International Journal of Engineering and Applied Physics (IJEAP)
Vol. 2, No. 3, September 2022, pp. 555~565
ISSN: 2737-8071

Structural and Electronic Properties of Gallium Phosphate Semiconductor in Wurtzite, Rock Salt and Zinc Blende

Solomon Tahiru Tonga[1], Yohanna Jacob Baro[2]
[1]Department of Physics, Taraba State University, Jalingo, Nigeria.
[2]Department of Theoretical and Applied Physics, AUST, Abuja, Nigeria

Article Info

Article history:

Received Jul 6, 2022
Revised jul 22, 2022
Accepted Sep 01, 2022

Keywords:

Gallium Phosphate
Pseudo-Potential
Band gap
Density functional theory
Semiconductor

ABSTRACT

First principle method was used to study the structural and electronic properties of Gallium Phosphate in Wurtzite, zinc blende and rock salt using the molecular dynamics density functional theory implemented on the Quantum Espresso software. For this work the choice of the pseudo-potential is the GGA, scf calculation was used for zinc blende and rock salt to test the convergence of kinetic energy cut-off, lattice parameter, number of k-point with respect to 1mRy energy and 0.5kbar pressure. The same was repeated in wurtzite but vc-relax was used, all the plots obtained for the three structure converges towards the set threshold, the plot of band structure and density of state reveals that rock salt is a metal due to absence of band gap while other are semi-conductors with an indirect band gap, a plot of energy versus enthalpy shows that there's a transition from zinc blende to rock salt with about 18.73% decrease in volume from zinc blende to rock salt and this occur at a pressure of 29.07GPa, it is noteworthy that Gallium Phosphate was found to be more stable in zinc blende

Corresponding Author:

Solomon Tahiru Tonga,
Department of Physics,
Taraba State University,
Jalingo, Nigeria.
Email: stahiru@aust.edu.ng

1. INTRODUCTION

Knowledge of physical properties of crystalline materials plays a vital role in developing new technologies. Such materials include III-phosphide binary compounds, namely boron phosphide (BP), aluminum phosphide (AlP), gallium phosphide (GaP) and indium phosphide InP, which are common-anion III–V semiconductors. At ambient conditions, these compounds crystallize in the zincblende structure with a space group F434m [1–3] and have an indirect band gap, with the exception of InP. Recently, these compounds have attracted a great deal of attention, anticipating fabrication of important electronic devices. Boron phosphide is classified as a refractory material and has resemblance with silicon carbide electronically [4,6]. Like boron arsenide and boron antimonide, BP shows a strong covalent nature and exhibits an unusual behavior due to small core and absence of p electrons in the core of the boron atom compared to other III–V compounds [5]. Similarly, GaP is in use as a material for light-emitting diodes, and InP has particular importance in the designing of transferred-electron devices [7]. Motivated by the

technological significance of these materials, III- phosphides have been the subject of various theoretical investigations, from empirical [8] to first-principles based on the density functional theory (DFT) [9,10]. Most of these studies have been undertaken using the pseudo-potential [11] or full-potential linearized-augmented plane wave (FP-LAPW) method; one of the most accurate computational schemes for the study of crystalline solids, within local density approximation (LDA) [12] or generalized gradient approximation (GGA) [13]. Although LDA and GGA give good results for ground state properties, usually they underestimate energy band gap values. Another form of GGA proposed by Engel and Vosko (GGA-EV) [13] successfully explains the electronic properties of different solids. To the best of our knowledge, GGA-EV has not yet been used for theoretical study of the electronic properties of III-phosphides. For structural properties only few computational investigations using GGA [13] have been reported. This article will focus on the study of gallium phosphide

2. COMPUTATIONAL DETAIL

Ab initio calculations were performed using numerical-atomic-orbital density- functional method and implemented in the QUANTUM ESPRESSO code [15,16]. We have used local density approximation with exchange correlation, as parameterized by Perdew and Zunger [16]. Semiconductor structures are obtained by minimization of the total energy using Hellmann Feynman forces including pulay-like corrections. Structural optimizations were performed using the conjugate gradient algorithm until the residual forces in the optimization are smaller than 0.04 eV/Angstrong.The choice of pseudopotential used was the ultra-soft non – relativistic and it was used for each of the element forming the compound semiconductor, using the above pseudopotential a reasonable value of lattice parameter in (au) and brillioun zone sampling was fixed and kinetic energy cutt-off was varied unless a convergence was reached, with the converged value of energy cut-off fixed number of kpoints and lattice parameter too were varied unless a convergence was achieved. For the purpose of this article a convergence of 1mRy and 0.5kbar with respect to energy and pressure was considered. For the case of the wurtzite structure, it has two lattice parameter (c=12.56au and a=7.40au so that c/a=1.70) after fixing the two converge value of the lattice parameter, vc-relax was used and pressure was also varied. For the remaining structures, scf was used and convergence was reached. With all the parameters fixed the energy volume dependence was investigated and the plot of band structure and density of state reveals some properties of the compound its transition from one phase to another.

3. RESULTS AND DISCUSSIONS

3.1. X-crysden structure for Wurtzite, Zinc Blende and Rock Salt

The crystal structure of GaP was viewed using the x-crysden instruction[17-21] in the Quantum Espresso package based on the information provided. Below are the different structures of GaP.

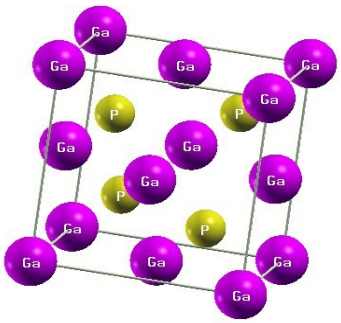

Figure 3.1: GaP in a Wurtzite

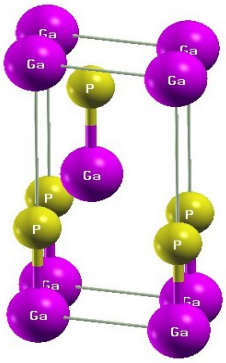

Figure 3.2: GaP in a Zinc-Blende

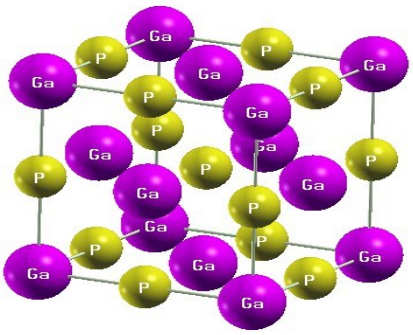

Figure3.3: GaP in a Rock-Salt

3.2 Convergence of kinetic energy cut-off

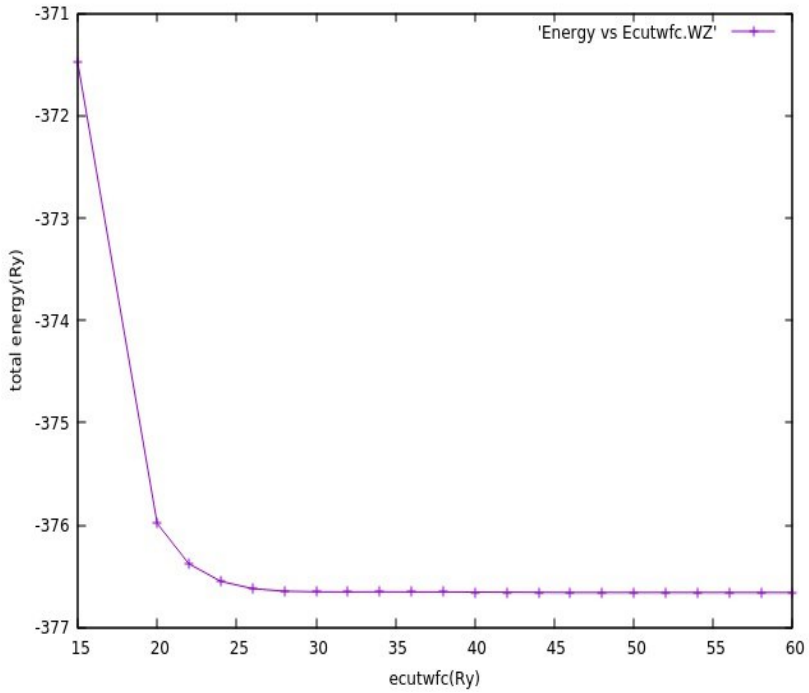

Figure 3.4 ecutwfc for wurtzite

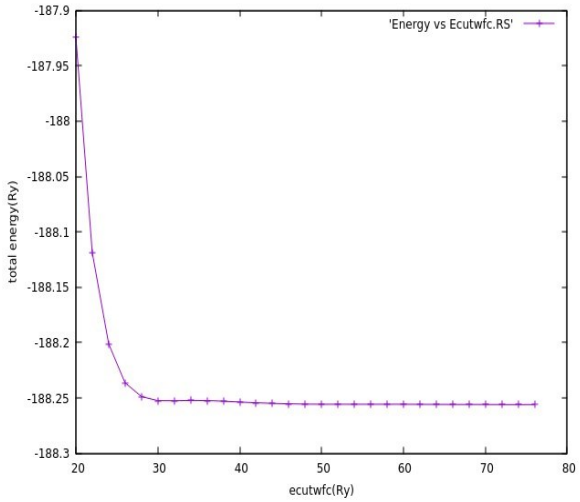

Figure 3.5 ecutwfc rocksalt

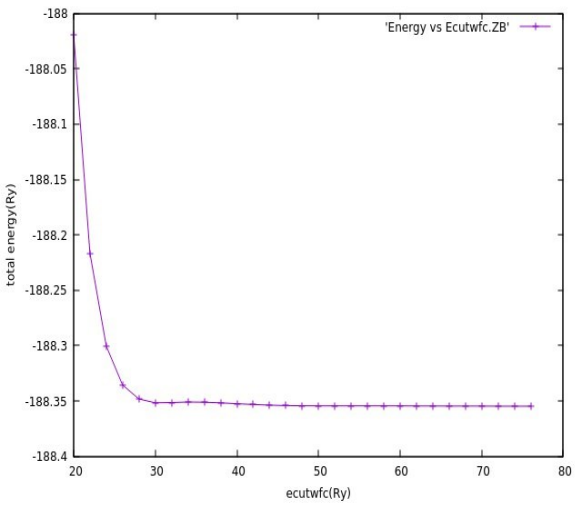

Figure 3.6 ecutwfc zincblende

3.3 Convergence with respect to number of k-point

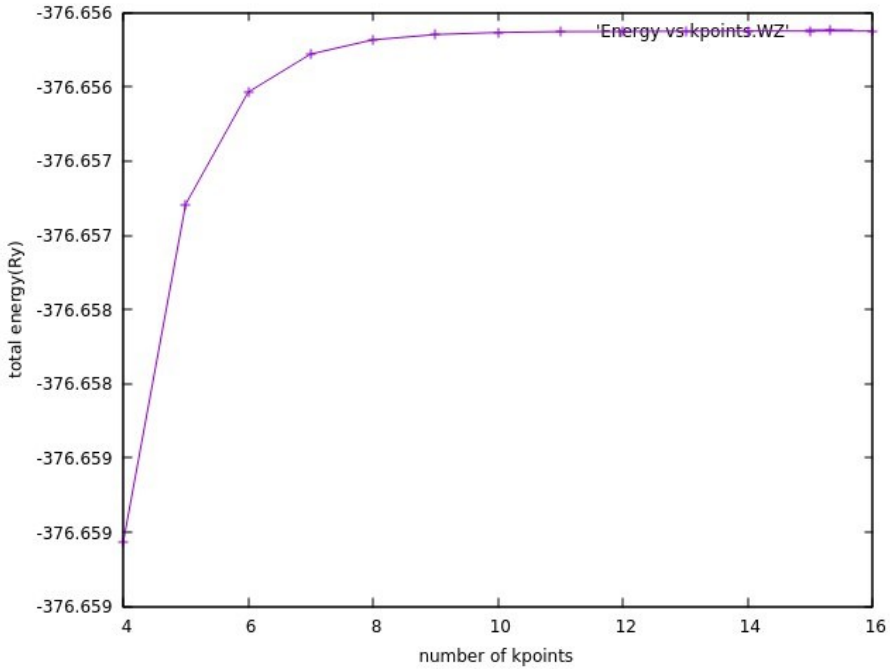

Figure 3.7: number of kpoints for wurtzite

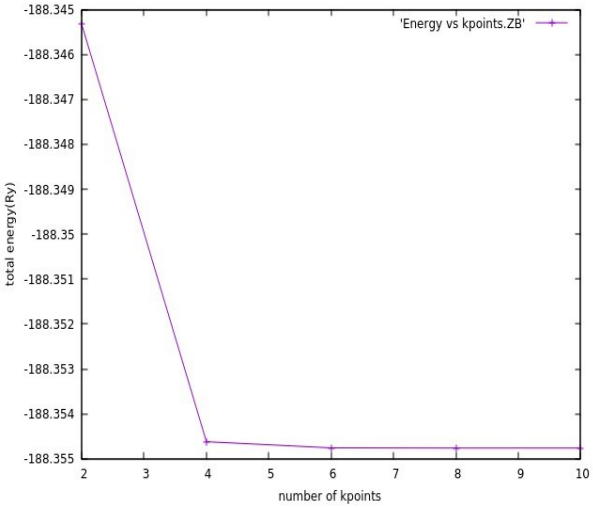

Figure 3.8: number of kpoints for zincblende

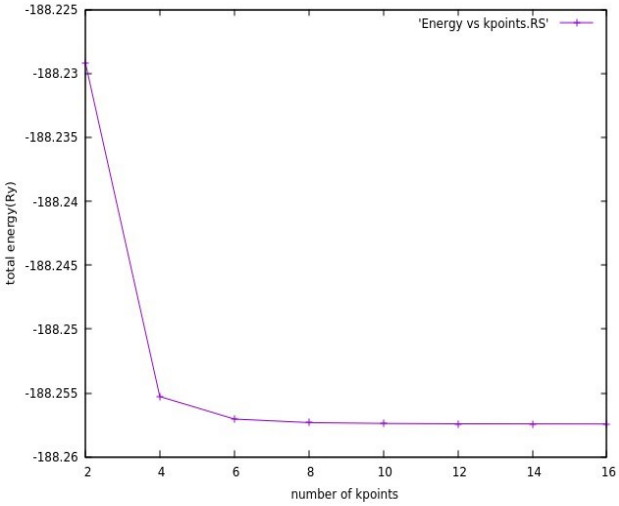

Figure 3.9: number of kpoints

3.4 Convergence with respect to lattice parameter

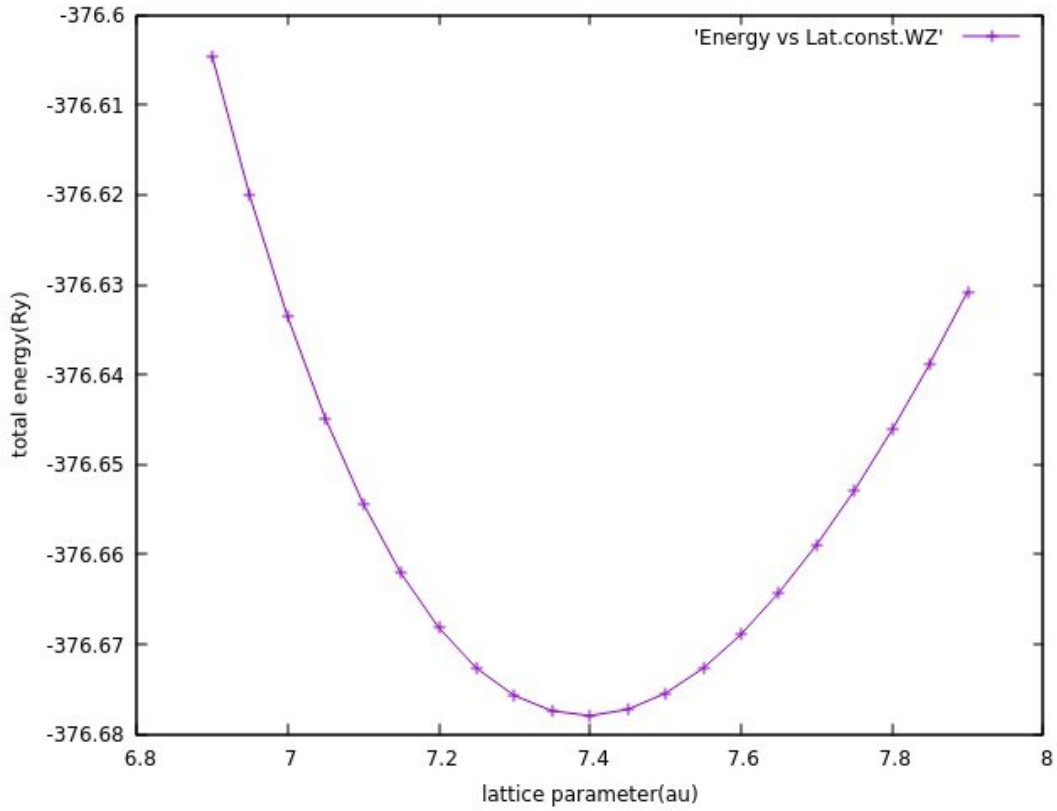

Figure 3.10 lattice parameter for wurtzite

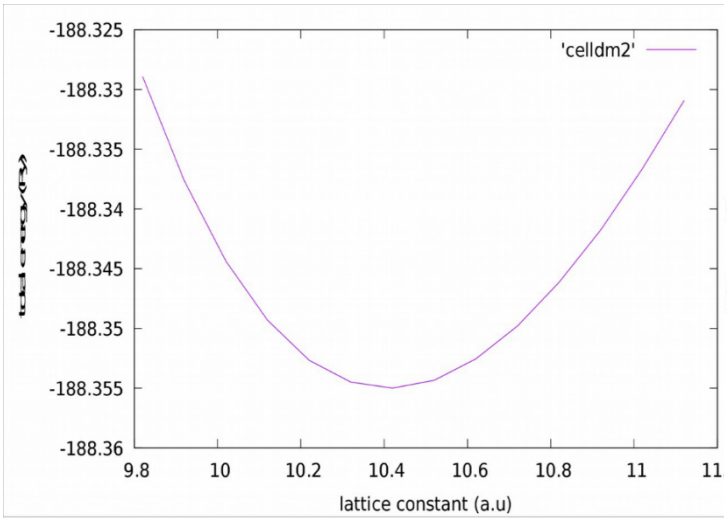

Figure 3.11: alat for zincblende

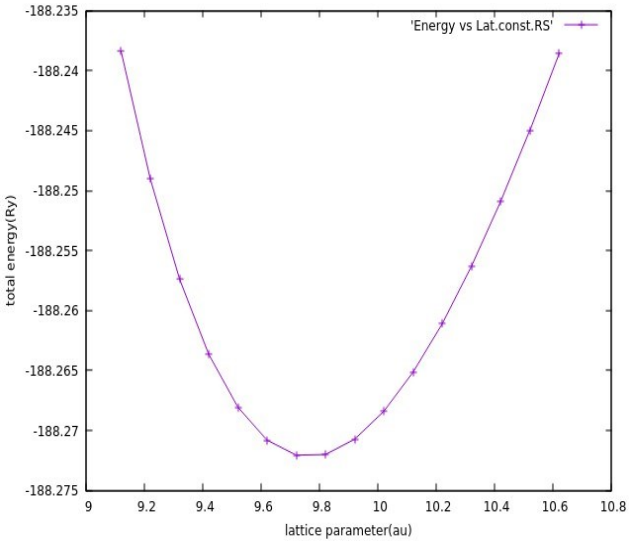

Figure 3.12: lattice alat for rocksalt

3.5 Enthalpy-Pressure for the three structures

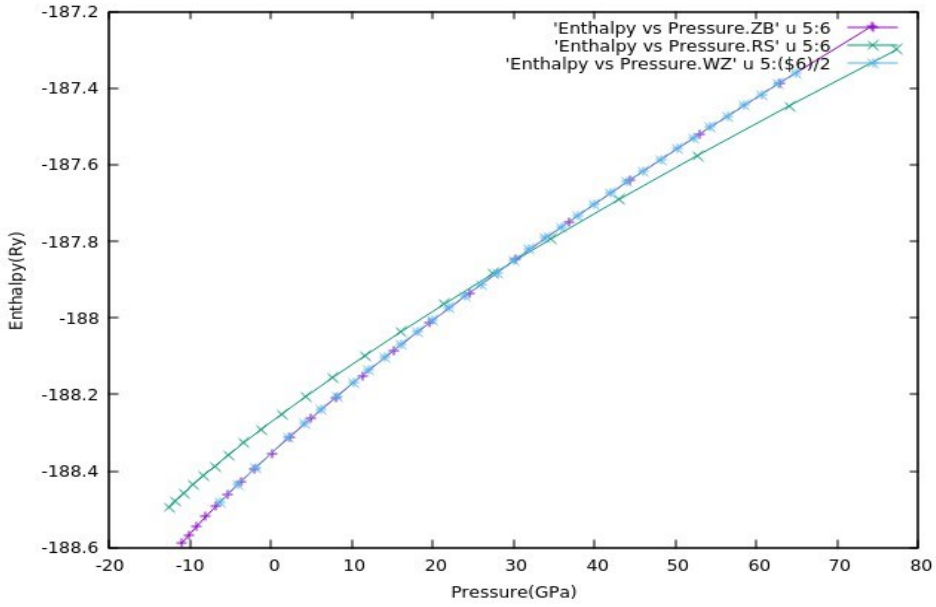

Figure 3.13 Energy – Enthalpy for the three structures

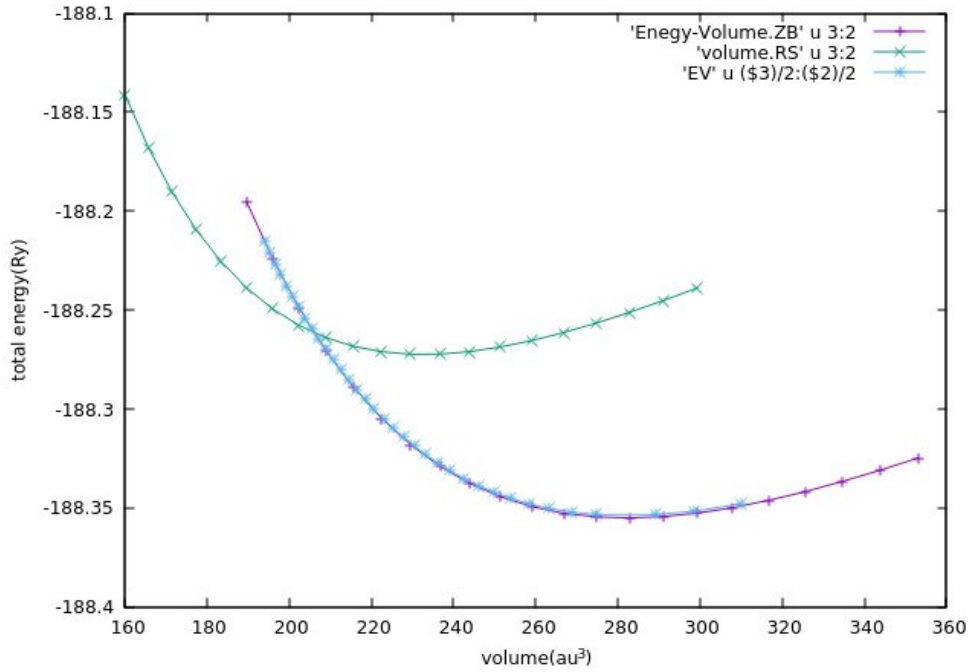

Figure 3.14 Energy-Volume for the three structures

3.6 Density of State

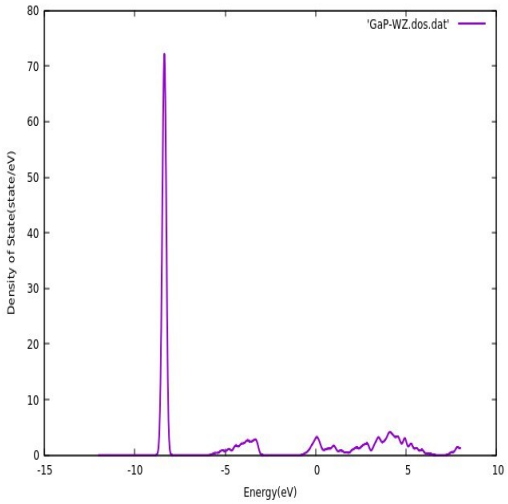

Figure 3.16 Density of State for wurtzite

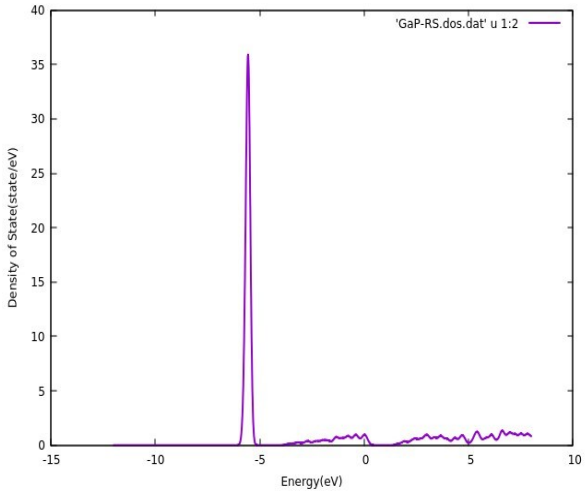

Figure 3.17 Density of State for Rock Salt

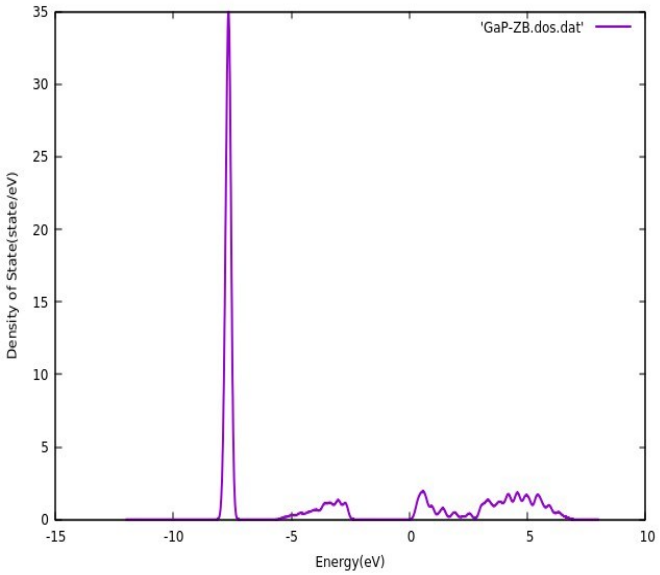

Figure 3.17 Density of State for Rock Salt

3.7 Band Structure

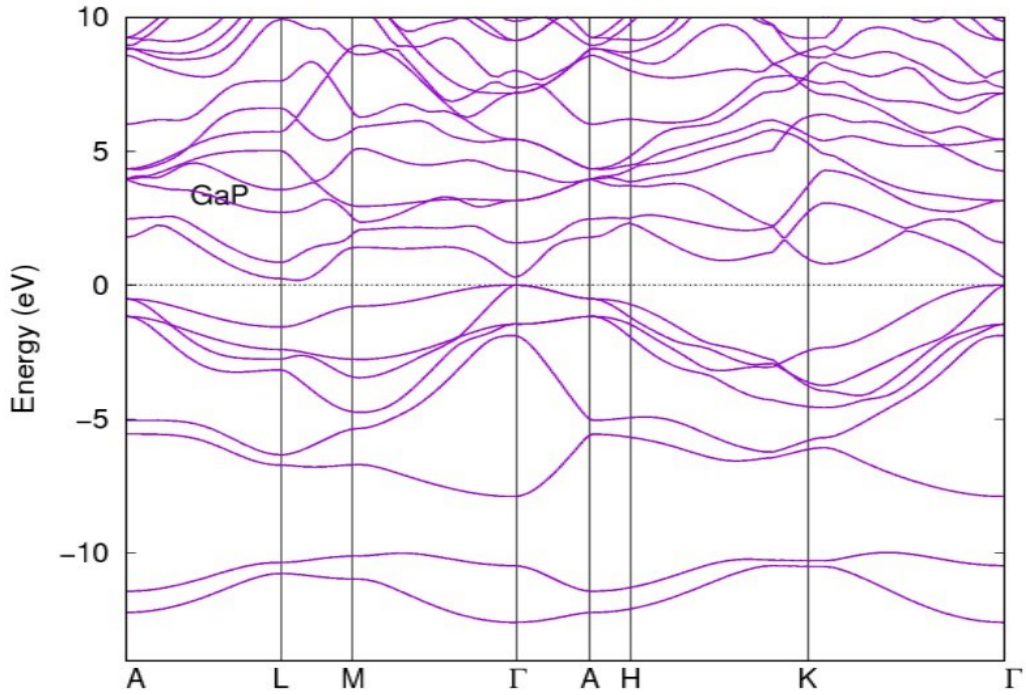

Figure 3.19: Band Structure for Wurtzite

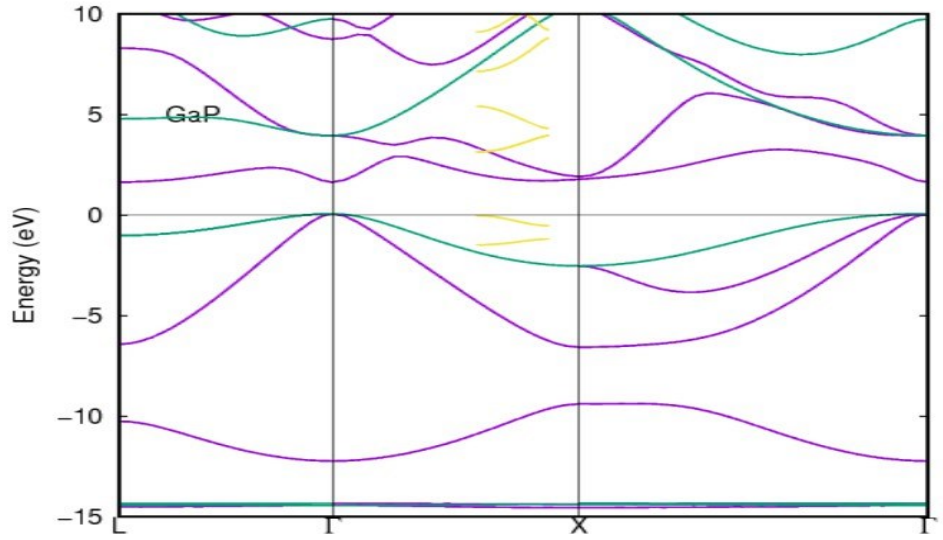

Figure 3.20: Band Structure for Zinc Blende

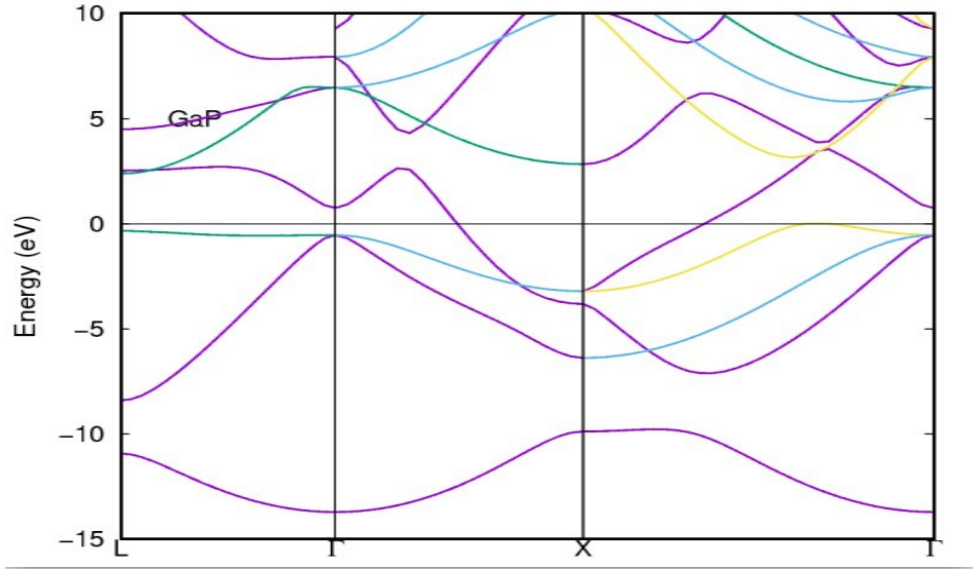

Figure 3.21: Band Structure for Rock Sal

Table 3.1: Comparison between current and experimental value of lattice parameter and band gap

Structure	Lattice Parameter - alat(au)		Band GaP (eV)		Type
	Current value	experimental value	Current value	Experimental value	
Wurtzite	7.40 (a)	7.11(a)	0.2	1.40	Indirect
	1.70(c/a)	1.64(c/a)			
Zinc Blende	10.40	10.30	1.97	2.26	Indirect
Rock Salt	9.77	9.37			

The above table shows the comparison between current i.e values used in this work and the experimental value of lattice parameter and the band gap for the three structures. The type of the band gap in this work is the indirect band gap I, hence the use of I in table 3.1

3.8 Discussion

Convergence test

In figure 3.4 above (wurtzite) it can be seen that the plot of the kinetic energy cut – off converges to a value of 46 Ry when the convergence of 1mRy was considered so also the same result was realized for the case of zinc blende in figure 3.6 above but this is different for the case of rock salt in figure 3.5, when convergence with respect to 1mRy was considered, the ecutwfc was found to converge at 48Ry.

For the number of kpoints there was a convergence at (6*6*6) ,(8*8*8) and (8*8*8) for wurtzite, zinc blende and rock salt respectively as in figure 3.7, 3.8 and 3.9 of the plots.

The lattice parameter values 'a' in the unit of atomic unit(au) that corresponds to the minimum energies for wurtzite, zinc blende and rock salt are 7.40, 10.40 and 9.77 respectively as in figure3.10, 3.11 and 3.12

Stability

The plot of energy versus volume in figure 3.17 shows the stability of zinc blende in which form the original compound semiconductor was found.

Phase Transition

Using the first principle (PP-PW) method the electronic structure of GaP in wurtzite, zinc blende and rock salt was studied at various pressure ranges as in figure 3.16.

The phase transition that occurs in this case was from zinc blende to rocksalt which occurs at pressure of 29.07GPa which exhibit 18.73% volume decrease of ZB to RS. From other literature search the transition occur at 21.9GPa and 14.11% volume decrease of ZB to RS was exhibited but the method used was full potential linearized augmented plane wave (FP-LAPW) that could possibly be the cause for the disparity

Band structure and density of state

The density of state and the band structure for the three structures was plotted as seen in figure 3.15, 3.16, 3.17, 3.18, 3.19 and 3.20 which reveals that the rock salt structure is metallic due to the absence of band gap and zinc blende is a semiconductor with a band gap of approximately 1.97 eV which is bigger than that of wurtzite also a semiconductor which was found to be approximately0.2eV far less than the experimental value of about 1.40eV this could possibly be due the fact that LDA and GGA underestimate the value of band gap.

1. CONCLUSION Conclusion

The aimed of this work has been achieved since the various converged parameters were used to confirmed the stability of Gallium Phosphide in zinc blende structure and the band gap was found to be just a little less than the experimental value which is due to the fact that LDA and GGA underestimate the values of band gap and even other parameters applies.

ACKNOWLEDGEMENTS

We want to acknowledge African University of Science and Technology, Abuja-Nigeria for giving us the opportunity to conduct this research

REFERENCES

[1] R.W.G. Wyckoff, Crystal Structures, second ed., Krieger, Malabar, (1986).

[2] O. Madelung, Semiconductors: Data Handbook, Springer, Berlin, (2004).

[3] O. Madelung, Landolt-Bornstein, Numerical Data and Functional Relationships in Science and Technology New Series, Springer, Berlin, (1982).

[4] E. Schroten, A. Geossens, J. Schoonman, J. Appl. Phys. 83 (3) (1998) 1660 (references given therein).

[5] B. Bouhafs, H. Aourag, M. Cartier, J. Phys.: Condens. Matter 12, 5655 (2000)

[6] R.M. Wentzcovitch, M.L. Cohen, J. Phys. C: Solid State Phys. 19, 6791 (1986).

[7] L. Lin, G.T. Woods, T.A. Callcott, Phys. Rev. B 63, 235107 (2001).

[8] M. Ferhat, A. Zaoui, M. Certier, H. Aourag, Physica B 252, 229 (1998)

[9] P. Hohenberg, W. Kohn, Phys. Rev. 136, 864 (1964).
[10] W. Kohn, L.J. Sham, Phys. Rev. A 140, 1133 (1965).
[11] W.E. Pickett, Comput. Phys. Rep. 9, 117 (1989).
[12] J.P. Perdew, Y. Wang, Phys. Rev. B 45, 13244 (1992).
[13] J.P. Perdew, K. Burke, M. Emzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[14] E. Engel, S.H. Vosko, Phys. Rev. B 47, 13164 (1993).
[15] Y. Juan, E. Kaxiras Phys. Rev. B, 48, 14944, (1993).
[16] P. D. Ye, J. Vac. Sci. Technol. A, 26, 696, (2008).
[17] J. Phys.: Condens. Matter 14, 9579–9587 (2002).
[18] H.J. Kim, B.J. Kim, T.W. Kim, K.H. Yoo, Appl. Surf. Sci. 255, 5048 (2009).
[19] S. Fridjine, S. Touihri, K. Boubaker, M. Amlouk, J. Cryst. Growth 312, 202 (2010).
[20] S. Park, H. Kim, C. Jin, C. Lee, Curr. Appl. Phys. 12, 499 (2012).
[21] K.M.M. Abo-Hassan, M.R. Muhamad, S. Radhakrishna, Physica B 358, 256 (2005).