# Structural And Electronic Properties Of III-Nitride Semiconductor Alloys: A First Principle Study

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***Abstract: The present work focuses on the investigation of structural and the electronic properties of InN and BN alloys using the first principles within linear combination of atomics orbital method. This work has been with the use of CRYSTAL code. Some important parameters like bulk modulus, lattice constant and band gap have been calculated.***

***Keywords: LCAO, Density functional theory, first principles, InN, ternary alloy***

## 1. Introduction

Semiconductors are the most investigated today and are the basic building blocks of emitters and receivers in optoelectronic devices. Group-III nitrides have tremendous applications in various industries dealing with optoelectronic devices [1-4]. There are huge number of semiconductor devices made by intermixing elements from III and V group of the periodic table. These compounds are used for LED/LD, fiber communication and solar cells. The compounds which are made from GaN are very significant in lighting systems. Silicon is the most commonly used material in ICs. In, P, and Al are also commonly used for the similar purposes with higher operational efficiency. The operational efficiency pertains to its higher electron mobility [5-11]. Since these devices are efficient and operate with lower voltages, they are commonly used in space vehicles and satellites. A Laser made from InGaAsP emits radiation at 1.55 μm which is used for transferring streams of information in the form of digitally codes.

In this study, total energy were calculated via first principle to investigate structural and electronic properties of $In_xB_{1-x}N$ (x=0.25, 0.50, 0.75) using LCAO method [12, 13].

The article is organized as follows: In section 2 we give a description of computational method. In section 3, result and discussions for structural properties are presented. Finally, the conclusion has been presented in section 4.

## 2. Computational method

The properties of the alloys $In_xB_{1-x}N$ (x = 0.25, 0.50, 0.75) have been investigated with the quantum mechanical simulation i.e. density functional theory (DFT) [14]. The optimization was executed by minimizing the total energy in reference to volume of cell for each composition. The function of exchange and correlation of Becke [4] and PBE

[5] has used. For the coding purpose, the Gaussian basis set has been used [6]. The lattice constant (a), bulk modulus ($B_0$), pressure derivative of bulk modulus and band gap have been calculated. The 165 k points are used with adequate tolerance. The 45 % mixing is used for consecutive cycles. Within the 15 cycles the self-consistency is attained.

## 3. Result and Discussion

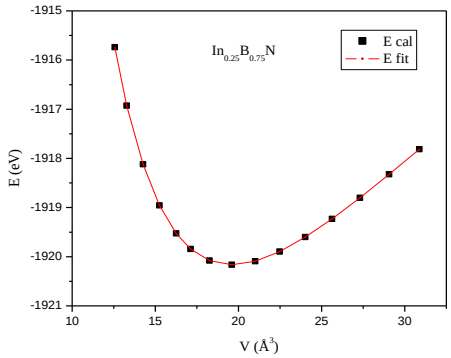


Fig 1: E vs. V curve for x=0.25

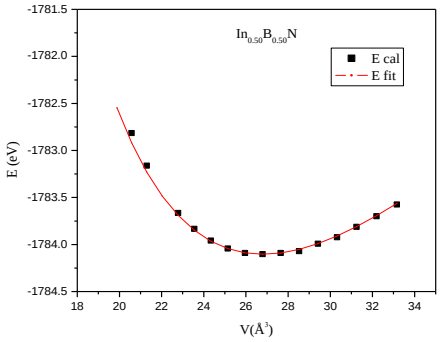


Fig 2: E vs. V curve for x=0.5

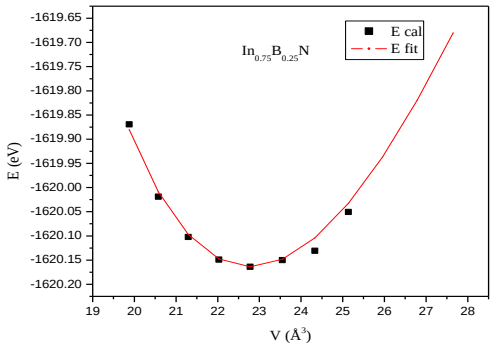


Fig 3: E vs. V curve x=0.75

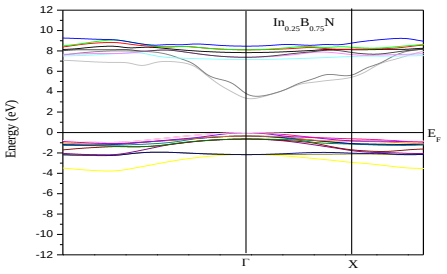


Fig 4: Band structure for $In_{0.25}B_{0.75}N$

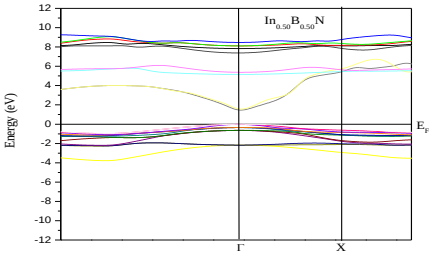


Fig 5: Band structure for $In_{0.50}B_{0.50}N$

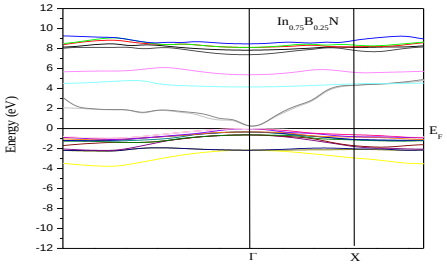


Fig 6: Band structure for $In_{0.75}B_{0.25}N$

The structural parameters of the InN and BN alloys in Zinc blende (B3) phase have been computed by calculating the total energy optimization with the variation of volume of primitive cell of the crystal [12-15]. Figure 1 to 3 represents the energy versus volume curve for $In_xB_{1-x}N$ (x = 0.25, 0.50, 0.75), the dots represent the calculated energies through DFT software and the curves represent the fitted energies to the Brich Murnaghan equation of state [10, 19-21]. The results of structural parameters are summarized in Table 1 The electronic band structure has been considered at the lattice constant at equilibrium position is revealed in Figures 4 to 7. The different symmetry points taken into consideration are W, L, Γ, X, W, Figures 4 to 7 reveal direct band gap decreases as the concentration of In increases.

**Table 1 : Structural parameters**

| | | Present | Theoretical | Experimental |
|---|---|---|---|---|
| InN | a (Å) | 5.03 | 4.98 [8], 5.08 [8] 5.04-4.94 [8] | 4.98 [10] |
| | B(GPa) | 123 | 155.35 [8], 127.71 [8] 133-146 [9] | 137[11] |
| | B' | 5.2 | 4.49 [8], 3.40 [8], 3.36-4.48 [9] | |
| $In_{0.25}B_{0.75}N$ | a (Å) | 4.28 | 4.26 [17] | |
| | B(GPa) | 258 | | |
| | B' | -- | 3.48 [17] | |
| $In_{0.50}B_{0.50}N$ | a (Å) | 4.50 | 4.61[17] | |
| | B(GPa) | 200 | | |
| | B' | -- | 3.55 [17] | |
| $In_{0.75}B_{0.25}N$ | a (Å) | 4.75 | 4.91[17] | |
| | B(GPa) | 166 | | |
| | B' | -- | 3.91 [17] | |
| BN | a (Å) | 3.65 | 3.58 [8], 3.36 3.57-3.64 [12, 13] | 3.61 [14] |
| | B(GPa) | 369 | 408.89 [8], 395.74 [8] 397-366 [12, 13] | 369 [12, 13] |
| | B' | 4.0 | 3.65 [8], 2.94 [8] 3.97 [11] | 4.0 [12] |

**Table 2: Electronic structure- band gap(in eV)**

| | Present | | Experimental | Other Theoretical calculations | |
|---|---|---|---|---|---|
| | Direct | Indirect | | Direct [8] | Indirect [8] |
| BN | 8.077 | 3.896 | 6 [14] | 8.677 | 3.953 |
| $In_{0.25}B_{0.75}N$ | 3.208 | 5.408 | | 2.716 | 3.582 |
| $In_{0.50}B_{0.50}N$ | 1.107 | 5.308 | | 0.855 | 2.362 |
| $In_{0.75}B_{0.25}N$ | 0.189 | 4.308 | | 0.208 | 2.597 |
| InN | 0.106 | 5.208 | 1.9 [16] | 0.00 | 2.765 |

## 4. Conclusion:

In summary, LCAO method has been applied to investigate the various properties of III-N compounds i.e. structural and electronic. The InN and BN alloys $In_xB_{1-x}N$ (x = 0.25, 0.50, 0.75), have been investigated in the zinc blend (B3) phase. In addition, it has studied that with the different doping concentration of In dopant into the BN compound three parameters changes linearly. With the increasing concentration the lattice constant changes directly and the bulk modulus and the energy band-gap changes inversely. It was observed that calculated results are in good agreement with previous investigations.

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