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First-Principles Study of Electronic and Structural Properties and Examining the Effect of Pressure on Energy Gap in InN Phases

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Abstract

The electronic and structural properties of both zinc-blende and wurtzite phases of InN were investigated by using full potential linearized augmented plane wave method within density functional theory. For the exchange correlation potential, generalized gradient approximation (PBE-GGA) and an alternative form of GGA proposed by Engel and Vosko (EV-GGA) have been used. Results obtained for band structure of these compounds have been compared with experimental results as well as other first principle computations. Our results show a significant improvement over other theoretical work and are closer to experimental data. The lattice constants, bulk modulus and its pressure derivative are calculated for both phases. We have also investigated the structural transitions of InN and have calculated the transition pressure between zinc-blende and rocksalt phases.

Introduction

Computer simulations have made it possible to compute with great accuracy a large number of electronic and structural properties of solids from first principles. It is now possible to explain and predict properties of solids under conditions, which are inaccessible to experiment [1].

InN is a III-V semiconductor compound. III-V compounds, specially the III-nitride semiconductors such as InN, AlN and GaN materials are of current interest on their potential use in optoelectronic and high power/temperature electronic devices including light emitting diodes, laser diodes [2,3] solar blind photo detectors [4] and heterostructure field effect transistors [5,6]. These compounds show considerable resistance to corrosion in aqueous solutions [7-9], therefore it is useful to know the band gap of these nitride compounds.

InN crystallizes in zinc-blende (zb) and wurtzite (wz) structure. The space group of zb structure is $F\bar{4}3m$ and that of wz is P63mc. InN, in the zb and wz structures, has a direct band gap. The wz phase is stable and the zb phas is metastable [10, 11]. Recent measurements [12-16] suggest that the band gap of InN is smaller (~0.8eV [17]) than the commonly accepted (~1.9eV[18]) band gap which was assumed in order to obtain agreement with the experimental data [3].

Small band gap value of InN is particularly useful as it will provide an extra direction in the applications of this compound. As a small band gap material, InN and its III-nitride alloys could be suitable for low future-generation solar cells.

Significant role of nitrogen in these compounds is in the formation of their physical properties similar to other wide band gap semiconductors such as diamond [19].In this paper, we investigate theoretically the structural and electronic properties of zb and wz phases of InN.

Computational methods

The electronic configuration of InN is, **In:** Kr $4d^{10}5s^25p^1$and that of **N:** He $2s^22p^3$. In our computational work, we distinguish between the inner-shell electrons of In ($1s^22s^22p^63s^23p^63d^{10}4s^24p^6$), N ($1s^2$) and the valence band electrons of the In ($4d^{10}5s^25p^1$) and N ($2s^22p^3$). We have used the full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory.The exchange-corrolation potential is calculated using local density approximation (LDA)[21] and generalized gradiant approximation (PBE-GGA , EV-GGA) [20, 22]. The computation has been carried out using the Wien2K code [23]. In this code the unit cell is divided into non overlapping muffin-tin spheres of radius R_{MT} and an interstitial region, where the Kohn – Sham wave functions are expressed in spherical harmonics within spheres and in plane waves in the remaining space of the unit cell. We use the value 7 for the parameter $R_{MT}K_{MAX}$ which determines the matrix size (convergence), where K_{MAX} is the cut-off wave number for the plane waves, and R_{MT} is the smallest

value of all atomic-sphere radii. Basis functions, charge density and potential were expanded inside the muffin-tin spheres in spherical harmonic function with cut-off l_{MAX} and in Fourier series in the interstitial region. The values of muffin tin radius (R_{MT}) for In and N atoms are chosen respectively 2.0 and 1.8, and the K-Point number is chosen 800.

Results and discussion
Electronic properties

In this section we have calculated the band structure of zb and wz phases of indium nitride. In both phases, the band gap is at Γ direct (Fig 1, 2) but there is a difference in the value of the band gap between valance and conduction bands. Our calculation with EV-GGA gives the band gap value of 0.16eV for zb. and 0.33eV for wz. We note that our results are not in good agreement with experimental values [17, 24]. The reason of this discrepancy is the high electronegativity existence on Nitrogen atom. In these conditions, a great potential is applied on 4d electrons of In atom. So our calculated values by using LDA and PBE-GGA approximations isn't in good agreement with experimental results. Then we used the EV-GGA, and a better band gap was obtaind. To obtain a better band gap, we optimized the muffin-tin radius. By increasing the muffin-tin radius of In atom, the potential which was applied on 4d electrons became spherical. So the results show more reality.

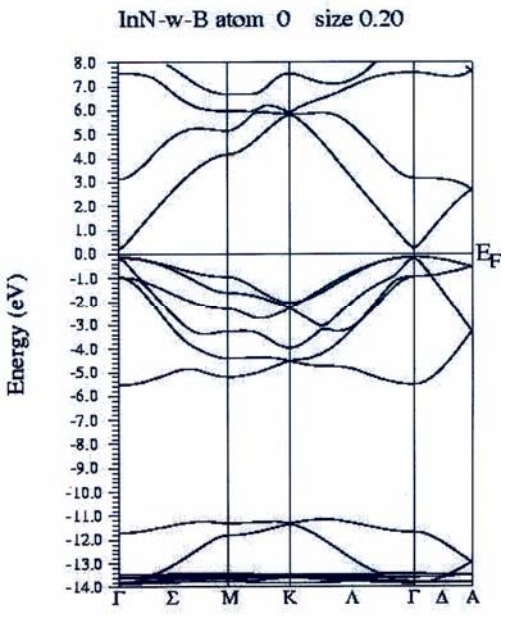


Fig.1: Band structure of InN wz (GGA-EV)

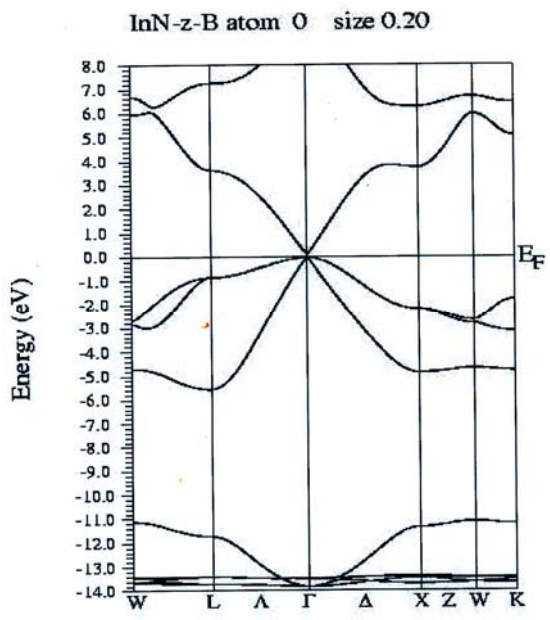


Fig. 2: Band structure of InN zb (GGA-EV)

Our results support remarkably the latest experimental results [17, 24] of the band gap of InN, in comparison with the results of band gap already mentioned in literature [25]. Calculations based on GGA and LDA give lower values for the band gap compared to EV-GGA. GGA and LDA are not flexible to reproduce accurately exchange correlation energy and its density derivative simultaneously.
The general results for band structure are as follows:
1- The occupied bands for two phases are respectively separated into two sub-bands with gaps of 6.0eV and 6.5eV for zb and wz respecktively.
2- The values of the band gaps of the semiconducting phases calculated by using EV-GGA agree with the other results.
3- The band gap (valance-conductions) is decreasing from wz to zb.

Density Of State (DOS)

The total and partial DOS of the InN in both phases have been calculated by means of the tetrahedral method [26]. The total DOS of InN in the wz phase is shown in (Fig.3.a). The partial DOS of the s,p and d orbitals of In are presented in (Fig.3.b) and the partial DOS of the s and p orbitals of N are presented in (Fig.3.c).

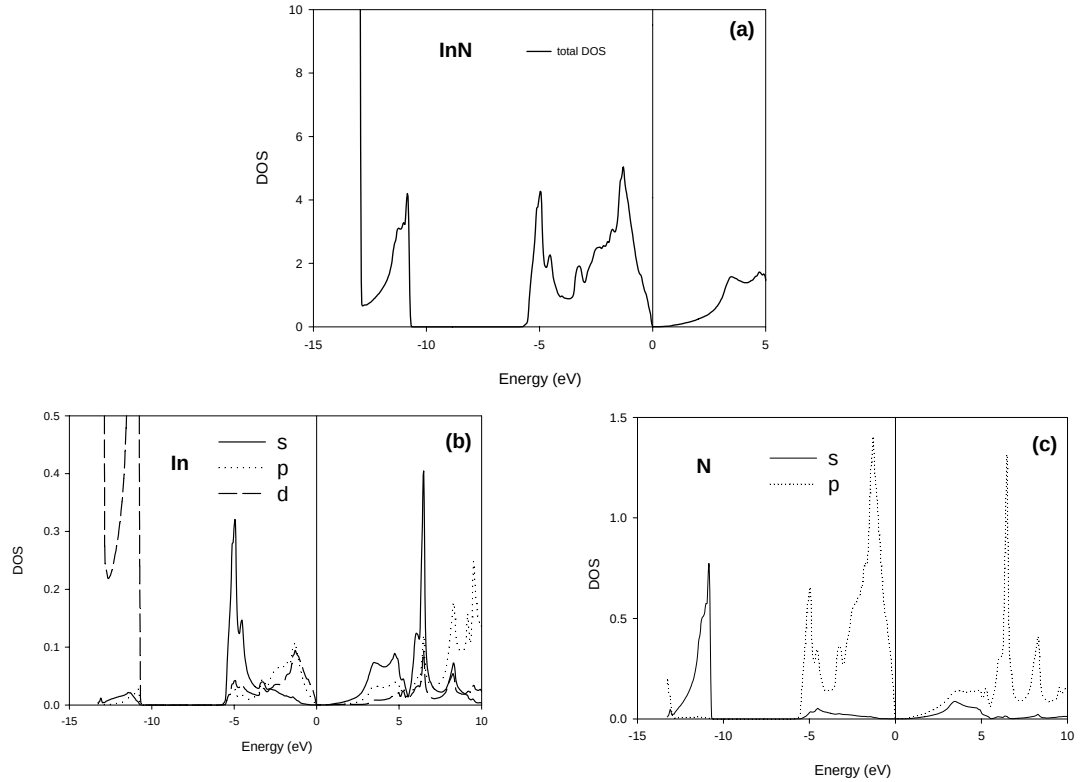


Fig. 3: Total DOS and PDOS of wz phase in zero-pressure

The positions of the peaks are in reasonable agreement with earlier calculations. It is further observed that the first peak encountered in the total DOS for InN in (Fig.3.a) is small but relatively broadly centered around -11.0eV. The peak arising almost entirely from N 2p states is seen from the partial DOS for N (Fig.3.c). This peak corresponds to the lowest lying band in (Fig.1) with its width arising from the dispersion in regions around the Γ point in the Brillouin Zone. The peak at -5.0eV correspons to the In 5s states (Fig.3.b) that are mixed with the N 2p states (Fig.3.c). The hump between -2.0eV and zero energy corresponds to the N 2p states (Fig.3.c) that are mixed with In 5p states (Fig.3.b). The peak at 7.0eV (above the Fermi level) is due to equal contributions of the In 5s and N 2p states (Fig.3.b, c). On the whole, it is seen that below and close to the Fermi level the N 2p states dominate, whereas above and close to Fermi level In 5s stated dominate.

The effect of pressure on the energy gap

We also have calculated the band gap values of wz and zb by putting pressure on InN crystal. We can see that the band gap increases when we put pressure on the InN crystal. The nearest neighbor atoms overlap with each other more than before and the repulsive potential between electrons charges their states, therefore the band gap increases (Fig 4). Under these conditions, the electrons density of states is broadened (Fig. 4).

In Fig. 5 shows these values for wz and zb. When the pressure is applied and the value of the unit cell is reduced by 20% (a=3.28A$^{\circ}$), the wz phase band gap is 1eV, and when the pressure is zero (a=3.544A$^{\circ}$), its band gap is 0.33eV. These results are shown in zb phase too. At high pressures when the volume is reduced by 20% (a=4.55 A$^{\circ}$), the band gap is 0.77eV and in zero pressure the band gap is 0.16eV (Fig .5).

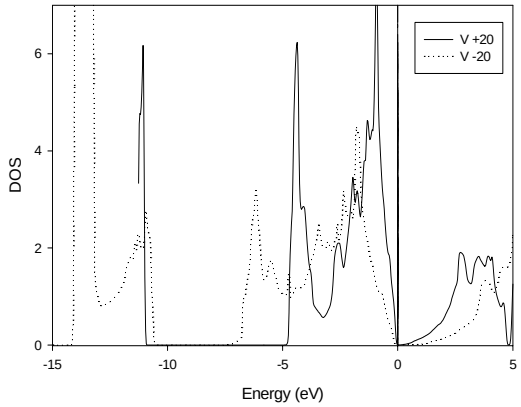


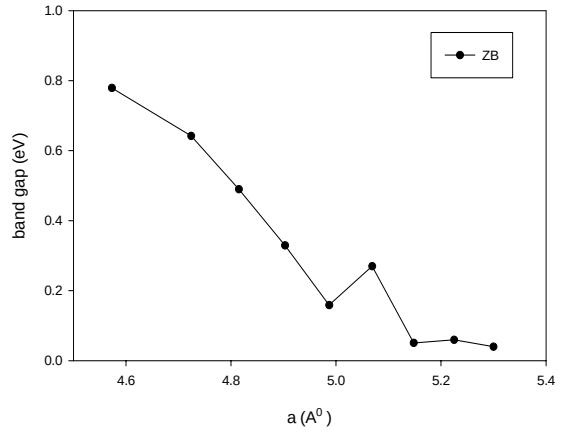
Fig. 4: Total DOS of wz phase under zero-pressure (dotted curve) and high-pressure (lined curve)

Equilibrium structural properties

The ground-state properties of InN at high pressure were obtained by calculating the total energy (E_{tot}) as a function of volume (V). Fig.6,7 show the E_{tot} versus V for the zb, wz and rock-salt phases of InN by using GGA and LDA approximations. These curves were obtained by calculating E_{tot} at several different volumes and by fitting the calculated values to Murnaghan equations of state [27]. It shows that the wz phase is more stable than other phases, and the zb is a metastable phase. This result is in agreement with other reports [10, 11]. From the total energy versus volume curves the zero-pressure equilibrium lattice constant (a_{eq}), the Bulk modulus ($B_\circ$) and pressure derivative of the Bulk modulus (B') have been obtained. These results have been obtained using the LDA, GGA and EV-GGA approximations and are reported in table 2. Our calculations by LDA approximation are in good agreement with the experimental and other theoretical data. Our results show that the EV-GGA isn't suitable for structural parameters.

Phase transformations under high pressure

The (negative value of the) gradient of the common tangent of two energy-volume curves corresponding to two different phases gives the transition pressure (P_t) between those two phases. We have shown that in low pressure the wz phase is stable and in high pressure, at first, the zb phase exist and then by increasing the pressure, this phase loses it's stability and transforms to a rock-salt (ro) phase. We've calculated the transition pressure from zb phase to ro phase by using GGA approximation as 10.8GPa (Fig.6). It means that the zb



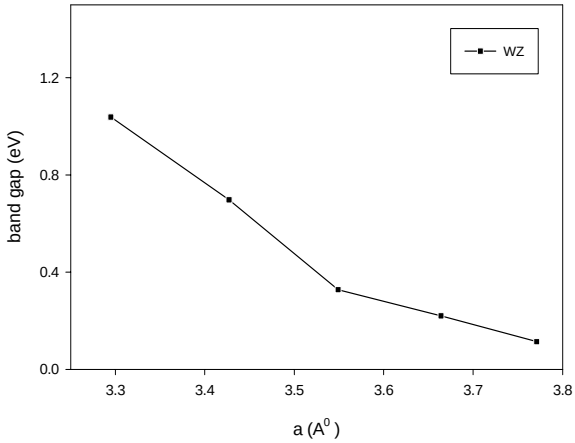


Fig. 5: increasing of band gap by reducing the volume of 1 to unit cell

phase loses it's stability at high pressure and ro phase shows itself in higher pressures. No transition from the wz phase to other phases are seen. Very clearly, these two phases, zb and ro show themseleves at high pressures. But at normal pressure the wz phase is more stable. All the above calculations have been repeated by LDA approximation (Fig.7) and similar results have been achieved by GGA approximation too. Calculated transition pressure with LDA approximation for transition from zb to ro phase comes out to be 8Gpa, i. e. less than that of the GGA approximation. In comparision with pervious calculations [28] (showing GGA to be more exact than LDA), we argue that GGA results are more exact.

Table.1: The calculated equilibrium parameters for wz and zb phases

structure	lattice costant(A°)	B(GPa)	B′	Min Energy(eV)
wz				
present work (GGA)	a=3.61,c=5.83	116.99	4.87	-23752.03
present work (LDA)	a=3.54,c=5.7	142.56	5.23	-23729.89
present work (EV)	a=3.88,c=6.26	56.86	4.50	-23763.06
other works	a= 3.59[28],3.52[29]	152[29]	3.4[31,32]	
	c=5.81[28],5.67[36]	139[30]		
Expriment	a=3.544[29,30]	125.5[32]	12.7[32]	
	a=3.533[31]	139[30]		
	c=5.718[29,33], 5.76[34]			
zb				
present work (GGA)	a=5.09	122.92	4.37	-11876.01
present work (LDA)	a=4.99	144.99	4.77	-11864.95
present work (EV)	a=5.47	55.99	4.45	-11881.52
other works	a=4.97[28],4.932[30]	144[30]	4.3[32]	
	a=5.03[35]			
Experimental	a= 4.98[28,30,32,34]	137[30] , 125.5[35]		
	a=4.97[35]			

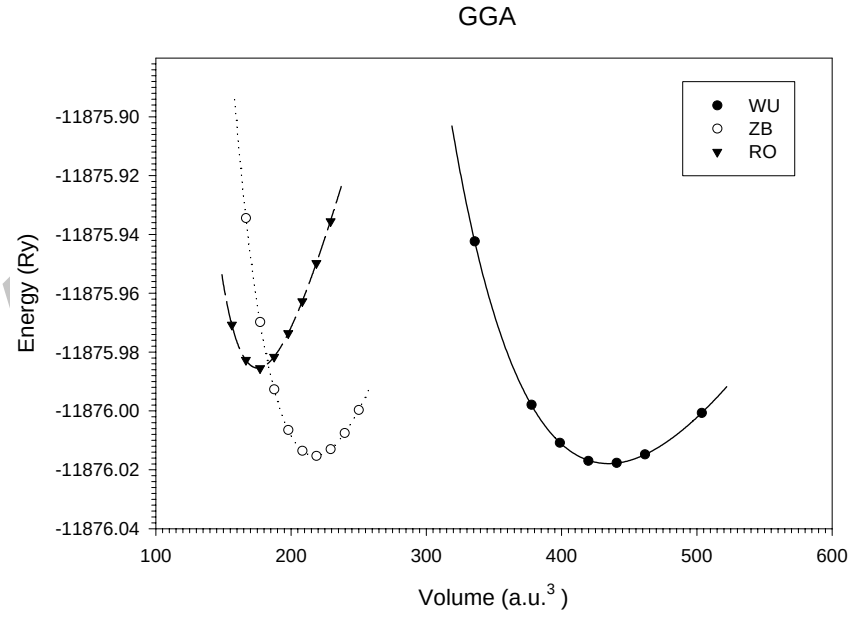


Fig. 6: Total energy versus volume curves of wz, zb and ro phases of InN by GGA

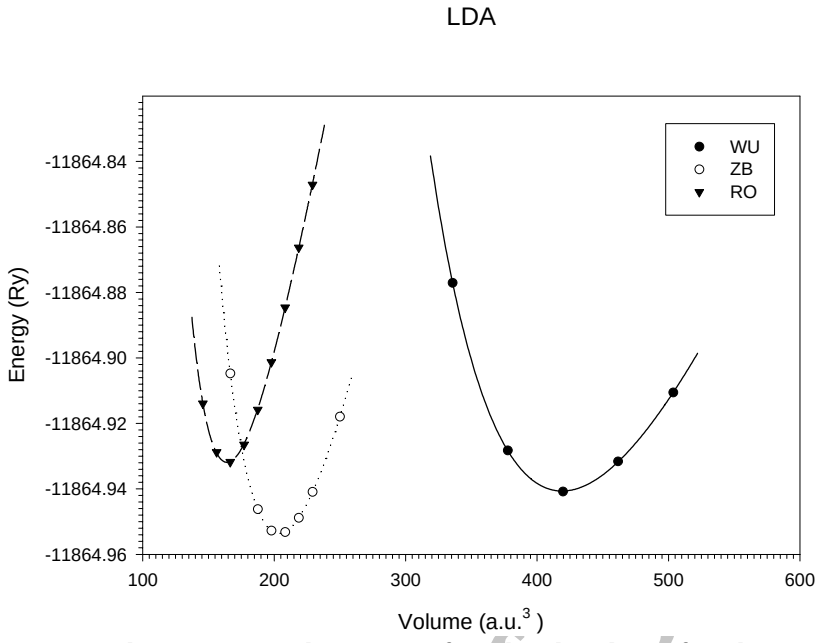


Fig.7: Total energy versus volume curves of wz, zb and ro phases of InN by LDA

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