Study of electronic and optical properties of aluminium pnictides (AlX, 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 aluminium pnictides is presented by applying the full-potential linearized augmented plane wave (FP-LAPW) method within density-functional theory (DFT) as implemented in WIEN2k code. 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 10 eV. The results are compared with other existing calculations and experimental data and agreement was found.

Key words: AlX; FP-LAPW; band structure; optical properties; WIEN2k.

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

INTRODUCTION

Recently, III–V zinc blende semiconductors compounds occupy a privileged position in the domain of materials science. These compounds semiconductors are favorite hosts for photonic and optoelectronic devices. These semiconductors have higher electron mobility and have wider band gaps than silicon. In the past two decades, remarkable progress has been made toward accurate calculations of the total energy, using density functional theory in the local density approximation[1] and more recently in the

generalized gradient approximation[2]. In the present work we use the full potential linear augmented plane wave (FP-LAPW) method which has proven to be one of the most accurate methods[3] for the computation of the electronic structure of solids within density functional theory (DFT). Hence the effect of the full potential on the linear optical properties can be ascertained.

Although there have been numerous calculations of the electronic and optical properties of AlX (X=P, As, Sb) using different methods, to our knowledge there is only one report had been used the full potential calculation[4] to calculate the electronic structures. Our calculations will highlight the effect of replacing P by As and As by Sb on the electronic and optical properties of

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the investigated compounds.

The aim of this paper is to give a comparative and complementary study of electronic and optical properties to both experimental and other theoretical works by using FP-LAPW method for AlX.

METHOD

The calculation of optical properties of AlX was based on the FPLAPW method[5] as implemented in the WIEN2K package[6]. We choose the exchange-correlation potential parameterized by Perdew *et al.,*[2] 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. We have chosen sphere radii of 2.1 Å for Al, 2.3 Å for P, 2.5 Å for As and 2.8 Å for Sb. For our calculation, we used lattice parameters a = 5.4635 Å, 5.66139 Å, and 6.09593 Å for AlP, AlAs and AlSb respectively[7]. The values of Kmax × RMT = 7.0 (where RMT is the atomic sphere radius and Kmax 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. The compound AlX crystallized in the zinc-blende structure. The space group is F-43 m. The Al atom is located at the origin and the X atoms are located at (1/4, 1/4, 1/4).

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[8]. While the real part $\varepsilon_1(\omega)$ can be obtained from the imaginary part $\varepsilon_2(\omega)$ by using the Kramers-Kronig dispersion relation.[9]

RESULTS AND DISCUSSION

Band structure and density of states

The calculated total density of states, the partial density of states and band structures for aluminum pnictides are shown in Figures 1, 2 and 3. The band structure and TDOS can be divided into three main groups/structures. From the partial DOS we are able to identify the angular momentum character of the various structures. The lowest energy group has mainly X-s states. The second group is mainly Al-s and X-p states. The third group is mainly from p state of Al and X. From the partial DOS, we note a strong hybridization between Al-s and X-p states below and above E_F. The valence band maximum (VBM) is located around Γ and the conduction band minimum (CBM) is located around X resulting in an indirect energy bad gap of 1.58 eV,

Table 1. Indirect energy band gap values and the experimental and theoretical band gap (all values are in eV).

System study	Expt. band gap	Theoretical band gap			Our calculated band-gaps GGA
		TB	LDA	GGA	
AlP	2.50[a]	2.45[b]	2.17[a], 1.49[c]	1.638[d]	1.58
AlAs	2.3[a]	2.153[b]	1.37[a], 1.39[c]	1.494[d]	1.46
AlSb	1.87[a]	1.615[b]	1.23[a], 1.17[c]	1.214[e]	1.20

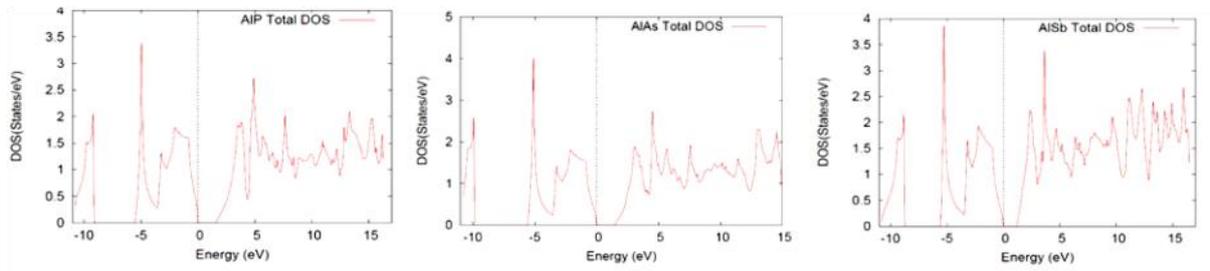[a]Ref. 11; [b]Ref. 10; [c]Ref. 12; [d]Ref. 13; [e]Ref. 14.

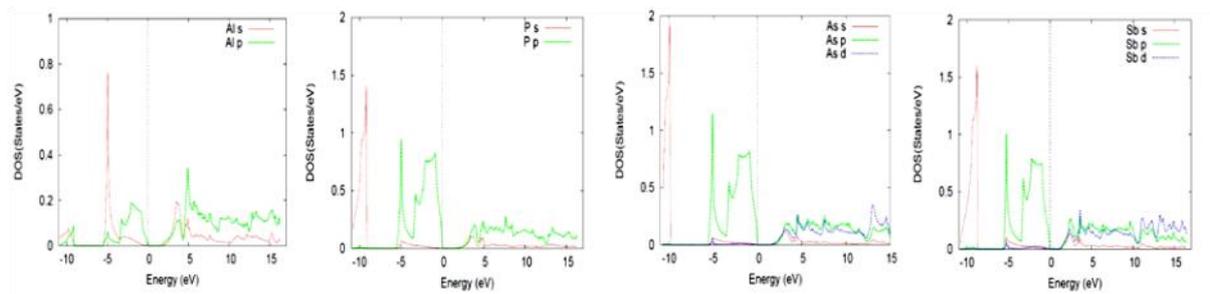Figure 1. Total density of states for AlP, AlAs and AlSb.

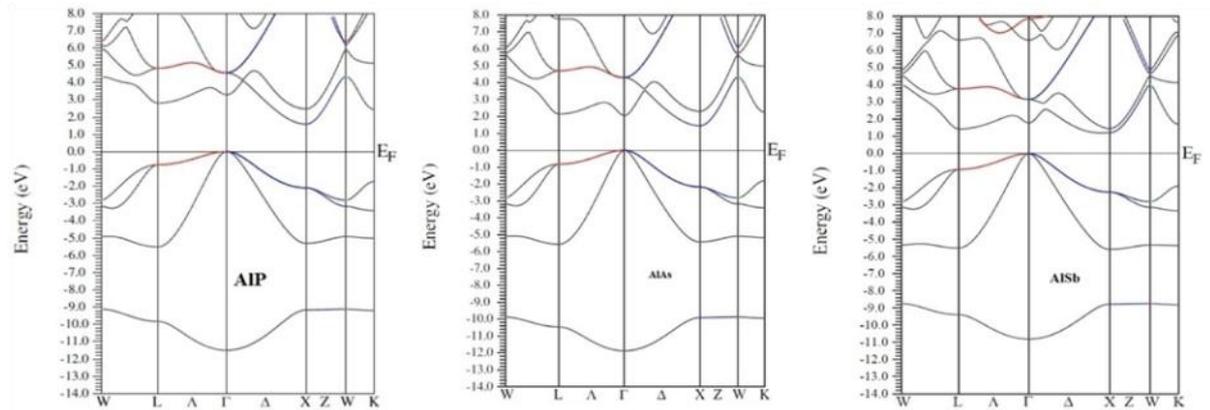Figure 2. Partial density of states for AlP, AlAs and AlSb.

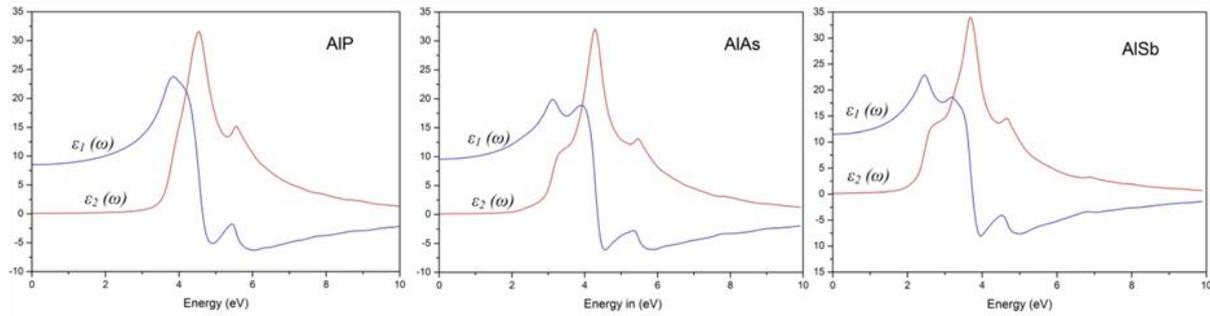Figure 3. Band structure for AlP, AlAs and AlSb.

Figure 4. Real and imaginary part of dielectric function for AlP, AlAs and AlSb.

1.46 eV, 1.2 eV for AlP, AlAs and AlSb respectively. 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 (TB) [10]. Our results are in a good agreement with the other theoretical work with the same exchange correlation approximation of LDA [11,12] and GGA [13,14]. We note that the energy gap decreases when P replaced by As and As by Sb in agreement with the previous theoretical calculations and experimental data.

Linear optical properties

The detailed variation of real, $\varepsilon_1 (\omega)$ and imaginary $\varepsilon_2 (\omega)$ parts of the dielectric function for AlX with photon energy are shown in Figure 4. Since the investigated compounds have cubic symmetry, we need to calculate only one dielectric tensor component to completely characterize the linear optical properties. This component is $\varepsilon_2 (\omega)$ the imaginary part of the frequency dependent dielectric function. We note that $\varepsilon_2 (\omega)$ shows a large peak located at 4.5 eV for AlP, 4.3 eV for AlAs, and 3.7 eV for AlSb. All the structures in $\varepsilon_2 (\omega)$ are shifted towards the lower energies when P is replaced by As and As by Sb. This is attributed to the increases in the band width of the conduction bands when we move from P to As to Sb. We note that the peak heights are increases when we move from P to As to Sb. We compare our calculated $\varepsilon_2 (\omega)$ with the most recent calculations of Huang and Ching [11]. Previous calculations [11] underestimate the magnitude of $\varepsilon_2 (\omega)$ in the low energy regime. This could be due to an inaccurate representation of the wave functions.

CONCLUSION

The calculations of band structure, DOS and linear optical response for AlP, AlAs, and AlSb compounds using FP-LAPW method based on the DFT in GGA are presented in this work.

Our results for band structure and DOS, show that these compounds have similar structures and the energy gap decreases when P is replaced by As and As by Sb. This is attributed to the fact that the bandwidth of the conduction bands increases on going from P to As to Sb. All the structures in the imaginary part of the dielectric function $\varepsilon_2 (\omega)$ are shifted towards lower energies when P is replaced by As and As by Sb. We compare our calculated $\varepsilon_2 (\omega)$ with the previous theoretical calculations and found good agreement. We also identified the microscopic origin of the main features in the optical spectra and found that transitions between highest lying valence band (HVB) and lowest lying conduction band (LCB) are responsible for most of the optical absorption in AlX. It is an established fact that indirect band gap materials are bad emitters of light because phonons are involved in the de-excitation of electron and hence the absorbed photon energy is trapped. Due to this disadvantage, AlX are ineffective for optoelectronic industry. In order to use these compounds in the green, blue and ultra violet (UV) optical devices the indirect band gaps of these materials must have to be transformed into direct ones through band gap engineering (i.e. doping, creating, applying external pressure or current etc.).

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