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Energy Band Structure Studies Of Zinc-Blende GaAs and InAs

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Abstract

A self-consistent calculation of the structural and electronic properties of zinc blende GaAs and InAs has been carried out. The calculations were done using the full potential-linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). The exchange-correlation energy used is the generalized gradient approximation as parameterized by Perdew-Burke and Ernzerhof (PBE-GGA). Energy band structures, density of states and structural parameters of all the compounds are presented and discussed in context with available theoretical and experimental studies. Our results show that the energy band gaps of the semiconductors are underestimated. But overall our results show reasonable agreement with previous results even though sufficient experimental results are not available for more realistic comparison.

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1.0 Introduction

With advances and sophisticated developments in computer technology, it is now possible to compute various properties of solids from first-principles methods. The properties of interest in condensed matter physics include structural, electronic, optical, elastic etc.
A tested and proved first-principles method is the density functional theory [1].
The electronic and structural properties of III-V semiconductors have been the subject of considerable as well as experimental investigation. The importance of these materials lies in their great potential for technological applications. GaAs is the most widely used semiconductor in technology. It is used mainly for microwave and photonic applications while ternary compounds such as GaInAs form heterojunction photodetectors at long wavelengths[2]. Interestingly it has been shown that Al deposited on GaAs is a prototype Schottky barrier.
In view of all these possible applications there is need to still continue to study extensively these compounds both experimentally and theoretically. To understand some of the physical properties of these compounds, a detailed description of electronic structure of these compounds is necessary.
In this paper we intend to give a complimentary study of the structural and electronic properties to both experimental and other theoretical works for GaAs and InAs using the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT). The layout of the remaining part of the paper is as follows: in section 2 we describe the method of the calculation of the structural and electronic properties based on the FP-LAPW. In section 3 we present the results of our calculations and compare them with experimental and other existing theoretical results. The conclusion is given in section.

2.0 Description of The Method

In DFT, the problem of interest is a system of N interacting electrons described by the Hamiltonian

$H = T + V + V_{ee}$

$$= \sum_{i=1}^{N} \frac{\nabla_i^2}{2} + \sum_{i=1}^{N} v(r_i) + \frac{1}{2}\sum_{i-1}^{N}\sum_{\substack{j=1 \\ i \neq j}}^{N} \frac{1}{|r_i - r_j|}$$

(2.1)

where T, V and V_{ee} are the kinetic, potential and interaction energy operators respectively.
The primary objective of DFT is to determine theoretically the ground – state properties of an interacting many – electron system in an external potential using the particle density as the key variable. It replaces the many – body problem with effective one – electron equations, the so called Kohn – Sham (KS) equations (2.3)

$$\left[-\frac{\nabla^2}{2} + v_{eff}(r)\right]\varphi_i(r) = \varepsilon_i \varphi(r)$$

(2.2)

and the ground state density n(**r**) of the N – electron system is

$$n(r) = \sum_{i=1}^{N} \varphi_i(r) * \varphi_i(\bar{r})$$

(2.3)

The effective potential is given by

$$v_{eff}[n](r) = v(r) + \int d^3r' \frac{n(r')}{|r - r'|} + v_{xc}[n](r)$$

(2.4)

where the exchange correlation potential v_{xc} is defined by

$$v_{xc}[n](r) = \frac{\delta E_{xc}[n]}{\delta n(r)}$$

(2.5)

Equations 2.2, 2.3 and 2.4 are solved self – consistently.
Approximation enters the DFT through the exchange correlation energy term. One of such approximates is the generalized gradient approximation, GGA where the exchange – correlation energy for spin unpolarised systems is written as

$$E_{xc}^{GGA}[n] = \int d^3r f(n(r), \nabla n(r))$$

(2.6)

The full potential linearized augmented plane wave (FP – LAPW) [4] is used in solving the Kohn – Sham equations for the ground state density, total energy and eigen values of a many – electron system by introducing a basis set which is especially adapted to the problem. To realize this adaptation, FP – LAPW partitions the unit cell into two parts: non – overlapping atomic spheres (centred at atomic sites) and an interstitial region.
The LAPW expands potential in the form

$$V(r) = \sum_{l,m} V_{lm}(r) Y_{lm}(\hat{r}) \qquad \text{inside sphere}$$

(2.7)

$$= \sum_{k} V_k \exp(ik.r) \qquad \text{outside sphere}$$

(2.8)

and expands the charge density as

$$n(r) = \sum_{l_1 m} n_{lm}(r) Y_{lm}(r) \qquad \text{inside sphere}$$

(2.9)

$$= \sum n_k \exp(ik.r) \qquad \text{outside sphere}$$

(2.10)

The unit cell has one molecule with either Ga or In at (0,0,0)a while As is located at (¼,¼,¼)a where a is lattice constant. The sphere radii used in the calculations are 2.2 and 2.4atomic units for Ga and In respectively while radius of 2.1a.u. is used for As in both compounds. In this work we have employed the FP-LAPW as embodied in WIEN 2k code[5]. The Perdew-Burke-Ernzerhof (PBE) scheme[6] within the GGA is used to calculate the exchange-correlation part of the potential.

The Brillouin zone integrations for the calculations were done using the tetrahedron method [7] with 91- and 116- k-points respectively in the irreducible part of the Brillouin zone. Both the muffin-tin sphere radius and the number of k-points are varied to ensure convergence. Well converged solutions were obtained for $R_{MT} K_{max} = 8$ where R_{MT} is the atomic sphere radii and K_{max} is the interstitial plane wave cut-off.

3. RESULTS AND DICUSSION

The total energies of GaAs and InAs were calculated for different volumes along the equilibrium cell volume in the zinc blende structure using the FP-LAPW method in the GGA form of exchange and correlation. The calculated total energies are fitted to the Murnaghan's equation of state [8] in order to determine the equilibrium lattice constant, bulk modulus and the pressure derivative of the bulk modulus. The results are tabulated in Table 3.1.

Table 3.1: Structural properties of GaAs and InAs

GaAs				
a(Å)	5.7484	5.72[10]	5.79[11]	5.65[9]
B(Mbar)	0.6574	5.77[12]		0.75[9]
B′	4.4010	0.58[10]	0.61[11]	
		0.68[12]		
InAs				
a(Å)	6.1900			6.036[9]
B	0.5080	0.61[13]		0.60[9]
B′	4.4821			

It can be seen that the calculated results are in good agreement with experiment and previous results. The calculated lattice constant values are 2.55% and 1.68% higher than experimental values. The values of the bulk modulus also compare favourably with both experimental data and results by earlier workers where available. The slightly greater values for the lattice constants are characteristic of the GGA.

The relativistic band structures are displayed in figures 3.1 and 3.2. The graphs are for a plane through the Brillouin zone, surrounded by the high symmetry k-points W-L-Λ-Γ-Δ-X-Z-W-K. The zero of the energy scale shows the position of the Fermi level. The positions of symmetry points are indicated by vertical lines.

For GaAs the valence band maximum and the conduction band maximum occur at Γ. The same trend was observed for InAs. So, these semiconductors are predicted to have direct band gap at Γ for the zinc blende structure. The results of the energy band for GaAs and InAs show a wide deviation of 64%and 58% below the experimental values. This underestimation of band gap with GGA has been noted by earlier workers.

In figures 3.2and 3.3 we show the total density of states (DOS) for GaAs and InAs. The DOS energy spectra are plotted in the range -15eV to +15eV. The dashed line is the Fermi energy. The energy gaps observed from the DOS are reported in Table 3.2.

Table 3.2: Energy band gaps (eV) for GaAs and InAs
(Experimental values are taken from ref.9 while other calculated values are from ref. 14)

	Present work	Experiment	Other calculated values
GaAs	0.5134	1.42	0.42, 1.16, 1.17
InAs	0.1769	0.42	0.00, 0.76, 0.78

The total density of states was computed using the modified tetrahedron method [7]. In this approach the Brillouin zone is divided into 48 tetrahedra cells.
The peaks in the DOS are in correspondence with the energy bands in the band structure. The positions of the conduction band minimum, the valence band maximum and the peaks in the total density of states are also in good agreement with that by earlier workers. The overall profile for GaAs and InAs are similar, showing three prominent
peaks. The first peak appears around -10eV and arises mainly from the As while the second at about -5eV is due to the Ga and In. The peak at about +5eV is due to the Ga and In. The peak at about +5eV in the conduction band are contributed by both elements of the semiconductors.

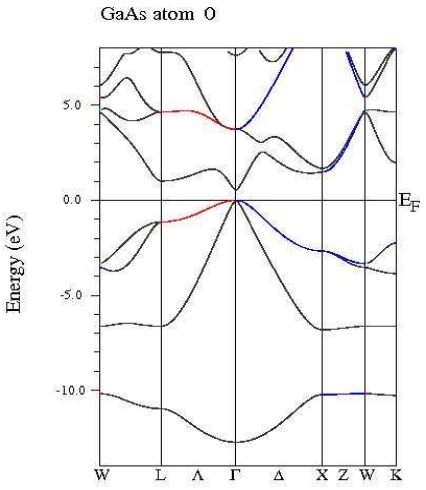

Figure 1: Electronic band structure of GaAs

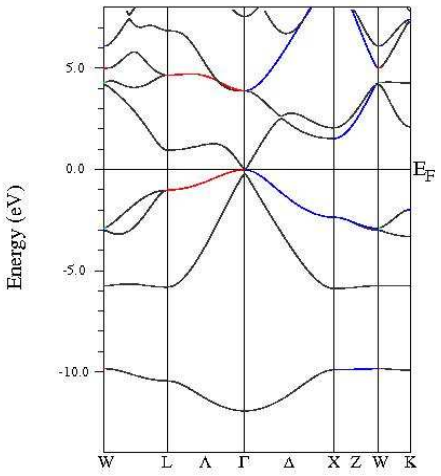

Figure 2: Electronic band structure of GaAs

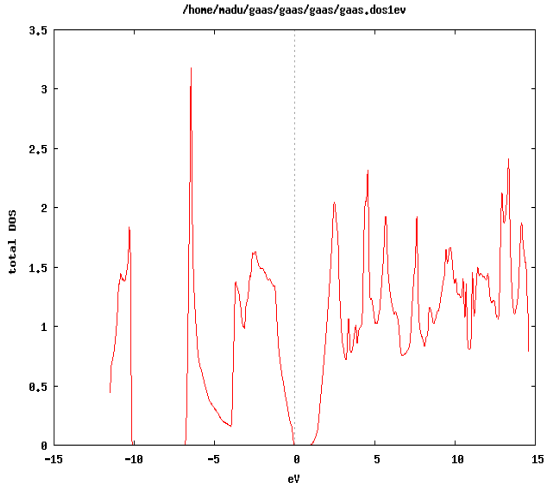

Figure 3: Total Density of States for GaAs

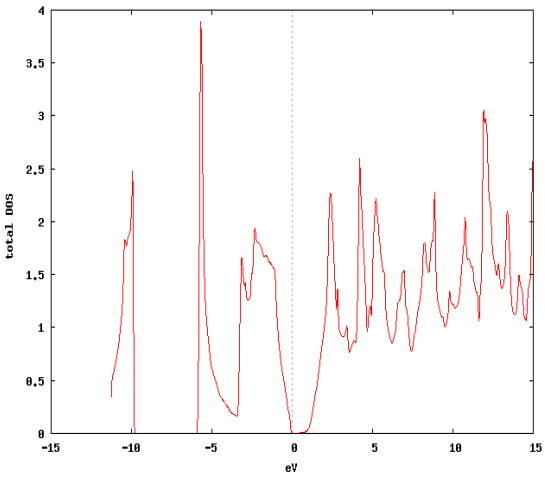

Figure 4: Total Density of States for InAs

4. Conclusion

We have presented the calculation of structural and electronic properties of group III-V semiconductor compounds, GaAs and InAs in the zinc blende structure using FP-LAPW method within the GGA estimation. The calculated equilibrium lattice constants, bulk moduli and energy gaps were compared with experimental values and the results obtained by earlier workers. The overall band profile for all the compounds is in agreement with the earlier band structure results. GaAs and InAs were found to have direct gap (Γ) in agreement with experiment and earlier results . However our results show that the band gap is underestimated. Recently a revised form of Perdew Burke-Ernzerhof GGA called PBE sol [15] that improves equilibrium properties has been introduced.

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