1.459 eV to 12 eV and they are separated by a relatively small indirect energy gap (less than 4 eV).

The presence of a small energy separation means that the element (AlAs) has a semi-conducteur property.

The results obtained for the energy interval (energy gap)  $E_g$  for the basic energy band X,  $\Gamma$  for the LDA approximation) were non-existent. As for the two approximations (GGA-PBE), (GGA-PBEsol), its value was= 1.609 eV,  $E_g = 1.459$  eV respectively. We note that these values were less than the experimental value  $E_g(\text{exp}) = 2.22$  eV Therefore, we decided to recalculate the value of the energy interval using (TB-mBJ) in order to approximate(GGA-PBEsol), its value was  $E_g = 2.259$ eV, and thus we approached the experimental value with an error of 1.76%.

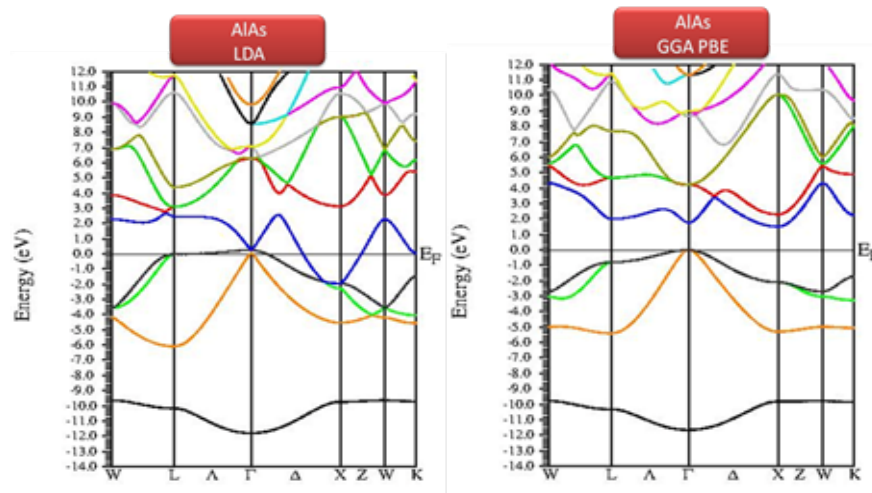


Fig. 3a: Variation of band gap energy for AlAs by the LDA, GGAPBE methods.

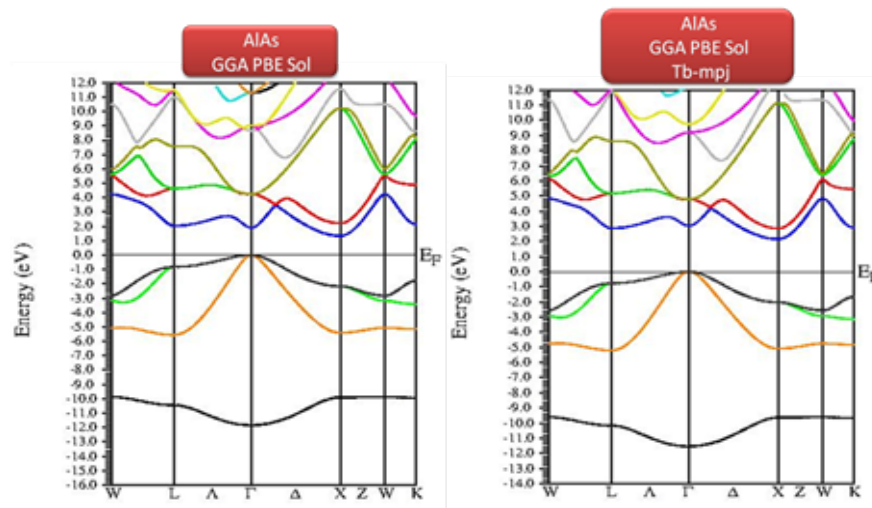


Fig. 3b: Variation of band gap energy for both methods, GGA-PBEsol, TB-mBJ.

We summarize all results in the following table:

Table 5. Results of gap energy by methods (LDA), (GGA-PBE), (GGA-PBEsol) (Tb-mbj).

	$E_g$ (LDA) eV	$E_g$ (GGA PPE) eV	$E_g$ (GGA PBE Sol) eV	$E_g$ (exp) eV	$E_g$ (Tb-mbj) eV
AlAs	0	1.609	1.459	2.22 [9]	2.259

## Conclusion

In this work, we have computed structural and electronic properties of AlAs semiconductor material. We employed first-principles calculations based on density functional theory and a systematically study. It was found that, the Lattice parameter constant and Band gap energy are consistent with previous studies.

The choice of the Murnaghan, Birch-Murnaghan, Vinet-Rose, equation of state was not Poirier-Tarantola, it is important because of the convergence of the results, as most of the results obtained with the four equations were convergent on the order of  $10^{-3}$ .

Calculate the structural properties from the crystal lattice constant  $a(\text{\AA})$ , the compressive modulus  $\beta$  and the first derivative of the compressive modulus  $\beta'$ , is not affected by the method used from the derivatives of the density function (LDA) (GGA-PBE), and (GGA-PBEsol), this means that the calculation of the structural properties is not affected by the choice of the density function of the state.

For the electronic study,  $E_g$  should be calculated for AlAs. The (LDA) method did not give any results compared to (GGA-PBE) derivatives. It gave close results that called us to use the TB-mBJ correction, which showed very close values to the experimental values.

## References

- [1] Annane F, Meradji H, Ghemid S and Hassan F E H 2010 *Comput. Mater. Sci.* 50 274 *Phys. B* 22 026201. <https://doi.org/10.1088/1674-1056/22/2/026201>
- [2] Rehamn G, Shafiq M, Saifullah M, Ahmad M, Asadadabadi S J, Maqbool M et al 2016 *J. Electron. Mater.* 45 3314; DOI: <https://doi.org/10.1007/s12034-018-1702-3>
- [3] Ziane M I, Bensaad Z, Labdelli B and Bennacer H 2014 *Sens. Transducers J.* 27 374. <https://doi.org/10.1063/1.5006170>
- [4] Ferreira L, Wei S H and Zunger A 1998 *Phys. Rev. B* 40 3197 *Phys. Rev. B* 40, 3197 – Published 15 August 1989. <https://doi.org/10.1103/PhysRevB.40.3197>
- [5] D. Singh, *Planes Waves, Pseudo-Potentials and the LAPW Method*, Kluwer Academic Publishers, Boston, Dortrecht, London, 1994. Hieder Al-Shami, Ahmed M. Salah, Mohamed Fathy Adel Ali *Open Journal of Modern Neurosurgery* Vol.10 No.3, May 8, 2020. <https://doi.org/10.4236/ojmn.2020.103034>
- [6] J.P. Perdew, K. Burke, Y. Wang, *Phys. Rev. B* 54 (1996) 16533. Received 14 February 1996. <https://doi.org/10.1103/PhysRevB.54.16533>
- [7] J.P. Perdew, S. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 77 (1996) 3865. Received 21 May 1996. <https://doi.org/10.1103/PhysRevLett.77.3865>
- [8] R.G. Greene, H. Luo, T. Li, A. Ruoff, *Phys. Rev. Lett.* 72, 2045 (1994) High pressure structural study of AlSb to 50 Gpa. [https://doi.org/10.1016/0022-3697\(94\)00231-2](https://doi.org/10.1016/0022-3697(94)00231-2)
- [9] B. Monemar, *Phys. Rev. B* 8, 5711 (1973) . Received 7 May 1973. <https://doi.org/10.1103/PhysRevB.8.5711>
- [10] Joyce J H, Docherty C J, Gao Q, Tan H H, Jagadish C, Hughes, J L et al 2013 *Nanotechnology* 24 214006. <https://doi.org/10.1007/s12034-018-1702-3>
- [11] Garriga M, Lautenschlager P, Cardona M and Ploog K 1987 *Solid State Commun.* 63 157 *Journal of Applied Physics* 42, 3499 (1971). <https://doi.org/10.1063/1.1660760>
- [12] Adachi S 1987 *Phys. Rev. B* 35 7454 *Phys. Rev. B* 35, 7454 – Published 15 May 1987 Received 10 November 1986. <https://doi.org/10.1103/PhysRevB.35.7454>

- [13] Joyce J H, Docherty C J, Gao Q, Tan H H, Jagadish C, Hughes J L et al 2013 Nanotechnology 24 214006 Semiconductor Science and Technology, Volume 31, Number 10 Citation Hannah J Joyce et al 2016 Semicond. Sci. Technol. 31 103003. <https://doi.org/10.1088/0268-1242/31/10/103003>
- [14] Garriga M, Lautenschlager P, Cardona M and Ploog K 1987 Solid State Commun. 63 157. <https://doi.org/10.1007/BF00615025>
- [15] Djuricic A B, Rakic A D, Kwok P C K, Li E H and Majewski M L 1999 J. Appl. Phys. 85 3638 Journal of Applied Physics 88, 2172 (2000). <https://doi.org/10.1063/1.1305544>
- [16] Ahmed R, Hashemifar S J, Akbarzadeh H, Ahmad M and Aleem F 2007 Comput. Mater. Sci. 39 580. <https://doi.org/10.1063/1.4757439>