

## Calculation of the effective masses of II-VI semiconductor compounds

A. Rubio-Ponce

Departamento de Ciencias Básicas, UAM-Azcapotzalco  
Av. San Pablo 180, 02200 México, D.F., México

D. Olgúin and I. Hernández-Calderón

Departamento de Física, Centro de Investigación  
y de Estudios Avanzados del Instituto Politécnico Nacional  
A.P. 14 740, C.P. 07300, México, D.F.

We present results on *ab initio* calculations of the effective masses for the II-VI zinc-blende wide band gap semiconductor compounds. The electronic band structure has been calculated using the full potential linearized augmented plane waves method. By computing the curvature of the principal band extrema at the  $\Gamma$ -point we have calculated the effective mass values. We show that our calculated values compare acceptably well with values reported in the literature.

*Keywords:* Plane-wave methods; Effective mass; Semiconductor compounds

### 1. Introduction

A number of important semiconductor properties require for their analysis detailed knowledge of effective masses at the main band extrema. However, even for most of the well-known materials we found an important dispersion of experimental and theoretical data existing in the literature. Although simple and formal expressions for the effective masses can readily be obtained from second order  $\overline{k \cdot p}$  perturbation theory, the important parameters in the model have been not known with accuracy sufficient to render the theoretical results reliable. The reason for this is connected with the different approaches to the band structure calculations, mainly in the empirical method, where the main objective is to reproduce energy values at high-symmetry points and the correct dispersion of the bands is not well predicted. Recent band structure calculations, based in *ab initio* methods, bring new tools to calculate the full dispersion of the bands and as a consequence the effective masses. In this work we present electronic band structure calculations of the II-VI zinc-blende semiconductor compounds using the full potential linearized plane wave (LAPW) method [1]. The method uses the LSDA as well as the the GGA [2] approach to solve the exchange-correlation part of the energy. We show that the tendency of our calculated values present better comparison with most of the values reported in the literature when we use the GGA correction than the LSDA calculations.

The paper is organized as follows: Section 2 describes briefly the method used, in Section 3 we present our results and we make a comparison with values reported in the literature, a final Section 4 presents our conclusions.

### 2. Method

In the framework of the density functional theory we have calculated the electronic band structure of the II-VI zinc-blende wide band gap semiconductors. The method used was the full potential augmented plane waves method [1]. The calculations were done using both the LSDA and GGA approach to compute the exchange-correlation energy. The spin-orbit corrections have been taken into account. We have verified the convergence of the calculations in terms of the number of  $k$ -points in the irreducible segment of the first Brillouin zone and in terms of the cutoff energy factor  $G_{\max}$ , the values used were 73 and 12, respectively. We have focused our attention in the Zn- and Cd-chalcogenides. The electronic structure configuration, including  $d$  orbitals, used for each atom as the valence states was Zn( $3p, 3d, 4s$ ), Cd( $4p, 4d, 5s$ ), Se( $3d, 4s, 4p$ ), Te( $4d, 5s, 5p$ ). Where the Zn  $3p$  states were treated in the local orbital extension of the LAPW method [1].

### 3. Results

We have computed the electron, heavy-, light-hole, and spin-orbit splitting effective masses in the [100] and [111]

**Table 1.** Calculated effective masses for the [100] directions. All the masses are given in units of the electron free mass.

Compound	LSDA calculations				GGA calculations			
	$m_e$	$m_{hh}$	$m_{lh}$	$m_{so}$	$m_e$	$m_{hh}$	$m_{lh}$	$m_{so}$
ZnSe	0.149	1.116	0.195	0.474	0.186	1.122	0.249	0.533
ZnTe	0.115	0.801	0.133	0.487	0.151	0.810	0.168	0.528
CdSe	0.057	1.174	0.069	0.322	0.116	1.217	0.150	0.428
CdTe	0.047	0.879	0.051	0.444	0.098	0.892	0.112	0.508

**Table 2.** Calculated effective masses for the [111] directions. All the masses are given in units of the electron free mass.

LSDA calculations Compound	LSDA calculations		GGA calculations	
	$m_{hh}$	$m_{lh}$	$m_{hh}$	$m_{lh}$
ZnSe	1.898	0.136	1.054	0.165
ZnTe	1.403	0.098	1.413	0.117
CdSe	1.925	0.051	2.046	0.105
CdTe	1.555	0.038	1.602	0.078

directions. For these two high symmetry directions there are six independent masses,  $m_e \equiv m_{e[100]} \equiv m_{e[111]}$ ,  $m_{hh[100]}$ ,  $m_{lh[100]}$ ,  $m_{hh[111]}$ ,  $m_{lh[111]}$ , and  $m_{so} \equiv m_{so[100]} \equiv m_{so[111]}$  [3]. The electronic bands near the  $\Gamma$ -point are defined as:

$$E_{so} = -\Delta E_0 - \frac{\hbar^2 k^2}{2 m_{so}}$$

$$E_{lh} = \frac{\hbar^2 k^2}{2 m_{lh}}$$

$$E_{hh} = \frac{\hbar^2 k^2}{2 m_{hh}}$$

$$E_e = E_0 + \frac{\hbar^2 k^2}{2 m_e}$$

where  $\Delta E_0$  is the spin-orbit splitting,  $E_0$  the band gap,  $m_i$  stands for the different associated masses, and the  $k$ -wavevector is evaluated in such a way that we are in the parabolic regime of the electronic band, usually around 0.5% of the full wavevector magnitude in each direction. From the above equations, the different effective masses are obtained from the expression

$$m^* = \pm \hbar^2 \left( \frac{d^2 E_k}{dk^2} \right)^{-1}$$

Tables 1-2 show our results both using the LSDA and GGA corrections. Table 1 shows the results for the [100] directions, Table 2 shows the results for the [111] directions.

For comparison, Table 3 shows some values found in the literature. Although the compilation given in Table 3 lacks for some entries, we can see that the published values for ZnSe, for instance, show noticeable dispersion. For CdTe the compiled data seems to be more consistent. For ZnTe and CdSe there are not enough data to establish a reasonable comparison.

Table 1 shows our calculated values for the conduction band. For the Zn-based compounds we found that our calculated values are, in general, in good agreement with the values collected in Table 3. For the Cd-based compounds our LSDA-calculated values represent almost one half of the reported values. However, the GGA-values show better agreement with the data of Table 3.

The calculated heavy hole masses for ZnSe are overestimated by a factor of two, comparing with the mean value of the data showed in Table 3. For the rest of the compounds our calculated values are almost 50% bigger than the collected values in Table 3.

The calculated light hole values for ZnSe show an acceptable agreement. For the Cd-based compounds the LSDA values are smaller than the reported ones. However, the GGA-calculated masses are in better agreement than the LSDA-values.

Although, the compiled spin-orbit splitting masses are not complete, our calculated values for CdTe compare acceptably well with the value shown in Table 3.

In summary, the tendency of our results show that the GGA-correction improves the density functional calculations in the semiconductor compounds, in comparison with the LSDA-correction, as it is accepted in the literature [2].

#### 4. Conclusions

We have calculated the effective masses of the II-VI zincblende wide band gap semiconductor compounds using *ab initio* calculations. We have used the LSDA and GGA correction to calculate the exchange-correlation part of the energy. Although, we have found that for some compounds the reported values present large dispersion, we have obtained that our GGA-calculations show better agreement with most of the published values than the LSDA-calculations.

**Table 3.** Reported effective masses for the [100] and [111] directions. All the masses are given in units of the electron free mass.

Compound	[100] directions			[111] directions		
	$m_e$	$m_{hh}$	$m_{lh}$	$m_{so}$	$m_{hh}$	$m_{lh}$
ZnSe <sup>a</sup>	0.13	0.574	0.221	-	0.754	0.145 <sup>b</sup>
	0.15	0.530	0.144		1.197	
	0.16	0.495	0.177		1.613	
	0.16	0.334	0.162		0.485	
	0.16	0.813	0.182		2.703	
	0.165	0.321			0.617	
ZnTe <sup>c</sup>	0.174					
	0.145	0.49				
CdSe <sup>d</sup>	0.116	0.6	-	-	-	-
	0.12	0.6				
CdTe <sup>e</sup>	0.119	0.820	0.262	-	1.613	0.226
	0.11	0.45				
CdTe <sup>e</sup>	0.110	0.600	0.180	0.350	0.690	0.210
	0.99	0.600	0.120	-	0.690	0.110
	0.09	0.40				

<sup>a</sup>Ref.[4-6]<sup>b</sup>Ref.[7]<sup>c</sup>ref.[5,6,9]<sup>d</sup>Ref.[6, 10]<sup>e</sup>Ref.[6,8]

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