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INVESTIGATIONS OF STRUCTURAL AND ELECTRONIC PROPERTIES OF III – Bi SEMICONDUCTOR BINARY COMPOUNDS USING DENSITY FUNCTIONAL THEORY

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ABSTRACT

Study of semiconductors physics is very important as it forms the basis for power and low current engineering. Semiconductors and their compounds are of enormous importance to information technology (IT) and Opto-electronics. To this end, band-gaps play prominent role in determining some characteristic properties of these components and devices, such properties include conductivities and optical wavelengths (Madouri D. B., 2008). In this research, structural and electronic properties of binary compounds of III-Bi semiconductors were investigated with a view to know the influence of pseudopotentials on the investigated properties of the selected compounds using first-principles (ab initio) method as embedded in Quantum espresso package. The investigated results which agreed with experiments show that the bulk moduli decrease while lattice constants increase with increasing atomic orbital's from BBi to InBi. Interestingly, only BBi has direct energy gap while the d-orbitals have spin-orbit splitting, an attribute of spintronic devies. Though the band gaps were under estimated as predicted in some related published work, precision of the predictive power of the investigating software tool needs further improvement so that the data obtained will be better relied on and form the starting point for the manufacturing/fabrication industries in Nigeria where the alternative commercial ab-intio simulation software may prove too expensive.

Keywords: *First-Principles, Energy Gaps, Phonon Frequency, Band Structures, Pseudopotentials and Quantum Espresso.*

INTRODUCTION

Semiconductor family is important in the world of information technology both at micro and nano-scale levels, (Catalan, Seidel, Ramesh, & Scott, 2012). Literature revealed that III-V semiconductors are so far good materials for electronic devices fabrications. Technologies of fabrication with a view to increase efficiency of these devices become imminent in view of larger demand for high current devices that can withstand high temperature condition. Semiconductors can be made magnetic either by doping or sp-d exchange and III-V diluted magnetic semiconductors can be modeled using computational tools, (Ohno, 2011). One incentive for studies in the field of condensed matter was and still is the investigation and development of materials for the next generation of IBM computers (Ludwig, 2011). In section one introduction essence of the research have been enumerated. In section two, background to the study was dealt with methodology, results and discussions followed while the conclusion of the work ended the main body of the research. In Born-Oppenheimer approximation equation1, the nuclei as fixed at positions R_i and electrons

$$\widehat{H} = \sum_i \frac{P_i^2}{2m} + \sum_j \frac{P^2}{2M_J} + \frac{1}{2}\sum_j \frac{Z_j Z_j e^2}{4\pi\varepsilon_O |Rj - Rj|} - \sum_{j,i} \frac{Z_j e^2}{4\pi\varepsilon_O |r_i - R_j|} + \frac{1}{2}\sum_{i,j}^{/} \frac{e^2}{4\pi\varepsilon_O |r_i - r_i|} \ldots (1)$$

are separated into the valence and rigid particles called the frozen core electrons (filled shells). Green's function technique, in which one-and two-particle green's functions are used to calculate the measurable quantities, though can be applied to infinite system, requires a large computational effort unlike density functional theory which can treat these systems with less computational effort when applied on homogeneous systems like atoms, molecules and solids (Kohn, 1999). Kohn - Sham density functional theory is an empirical methodology which does not depend on the materials being studied a property associated with ab-initio theory or first principles methods, (Harrison, 2005). From the failure of Hohenberg-Kohn equation, Kohn and Sham developed a good approximation for the functional $F[n]$ by introducing an auxiliary system of non-interacting electrons which has the same ground state density as the interacting one (Kohn W. , 1999). In DFT, total energy of the system is expanded as a functional of the charge density $\rho(r)$:

$$E(\rho) = T_{KS}(\rho) + \int dr\, V_{ext}(r)\rho(r) + V_H + E_{xc}(\rho) \ldots\ldots\ldots\ldots\ldots\ldots (2a)$$

$$V_{KS} = V_{ext}(r) + e^2 \int \frac{\rho(r^{\prime})}{|r - r^{\prime}|} dr^{\prime} + \frac{\delta E_{xc}(\rho)}{\delta\rho(r)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2b)$$

$V_{xc}(r) = \frac{\delta E_{xc}(\rho)}{\delta\rho(r)}$.

The term V_{xc} and the corresponding E_{xc} are the only unknown in K-S approach to DFT.

LITERATURE REVIEW

To the best of our knowledge band structure calculations of (Al, Ga, and In)-V binary compounds (Remediakis & Efthmios, 1999), excluding (Al, Ga, In)Bi while bandgaps and ionicities of Boron-V compounds (Madouri & Ferhat, 2005) had been investigated. Bi-III

compounds had received little attention and from literature most of the Bi-III compounds should have a small or even negative band-gap. Combinations of Bi with III-V compounds yield interesting new semiconductor alloys which contain semiconductor and semimetal compounds. Therefore III-(Bi-V) alloys have been predicted to be strong potential candidate materials for the active region of diode lasers and photo-detectors operating in the infrared and near infrared, (Madouri & Ferhat, 2005). Band structure of the stable zinc-blende phase of BBi in the absence of spin orbit interaction, revealed that the compound is direct band-gap with a small optical transition of 0.13eV in contrast to other boron-V compounds which are indirect band-gaps. This unusual behaviour is a consequence of the relativistic contraction of the 6s orbital of Bi which has an effective chemical valence of 3 rather than 5 like other atoms of group V, (Madouri D. B., 2008).

METHODOLOGY

First-principles total energy calculations were performed within the frame work of density functional theory using Perdew and Zunger local density approximation and Perdew Born Enzhorf generalized gradient approximation. For each calculation, irreducible k-points were generated according to the Monkhorst-Park (MP) scheme. Since convergence with respect to energy cut-off is a property of pseudopotentials, it was carefully performed for each compound up to the energy difference of 0.0001Ry for hard pseudopotentials. Equilibrium lattice constants, (a_o), bulk modulus (B_o) and their pressure derivatives ($B_o^{\prime}$) were calculated using the standard procedure by fitting total energy-volume to a Murnaghan's equation of states.

RESULTS

Tables (I-V) below show the results of the calculations.

Table 1: Parameters for pseudopotential generation

Atoms	orbital's cut-off radius		
	s	p	d
Si	2.20*	2.40*	-
Ge	2.25*	2.55*	2.50*
In	1.90^{x}, 1.85*	2.30^{x}, 2.20*	1.80^{x}

In table I, s and p orbital's cut-off radii for Indium compared well with other work.

[x] (Xifan Wu, 2009), *This work

Table II: Comparison of calculated **Structural parameters with Experiments and Other Works**

Alloys	**Experimetal lat const(*Å*)**	**Calculated Lat const (*Å***	**B_o(GPa)**	**B_o'**
BBipz	-	5.40*, 5.416[2]	83.8*, 86.27[2]	5.08*, 4.73[2]
BBipbe	-	5.638*, 5.529[2]	66.5*, 72.209[2]	4.63*, 4.6[2]
AlBipz	-	6.289*	40.1*	4.25*
AlBipbe	-	6.409*, 6.45[15]	34.9*, 36.92[15]	4.45*, 4.56[15]
GaBipz	6.442[12]	6.195*, 6.304[01]	49.5*, 43.25[01]	3.62*, 4.84[01]
GaBipbe	6.442[12]	6.507*	28.9*	4.07*
InBipz	-	6.429*	30.08*	4.96*
InBipbe	-	12.47*	37.2*	3.62*

*This work, [x](Xifan Wu, 2009), [2](Madouri & Ferhat, 2005), [01] (Achour, Louhibi, Amrani, Tebboune, & Sekkal, 2008), [12] (Madouri D. B., 2008), [5] Mesharo yashimoto, et al (2004), [3]D.W Palmer, (2006).

Table III: Calculated energy gaps of III-Bismuth alloys at Γ, X and L symmetries.

Compound	BBi pz	BBipbe	AlBipz	AlBipbe	GaBipz	GaBipbe	InBipbe	InBipz
E_{CL}	0.65	0.33	0.29	0.14	-0.154	-0.39	0	-0.154
$E_{V\Gamma}$	0.16	0.083	0.43	0.34	0	0	0.29	0.154
$E_{C\Gamma}$	0.82	0.17	-0.43	-0.34	0	0	-0.29	-0.154
E_{CX}	0.48	0.67	0.57	0.682	0.69	0.8	0.86	0.92
E_{gL}	0.81	0.413	0.72	0.48	-0.154	-0.39	0.29	0
$E_{g\Gamma}$	0.98	0.253	0	0	0	0	0	0
E_{Gx}	0.64	0.753	1.0	1.022	0.69	0.8	1.15	1.074

DISCUSSIONS AND CONCLUSION

As can be seen in table II, bulk moduli of the compounds revealed that compressibility increases from BBi to GaBi. The fact that LDA and GGA values are different for the same compound revealed that pseudopotentials have great influence on their compressibility. Lattice constants also increase from BBi to InBi, with increasing atomic orbitals and the calculated results compared well with experimental values. In table III, only BBi has direct band gap and is a good material for photoemission devices. If the underestimated factor 0.3eV (Yan & Donald, 2009) is anything to go by, the calculated bandgaps will have compared favourably well with both experimental and published work as depicted in table IV. This work further revealed that III-V (d-orbital) compounds possess spin-orbit splitting which increases with orbital number, a requirement for spintronic devices, (Ohno, 2011).

In conclusion, energy gaps of III-Bi binary compound showed that only BBi can be used in opto electronics and the d-orbital compounds are potential candidate for spintronic devices. Though the band gaps were under estimated as predicted in some related published work, precision of the predictive power of the investigating software tool needs further improvement so that the data obtained will be better relied on and form the starting point

for the manufacturing/fabrication industries in Nigeria where the alternative commercial ab intio simulation software may prove too expensive.

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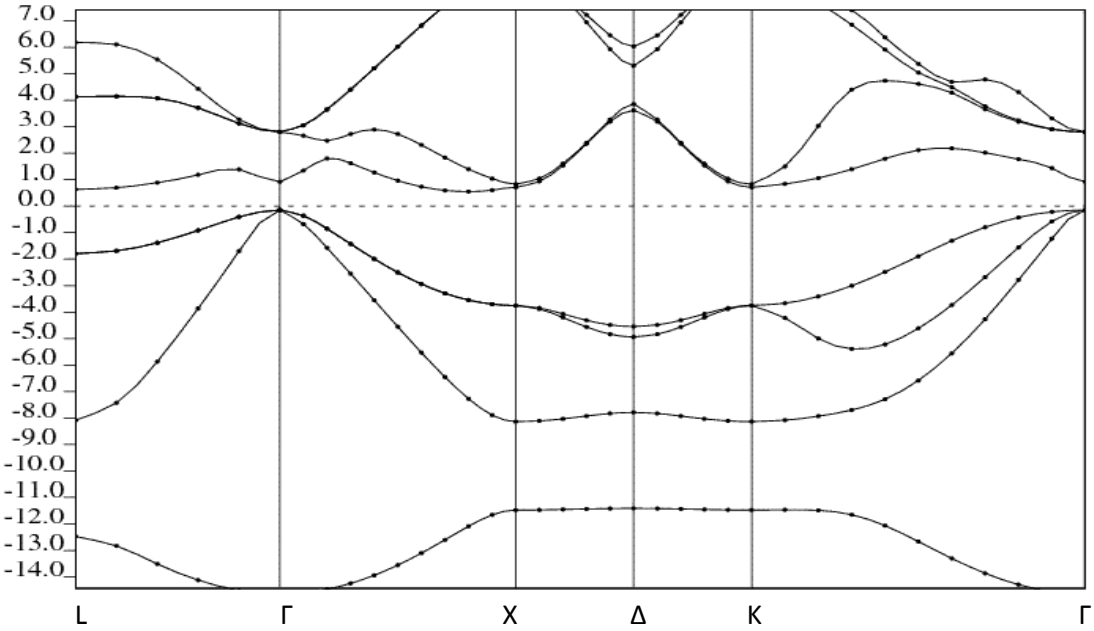
4.1 Bandstructures of III-Bismuth Semiconductors



Figa(i) Boron Bismuth (LDA)

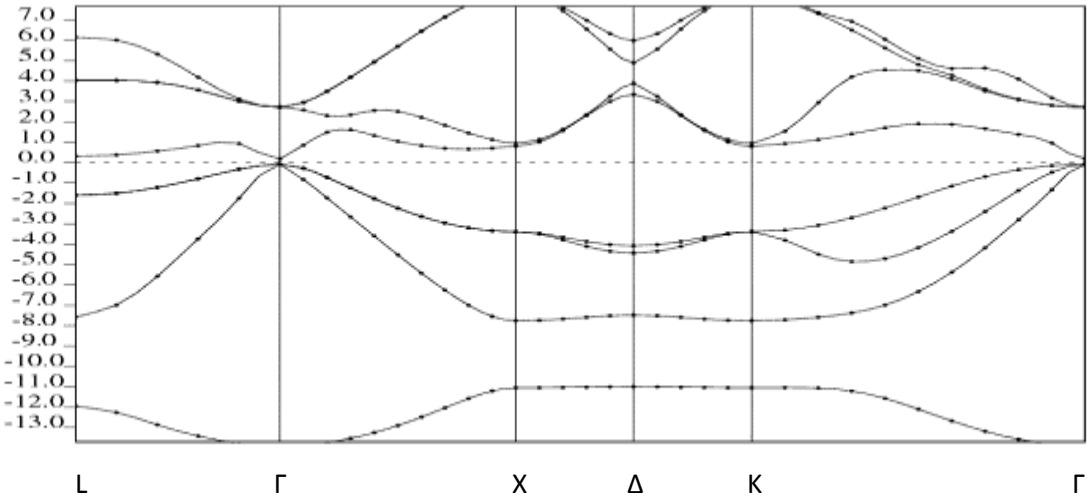
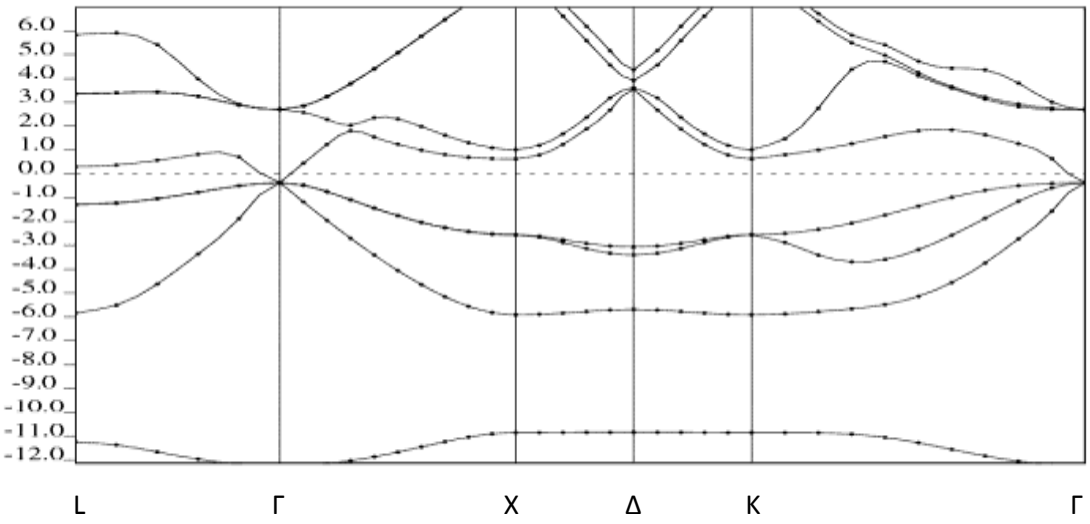
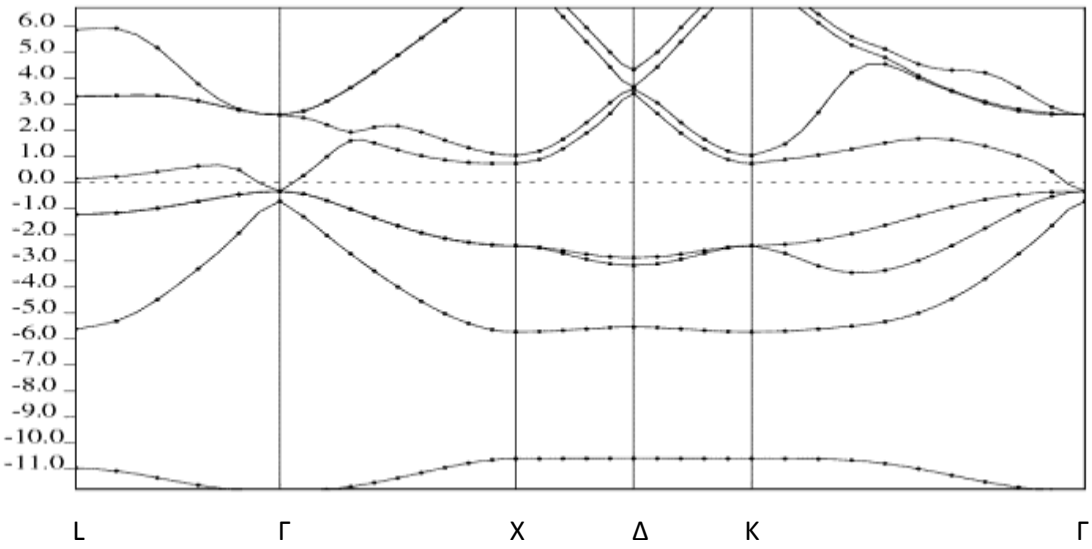


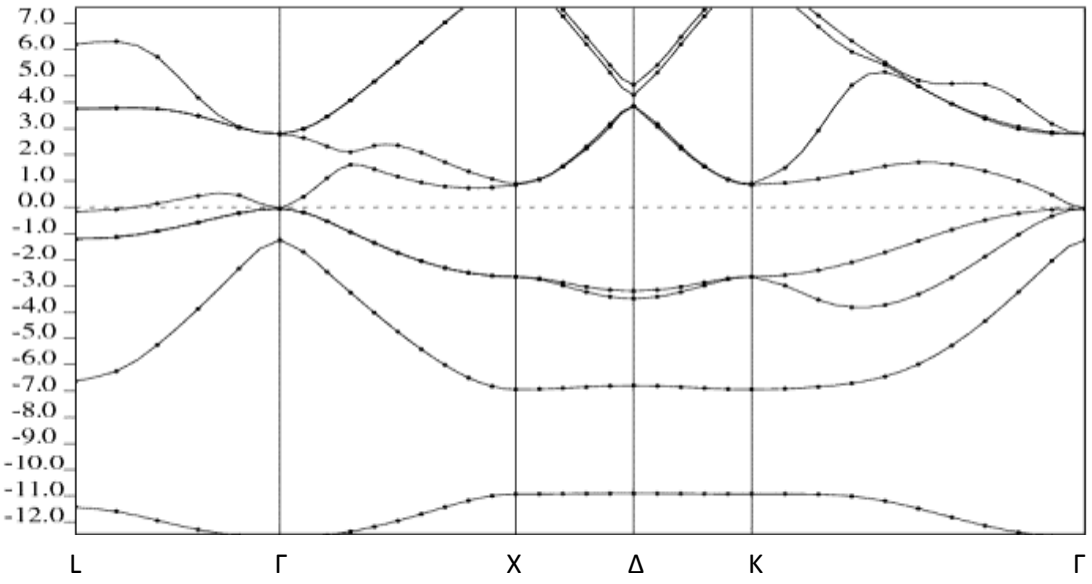
Fig.a(ii) Boron Bismuth (GGA)



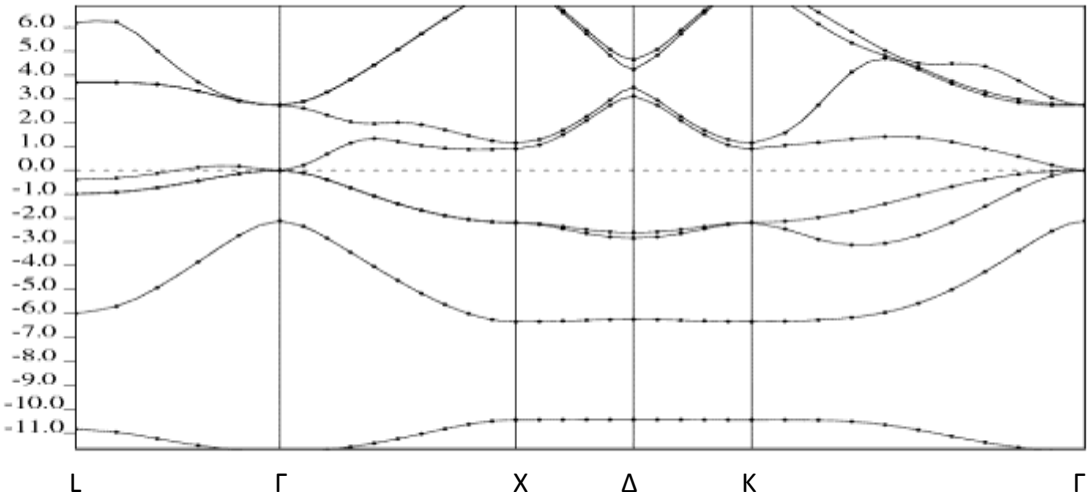
Figb(i) Aluminium Bismuth (LDA)



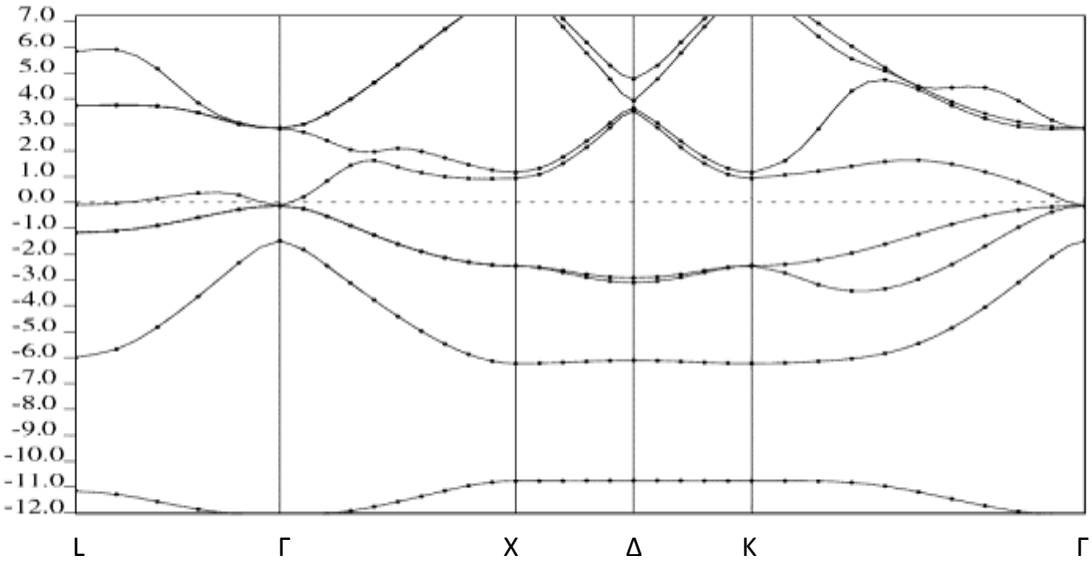
Figb(ii) Aluminium Bismuth (GGA)



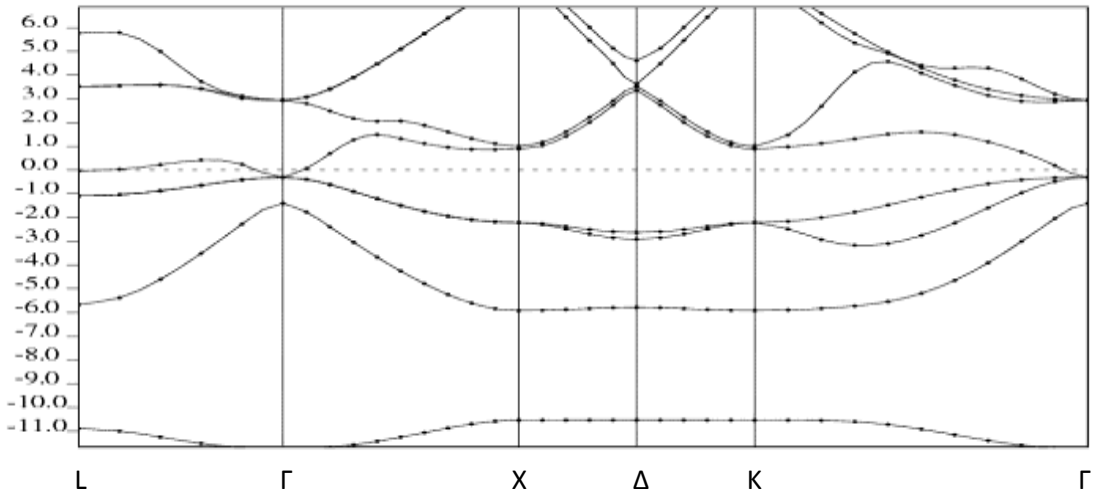
Figc(I) Gallium Bismuth (LDA))



Figc(ii) Gallium Bismuth (GGA)



Figd(i) Indium Bismuth (LDA)



Figd (ii) Indium Bismuth (GGA)

Investigations of Structural and Electronic Properties of III – Bi Semiconductor Binary Compounds using Density Functional Theory

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