

Study Of Electronic And Linear Optical Properties Of Indium Pnictides (InX, X = P, As, Sb)

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ABSTRACT

A comparative study of theoretical and experimental electronic properties and linear optical dielectric function of zinc blende structure of Indium pnictides is presented by using the full-potential linearized augmented plane wave (FP-LAPW) method within the DFT formalism. In this approach, the generalized gradient approximation (GGA) was used for the exchange-correlation potential calculation. Results are presented for the band structures, for the density of states, and for the real and imaginary parts of the linear dielectric functions for photon energies up to 15 eV. Detailed comparisons are made with published experimental and theoretical data and generally showed good agreement.

Key words: Band structure, FP-LAPW, InX, Optical properties, WIEN2k.

PACS Nos. : 71.15.Ap, 71.15.Mb, 71.20.Nr, 78.20.Ci

INTRODUCTION

In the last century considerable advances have been realized in the research and applications of semiconductors. It is well known that semiconductor technology has a great impact on our society. The III-V semiconductors are extensively used in the high-tech photonic and optoelectronic devices because of their wide range of band gaps. Narrow band gaps semiconductors Indium Pnictides InX (X=P, As, Sb) compounds have attracted much attention for their potential as new device materials [1].

There have been many electronic band structure calculations for III-V semiconductors. These include the empirical pseudopotential method (EPM)[2], the tight binding (TB)[3], full potential method[4], and the pseudopotential total energy

approach[5]. In the present work, we have reported the FP-LAPW calculations of the band structure, density of states and linear optical properties for the semiconductors InX (X=P, As, Sb,) compounds with zinc-blende structure. The exchange and correlation potential has been calculated using the generalized gradient approximation (GGA)[6] for the total energy calculations.

CALCULATION METHOD

The electronic configurations of elements in Indium pnictides are In: [Kr] $4d^{10} 5s^2 5p^1$; P: [Ne] $3s^2 3p^3$; As: [Ar] $3d^{10} 4s^2 4p^3$ and Sb: [Kr] $4d^{10} 5s^2 5p^3$. We have chosen sphere radii of 2.3 Å for In, 2.1 Å, 2.5 Å and 2.8 Å respectively for P, As and Sb. The calculations reported here were performed using the FPLAPW method [7] as implemented in the WIEN2K package [8]. We choose the exchange-correlation potential parameterized by Perdew et al.[6] which is derived by using the generalized gradient approximation (GGA). In the FPLAPW method, a basis set is obtained by dividing the unit cell into non-overlapping atomic spheres (centered on the atomic sites) and an interstitial region. Inside the atomic sphere, a linear combination of radial function times spherical harmonic is used, and in the interstitial region a plane wave expansion is augmented by an atomic like function in every atomic sphere. This method yields accurate energy eigenvalues and wavefunctions, therefore appropriate for calculating the electronic and optical properties of crystalline solids.

The Indium pnictides crystallize in the zinc-blende structure at ambient pressure and temperature with lattice parameter 5.8687 Å for InP, 6.0583 Å for InAs and 6.47937 Å for InSb[9]. The space group is F-43 m. The In atom is located at the origin and the X atom is located at (1/4, 1/4, 1/4). The values of $K_{\max} \times R_{\text{MT}} = 7.0$ (where R_{MT} is the atomic sphere radius and K_{\max} is the interstitial plane wave cut-off), In the atomic region, the basis set consists of spherical harmonics with angular quantum number $l = 10$ and a non spherical contribution with $l = 4$ are kept constant throughout the calculations. The self-consistent iterations are considered to be converged when the total energy of the system are stable within 10^{-5} Ry. A mesh point of 5000 k-points were used to obtain 111 special k -points in the irreducible wedge of the Brillouin zone for InP, InAs, InSb. Both the muffin-tin radius and number of k -points were varied to ensure total energy convergence.

The dielectric function of a solid is usually describes in terms of a complex parameter as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, in which the imaginary or the absorptive part of the dielectric function, $\varepsilon_2(\omega)$ can be obtained directly from the band structure calculation. While the real part $\varepsilon_1(\omega)$ can be obtained from the imaginary part $\varepsilon_2(\omega)$ by using the Kramers-Kronig dispersion relation[10].

RESULTS AND DISCUSSION

BAND STRUCTURE AND DENSITY OF STATES

Figures 1, 2 and 3 shows the calculated total density of states, the partial density of states and band structures for Indium pnictides InX (X=P, As, Sb). The band structure, partial and total DOS can be divided into three main groups. The lowest

energy group has mainly pnictide s states. The second group between -7 eV to E_F is composed of In-sp and pnictide p states. The last group from 0.7 for InP, 0.031 eV for InAs, and 0.01 eV for InSb and above has contributions from In-sp_d and pnictide p_d states. The valence band maximum (VBM) is located at Γ for all the three compounds. The valence band maximum (VBM) and the conduction band minimum (CBM) are located at Γ resulting in a direct gap in agreement with experiment and previous theoretical work [11]. The conduction bands shift towards Fermi energy (E_F) when moving from P to As to Sb.

A comparison of the experimental and theoretical band gaps are given in Table-I. It is clearly seen that the band gap obtained by GGA are lower than the corresponding experimental values and results obtained from Tight Binding method [12]. We note that DOS does show a larger energy gaps than the band structures. This is attributed to the fact that the DOS near the conduction band minimum is very small because of the small effective mass. Following Yamasaki *et al.* [13], we can define degree of hybridization by the ratio of In-d states and pnictide p states within the muffin tin sphere. Based on this we can say that the hybridization between In-d and pnictide p states is very weak.

Optical properties

The detailed variation of real, $\epsilon_1(\omega)$ and imaginary $\epsilon_2(\omega)$ parts of the dielectric function for InX with photon energy are shown in Figure 4. We note that $\epsilon_2(\omega)$ shows a large peak located at 4.3 eV for InP, 4.0 eV for InAs, and 3.5 eV for InSb in between two small peaks. All the structures in $\epsilon_2(\omega)$ are shifted towards the lower energies when P is replaced by As and As by Sb, in agreement with the experimental data [14]. This is attributed to the reduction in the band gaps. We compare our calculated $\epsilon_2(\omega)$ with the experimental data [14] and shows very good agreement in the matter of the peaks position and peaks height.

CONCLUSIONS

This paper has reported calculations of the energy bands structure, density of states and linear optical properties of InX (X=P, As, Sb) compounds using generalized gradient approximation (GGA) within the FP-LAPW method. Our result for band structure and DOS shows that these compounds are semiconductors with energy gaps of 0.7 , 0.031 , 0.01 eV. We note that the energy gap reduces when P replaced by As and As by Sb in agreement with the experimental data and pervious theoretical calculations. We compare our calculated linear optical properties with the experimental data [14]. This comparison shows very good agreement in the matter of the peaks position and peaks height.

Table 1: Our calculated direct energy band gap values and the experimental and theoretical band gap (all values are in eV)

Com- pounds	Expt. Band gap	Theoretical Band gap			Present work GGA
		TB	LDA	GGA	
InP	1.39 ^a , 1.35 ^b , 1.351 ^c	1.34 ^d	1.39 ^a , 1.804 ^e , 0.71 ^f , 0.7 ^g	0.85 ^g	0.7
InAs	0.42 ^a , 0.35 ^b , 0.356 ^c	0.35 ^d	0.55 ^a , 0.259 ^e , 0.03 ^f , 0.24 ^g	0.31 ^g	0.031
InSb	0.24 ^a , 0.18 ^b , 0.17 ^c	0.17 ^d	0.24 ^a , 0.00 ^e , 0.01 ^f , 0.14 ^g	0.18 ^g	0.01

^aRef. [11], ^bRef. [15], ^cRef. [16], ^dRef. [12], ^eRef. [17], ^fRef. [18], ^gRef. [19]

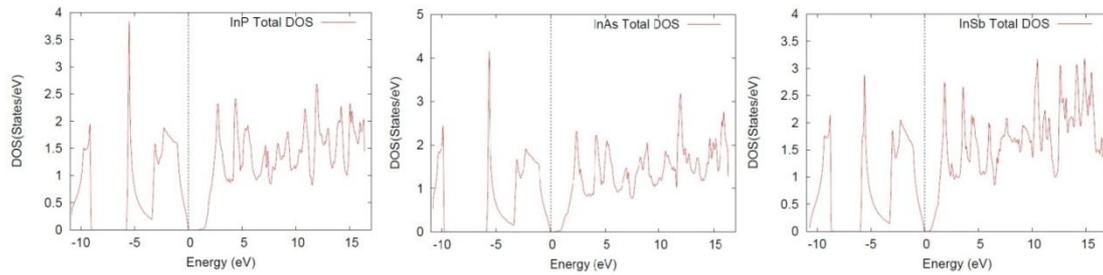


Figure 1: Total Density of States for InP, InAs and InSb

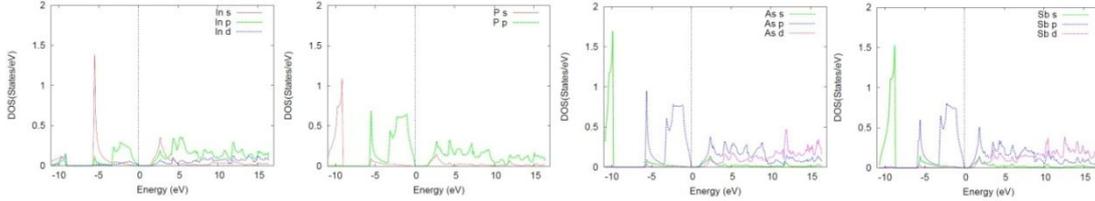


Figure 2: Partial Density of States for InP, InAs and InSb

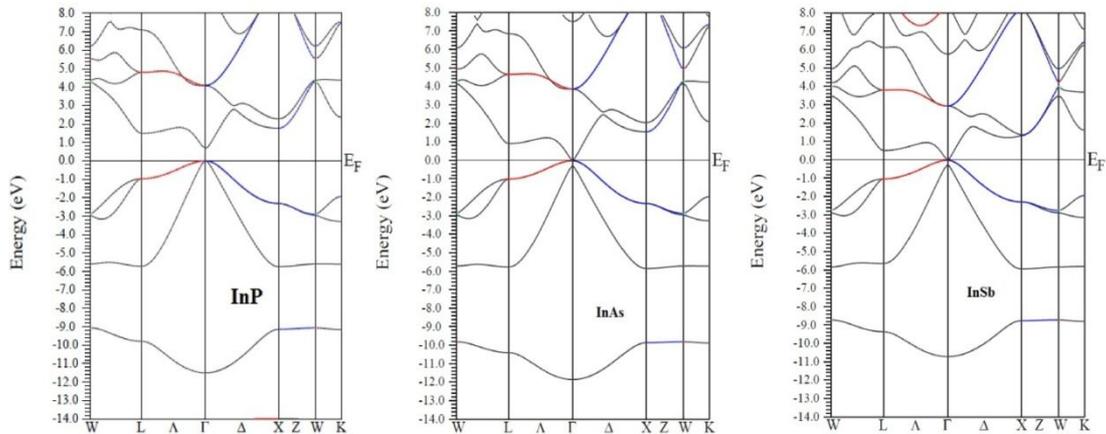


Figure 3: Band structure for InP, InAs and InSb

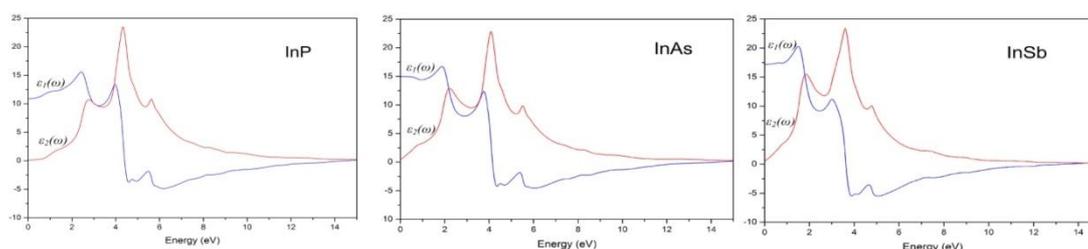


Figure 4: Real and Imaginary part of dielectric function for InP, InAs and InSb

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