



Study of the effect of spin orbit interaction on band structures in III-V semiconductor compounds

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ABSTRACT

We present a study of the effect of the spin-orbit interaction on the band structures in III-V binary semiconductor compounds like GaAs, GaP, GaSb, etc. Our calculations were performed using a self-consistent, full-potential linearized augmented plane wave (FP-LAPW) method as implemented in Wien2k code. We found that the inclusion of spin-orbit interaction affects on the band structures, and the splitting of degenerate valence band occurs on high symmetry G-point. We obtained the results on the band structures without and with the inclusion of spin-orbit interaction and compare the results. We also measured the value of the splitting energy and found that our results are similar to the calculated value of earlier results.

Key words: DFT, FP-LAPW; spin-orbit coupling; energy band structure; splitting energy.

INTRODUCTION

The spin-orbit interaction (also called spin-orbit effect or spin-orbit coupling) is any interaction of a particle's spin with its motion. Spin-orbit coupling makes the spin degree of freedom respond to its orbital environment. In solids this yields such fascinating phenomena as a spin splitting of electron states in inversion-asymmetric systems even at zero magnetic field and a Zeeman splitting that is significantly enhanced in magnitude over the Zeeman splitting

of free electrons.¹

The spin-orbit interaction is a relativistic effect whose magnitude increases with the atomic number. Consequently, it provides negligible contributions to the electronic structure of individual atoms and bulk materials made of light elements.² It is also the primary interaction responsible for most of the zero-field splitting and other properties of magnetic molecules.³ Several relativistic methods have been developed in various schemes for the all-electron calculations for solids: the augmented-plane-wave (APW) method,⁴ the linearized muffin-tin-orbital (LMTO) method,⁵⁻⁸ the Korringa-Kohn-Rostoker (KKR) method,⁹⁻¹³ and the linear-

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combination-of-atomic-orbitals (LCAO) method.¹⁴⁻¹⁸

In semiconductors, the spin-orbit interaction splits the edges of the valence and conduction bands¹⁹ and allows electrical manipulation of the spin direction.²⁰ This last effect is of paramount importance for the growing field of spintronics,²¹ which has certainly added more impetus to the inclusion of the spin-orbit interaction in the description of the electronic structure. The spin-orbit coupling determines the spin-relaxation time of electrons in ordinary semiconductors and in semiconductor heterostructures²² and also plays an important role in the physics of diluted magnetic semiconductors.²³ Finally, it is worth mentioning that electron spin manipulation using the spin-orbit interaction was recently demonstrated in the so-called spin-Hall effect,²⁴ which is a solid-state version of the Stern-Gerlach measurement.

It is therefore, clear that the spin-orbit interaction is becoming increasingly important for a number of applications, which also require the description of rather large mesoscopic systems.

FORMALISM

The Dirac Hamiltonian²⁵ can be written as

$$H_D = c\alpha^{\mathbf{r}} p + (\beta - 1)mc^2 + V(\mathbf{r}) \quad (1)$$

where $\alpha^{\mathbf{r}}$, β are 4x4 matrices:

$$\alpha^{\mathbf{r}} = \begin{pmatrix} 1 & \sigma^{\mathbf{r}} \\ \sigma^{\mathbf{r}} & 1 \end{pmatrix} ; \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (2)$$

$\sigma_x, \sigma_y, \sigma_z$ are the Pauli-spin matrices. Eigenvectors of (1) are four-component functions Ψ which are written in terms of two-component functions Φ, χ :

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} \quad (3)$$

In case of electrons, Φ is the 'large' and χ is the 'small' component of the wave function. Thus equations (1-3) lead to a set of coupled equations:

$$c(\alpha^{\mathbf{r}} p)\chi = (\varepsilon - V)\Phi \quad (4)$$

$$c(\alpha^{\mathbf{r}} p)\Phi = (\varepsilon - V + 2mc^2)\chi \quad (5)$$

From equations (4-5), we get the equation for the large component:

$$\frac{1}{2m}(\alpha^{\mathbf{r}} p) \left(1 + \frac{\varepsilon - V}{2mc^2} \right)^{-1} (\alpha^{\mathbf{r}} p)\Phi + V\Phi = \varepsilon \Phi \quad (6)$$

Using approximation and solving with some value, eqn. (6) leads to a differential equation for Φ given by

$$\left[\left(1 - \frac{\varepsilon - V}{2mc^2} \right) \frac{p^2}{2m} + V \right] \Phi - \frac{\hbar^2}{4m^2 c^2} (\nabla V \nabla \Phi) \Phi + \frac{\hbar^2}{4m^2 c^2} (\sigma^{\mathbf{r}} [\nabla V, \mathbf{p}]) \Phi = \varepsilon \Phi \quad (7)$$

If the potential has the spherical symmetry, eqn.(10) reduces to:

$$\left[\frac{p^2}{2m} + V - \frac{p^2}{8m^3 c^2} - \frac{\hbar^2}{4m^2 c^2} \frac{dV}{dr} \frac{\partial}{\partial r} + \frac{1}{2m^2 c^2} \frac{1}{r} \frac{dV}{dr} \begin{pmatrix} \mathbf{r} & \mathbf{r} \\ l & s \end{pmatrix} \right] \Phi = \varepsilon \Phi \quad (8)$$

The first and second term give non-relativistic Schrodinger equation. The third and fourth term are mass-velocity and Darwin correction, respectively. Finally, the last term corresponds to the spin-orbit coupling.

The four-component function Ψ is now written as:

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} = \begin{pmatrix} g(r)Y_{jl}^{j_z} \\ if(r)Y_{j'l'}^{j_z} \end{pmatrix} \quad (9)$$

where g and f are the radial function, $Y_{jl}^{j_z}$ is the r -independent eigen function of j^2, j_z, l^2 and s^2 formed by the combination of the Pauli spinor with the spherical harmonics, By solving eqn. (9) and eliminating f , we obtain

$$-\frac{\hbar^2}{2Mr^2} \frac{d}{dr} \left(r^2 \frac{dg}{dr} \right) + \left[V + \frac{\hbar^2}{2Mr^2} \frac{l(l+1)}{r^2} \right] g - \frac{\hbar^2}{4M^2r^2} \frac{dV}{dr} \frac{dg}{dr} - \frac{\hbar^2}{4M^2r^2} \frac{dV}{dr} \frac{1+\kappa}{r} g = \varepsilon g \quad (10)$$

The function f is given by

$$f = \frac{\hbar^2}{2Mc} \left(\frac{dg}{dr} + \frac{1+\kappa}{r} g \right) \quad (11)$$

The scalar relativistic approximation²⁶ is obtained by omitting the terms which depend on κ in eqns. (10, 11). The spin-orbit coupling may be then taken into account using the method described below. We denote the scalar relativistic approximation to f, g by f^0, g^0 :

$$-\frac{\hbar^2}{2Mr^2} \frac{d}{dr} \left(r^2 \frac{dg^0}{dr} \right) + \left[V + \frac{\hbar^2}{2Mr^2} \frac{l(l+1)}{r^2} \right] g^0 - \frac{\hbar^2}{2Mr^2} \frac{d}{dr} \left(r^2 \frac{df^0}{dr} \right) + \left[V + \frac{\hbar^2}{2Mr^2} \frac{l(l+1)}{r^2} \right] f^0 = \varepsilon g^0 \quad (12)$$

and f^0, g^0 satisfy the set of equations:

$$f^0 = \frac{\hbar^2}{2Mc} \frac{dg^0}{dr} \quad (13)$$

$$g^0 = -\frac{\hbar c}{\varepsilon - V} \frac{df^0}{dr} \quad (14)$$

The four-component wave function is now written as:

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} \quad (15)$$

where Φ is a pure spin state and χ contains mixture of up and down spin

The functions Φ are not eigen functions of the Dirac Hamiltonian (1) and their deviation from eigen function is used to define the spin-orbit Hamiltonian H_{so} :

$$H_0 \Phi = \varepsilon \Phi + H_{so} \chi \quad (16)$$

In the basis of functions (13), H_{so} has the form:

$$H_{so} = \frac{\hbar^2}{2Mc^2} \frac{1}{r} \frac{dV}{dr} \begin{pmatrix} r^l & 0 \\ 0 & 0 \end{pmatrix} \quad (17)$$

RESULTS AND DISCUSSION

We discuss here the results of the effect of spin orbit interaction on band structure in the case of binary semiconductor compounds like GaAs, GaP, GaSb and InP which are having zincblende structure. The calculations were performed using a self-consistent, full-potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2k code.²⁷ We have generated the band structures without spin orbit coupling and with spin orbit coupling. We compared each of these two results and measured spin orbit splitting energy on the valence band.

GaAs

Figure 1 (a) shows the band structure of GaAs without spin-orbit coupling. We can see that the valence band is degenerate in the high symmetry G point. But, if we include the spin orbit interaction, the splitting of valence band occurs on high symmetry G point which is shown in Figure 1(b). We have found that 0.35 eV is the spin splitting energy on GaAs compound, which is in good agreement with the earlier calculated result.²⁸

GaP

Figure 2(a) shows the band structure of GaP without spin-orbit coupling. It can be observed that the valence band is degenerate in the high symmetry G point. But, if the spin orbit interaction is included, the splitting of valence band occurs on high symmetry G point which is shown in Figure 2(b). We have also found that 0.08 eV is the spin splitting energy on GaP compound, which is in good agreement with the previous calculated result.²⁸

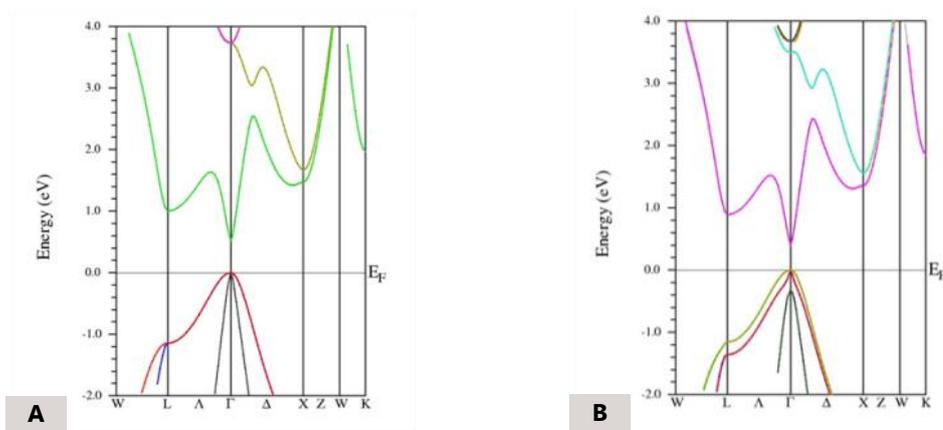


Figure 1. Band structures of GaAs. (a) Without spin-orbit coupling (b) With spin-orbit coupling

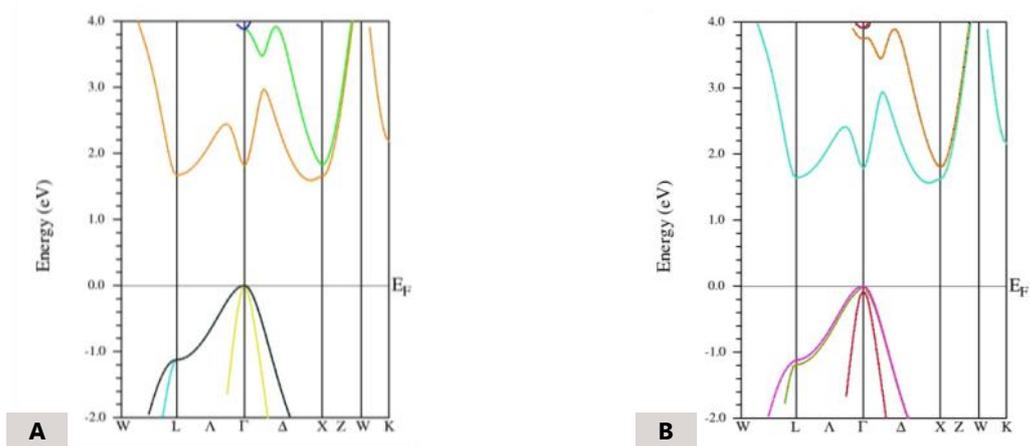


Figure 2. Band structures of GaP. (a) Without spin-orbit coupling (b) With spin-orbit coupling

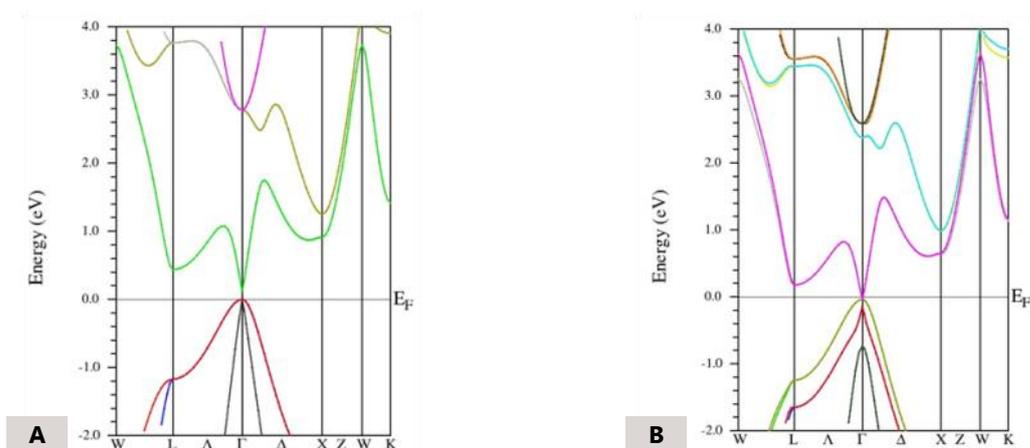


Figure 3. Band structures of GaSb. (a) Without spin-orbit coupling (b) With spin-orbit coupling

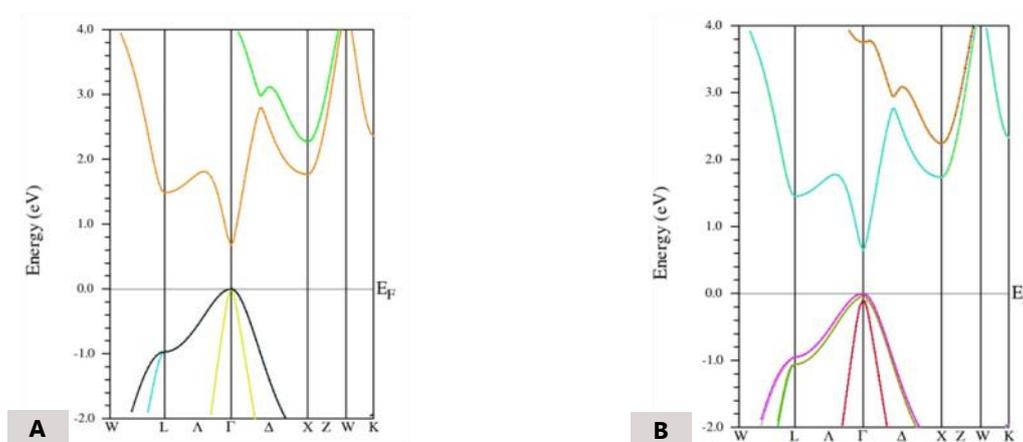


Figure 4. Band structures of InP. (a) Without spin-orbit coupling (b) With spin-orbit coupling

Table 1. Comparison of spin splitting energy in different binary compounds.

| Sl. No. | Name of compounds | Spin splitting energy (eV) | |
|---------|-------------------|----------------------------|---|
| | | Our calculated value | Ioffe physico-technical institute value (Ref. 27) |
| 1. | GaAs | 0.35 | 0.34 |
| 2. | GaP | 0.08 | 0.08 |
| 3. | GaSb | 0.80 | 0.80 |
| 4. | InP | 0.10 | 0.11 |

GaSb

Figure 3 (a) shows the band structure of GaSb without spin-orbit coupling. It can be observed that the valence band is degenerate in the high symmetry G point. But, if we include the spin orbit interaction, the splitting of valence band occurs on high symmetry G point which is shown in Figure 3(b). We have calculated that 0.80 eV is the spin splitting energy on GaSb compound, which is in a good agreement with the previous calculated result.²⁸

InP

Figure 4(a) shows the band structure of InP without spin-orbit coupling. It can be observed that the valence band is degenerate in the high symmetry G point. But, if we include the spin

orbit interaction, the splitting of valence band occurs on high symmetry G point which is shown in Figure 4(b). Again, we have found that 0.10 eV is the spin splitting energy on InP compound, which is in good agreement with the previous calculated result²⁸ like the case of GaAs, GaP and GaSb.

CONCLUSION

In this paper, we found that the spin-orbit interaction effect the valence band of III-V binary compound semiconductors. It is clear that the splitting energy of valence band is different in different compound and it values increases with atomic number. Table 1 below shows the comparison of spin splitting energy in different binary compounds and the comparison between our results and the previous calculated results.²⁸

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