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Ab initio studies of band parameters of A^{III}B^V and A^{II}B^{VI} zinc-blende semiconductors

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Electronic band-structure calculations have been performed for zinc-blende A^{III}B^V (AlP, AlAs, AlSb, GaP, GaAs, GaP, InP, InAs, InSb) and A^{II}B^{VI} (ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe) semiconductors by the *ab initio* pseudopotential method within the local-density approximation (LDA). The lattice parameters, band gaps, Luttinger parameters, momentum matrix elements and effective masses are studied in detail. It is shown that LDA calculations cannot give accurate band parameters systematically. It is found that LDA band parameters calculated using the experimentally determined lattice constants are more accurate than those using the LDA lattice constants. We found that inclusion of *d*-electrons of group-II atoms into the core gives more accurate band parameters.

1. Introduction

Density-functional theory (DFT) is a powerful tool for studying the electronic structure of solids. It is well known that the band gaps of bulk solids calculated within the theory are systematically underestimated compared to experimentally determined ones [1] because of its failure in the description of the excited-state properties and the problem rests not just with the local-density approximation (LDA). Following $\mathbf{k} \cdot \mathbf{p}$ theory (see e.g. Ref. [2]), however, one can say that if the fundamental excitation gaps are incorrect, then band dispersions should be too. This realization has been used by Cardona and co-workers [3–6] in generating corrected band parameters (Luttinger parameters, spin splittings) for a number of semiconductors. Nevertheless, there remains some dispute regarding this issue [7]. For instance, in 1992, Fiorentini and Baldereshi [8,9] using pseudopotential plane waves within LDA found that conduction-band masses (m_c) at the Γ point were very close to experimental values for GaAs, AlAs and Ge. However, the values of m_c found in Ref. [10] significantly differ from those determined experimentally for GaAs, GaSb, InP and InAs. Similarly, conduction-band effective masses calculated by Wang and Zunger [11] within LDA agree well with experimental data for Si, while for CdSe the masses were not very accurate and a semi-empirical modification led to somewhat better agreement. Kane [12], on the other hand, found that it is not possible to get the correct band gap and the cyclotron masses in Si by a local static potential such as the LDA. Fairly good agreement with experiment was obtained by Wang and Klein [13] for conduction and valence band effective masses of GaP, GaAs, ZnS and ZnSe using the linear combination of Gaussian orbitals within LDA. Systematic study of effective masses for 32 semiconductors by Huang and Ching [14] using the semi-*ab initio* technic shows much better agreement. Despite the importance of the effective masses, the question

as to whether the calculations within LDA give correct effective masses is, therefore, still open.

There is even less explicit work on the correctness of the momentum matrix elements (E_p) calculated within LDA, which are often claimed to be accurate. However, the validity of the statement has been less directly verified. The standard argument is that the pseudo-wave-function, in a pseudopotential approach, has a very high overlap with the true wave function [11]. The value of E_p for GaAs calculated by Winkler [15], and Kageshima and Shiraishi [16] within LDA is about ~ 1.7 times smaller than that determined experimentally [17,18]. Kageshima and Shiraishi [16] concluded that the wave functions calculated by the pseudopotential method lack a precise description around the atomic core regions and momentum matrix elements cannot be directly estimated from these wave functions, because the functions are smoother around the atomic cores, while the actual wave functions oscillate greatly. To fix the error, a core-repair term was added. By including the correction, significant improvement was indeed achieved for zinc-blende and wurtzite GaN. However, momentum matrix elements for poly-silane, siloxene and GaAs calculated with the correction and without it differ from each other by only 5.43, 3.0 and 1.8%, respectively. Wang and Zunger [11], on the other hand, had found a larger increase in the momentum matrix elements. To complicate matters, Levine and Allan [19] found that, even within the scissors approximation, the velocity operator gets renormalized.

It should be noted that correctness of the calculated and experimentally determined values of E_p is also being debated. Efros and Rosen [20], for example, concluded that $E_p = 14.98$ eV for bulk InP calculated by Fu, Wang and Zunger [21] using the direct diagonalization method is smaller than the measured value 20.6 eV, which indicates underestimation of the coupling between the conduction and valence bands, and overestimation of the influence of the remote bands. However, even the values of E_p extracted from experiments have an intrinsic scatter. For bulk InP, for

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example, the experimental values of E_p vary in the range from 16.6 (Ref. [22]) to 20.7 eV (Ref. [23]). So, the question as to whether the momentum matrix elements calculated by LDA are correct is still open.

It should also be noted that the above-mentioned problems are relatively less studied in $A^{II}B^VI$ semiconductors which have a cation d -band inside the main valence band playing a significant role in their electronic structures [24–29]. In $A^{III}B^V$ semiconductors the d -levels are below in energy to several eV than the lowest sp valence band states [30]. So the effect of the d -states on electronic structure of $A^{III}B^V$ compounds can be neglected. In the literature, the strong p – d coupling in the $A^{II}B^VI$ semiconductors has usually been taken into account by including the d -electrons (i) into the core, but including also nonlinear core corrections for exchange and correlation, and (ii) into the valence complex [24–26], but keeping the s and p semicore electrons in the core. Currently, description of the p – d coupling is still being improved. Despite numerous studies, the question as to which of the approaches related to the p – d coupling is correct and consistent with $\mathbf{k} \cdot \mathbf{p}$ band parameters is still open.

In this paper we provide the first systematic study of eigenvalues at Γ , X and L , Kane momentum matrix elements E_p and E'_p (defined as $2P^2/m_0$ in eV) corresponding to the fundamental direct p – s energy gap E_g and the p – p gap E'_g at Γ point, conduction-band effective masses m_c^{001} , m_c^{011} , m_c^{111} , heavy-hole effective masses m_{hh}^{001} , m_{hh}^{011} , m_{hh}^{111} , light-hole effective masses m_{lh}^{001} , m_{lh}^{011} , m_{lh}^{111} and Luttinger parameters γ_1^L , γ_2^L and γ_3^L and answer the question as to whether the band parameters calculated within the framework of LDA correct.

2. Computational details

2.1. Local-density approximation

Ab initio calculations were performed for $A^{III}B^V$ (AlP, AlAs, AlSb, GaP, GaAs, GaP, InP, InAs, InSb) and some $A^{II}B^VI$ (ZnS, ZnSe, ZnTe, CdS, CdS, CdSe, CdTe) semiconductors of zinc-blende structure. We did not study the $A^{II}B^VI$ compounds HgS, HgSe, and HgTe, because it is well known that spin-orbit coupling (which is not accounted for in this work) plays a significant role [24]. The unit cell considered consists of two atoms of group-III (II) at (0,0,0) and an atom of group-V (VI) at $(a/4, a/4, a/4)$, where a is the lattice constant.

Ab initio pseudopotentials have been generated using the method of Trouillier–Martins [31]. We have considered s , p and d as valence states to build the pseudopotential for the atoms of group-III and V using the p -potential as the local potential, while the s and d are taken as the nonlocal parts. We determined E_{cut} by requiring convergence of the total energy E_{tot} . For all the $A^{III}B^V$ semiconductors considered, $E_{\text{cut}} = 60$ Ry was used.

To study the $A^{II}B^VI$ compounds, s , p and d states were considered as valence states. Pseudopotentials for of

group-II atoms have been generated by two ways: including the d -electrons, which are inside the valence shell (i) into the valence complex, while keeping the semicore s and p states in the core, and (ii) into the core. For the latter case, we used $E_{\text{cut}} = 30$ Ry and nonlinear exchange correlation was included, which is known to give better agreement with experimental data [25]. For the former case, convergent results were obtained for $E_{\text{cut}} = 70$ Ry. The semicore d -electrons of $A^{III}B^V$ compounds have been included into the core, because, as discussed in Section 1, energy level of the electrons are much below the outermost sp -levels [30] and the electrons are not expected to effect significantly on band structure of the compounds.

Band-structure calculations were performed using the PETot code developed by L.-W. Wang [32], which uses the *ab initio* pseudopotential method within the LDA and neglects spin-orbit coupling. The Pulay–Kerker scheme has been used for self-consistent potential mixing. Also, g -space Kleinman–Bylander non-local pseudopotential implementations have been used with mask function scheme, without the need for preprocessing of the pseudopotentials. The LDA exchange-correlation contribution is accounted for by means of Perdew and Zunger’s parametrization [33] of the calculations by Ceperley and Alder [34]. The self-consistent solution of the one-electron Kohn–Sham equation has been performed by the planewave pseudopotential algorithm [35].

The potential for the unit cell considered was found by performing self-consistent calculations using 10 special k points in the Brillouin zone. Then, using the potential, eigenenergies at the special k points were found by non-self-consistent calculations.

2.2. Band parameters

Carrier effective masses are defined as:

$$\frac{1}{m_c(\mathbf{k}_0)} = \frac{1}{\hbar^2} \left. \frac{\partial^2 E(\mathbf{k})}{\partial k^2} \right|_{\mathbf{k}=\mathbf{k}_0} \quad (1)$$

for a direction \mathbf{k} about some point \mathbf{k}_0 in the Brillouin zone. We studied effective masses along [001], [011] and [111] directions in the vicinity of $\mathbf{k}_0 \equiv \Gamma(0, 0, 0)$ point. The masses can, in principle, be calculated by the $\mathbf{k} \cdot \mathbf{p}$ theory equation (see e.g. Ref. [2]). In this work, we calculate the band energies at a sequence of k points around Γ and calculate m_c from Eq. (1) directly.

We considered conduction-band effective masses m_c^{001} , m_c^{011} , m_c^{111} , heavy-hole effective masses m_{hh}^{001} , m_{hh}^{011} , m_{hh}^{111} and light-hole effective masses m_{lh}^{001} , m_{lh}^{011} , m_{lh}^{111} . To calculate the effective masses, 11 k -points were used in the ranges from $(2\pi/a)/(0, 0, -1/20)$ to $(2\pi/a)(0, 0, 1/20)$ for the direction [001], from $(2\pi/a)(0, -1/20, -1/20)$ to $(2\pi/a)(0, 1/20, 1/20)$ for the direction [011], and from $(2\pi/a)(-1/20, -1/20, -1/20)$ to $(2\pi/a)(1/20, 1/20, 1/20)$ for the direction [111]. Momentum matrix elements have been determined at the Γ point.

Table 1. Experimental (Ref. [37-40]) and LDA (a_0 , ad_0) lattice constants (Å) for the zinc-blende A^{III}B^V and A^{II}B^{VI} semiconductors for d -electrons of group-II atoms included into the core (a_0) and into the valence complex (ad_0)

	AIP	AlAs	AlSb	GaP	GaAs	GaSb	InP	InAs	InSb
a_0	5.4131	5.6246	6.0788	5.2836	5.5073	5.9380	5.6591	5.8564	6.2863
Experiment [39]	5.4670	5.6600	6.1355	5.4512	5.6533	6.0959	5.8687	6.0583	6.4794

	ZnS	ZnSe	ZnTe	CdS	CdSe	CdTe
a_0	4.8674	5.1706	5.6730	5.3038	5.5639	6.0517
ad_0	5.3404	5.6202	6.0072	5.8064	6.0572	6.4174
Experiment [37]	5.4102	5.6676	6.1037	5.8180	6.0520	6.4860
Experiment [38]	5.4110	5.6690	6.0890	5.8300	6.0840	6.4800
Experiment [40]	5.4100	5.6680	6.1000	5.8250	6.0520	6.4820

Following Ref. [36] and using the calculated effective-mass values, Luttinger valence-band parameters γ_1^L , γ_2^L and γ_3^L have been calculated as:

$$\gamma_1^L = \frac{1}{2} \left(\frac{1}{m_{lh}^{001}} + \frac{1}{m_{hh}^{001}} \right), \quad (2)$$

$$\gamma_2^L = \frac{1}{4} \left(\frac{1}{m_{lh}^{001}} - \frac{1}{m_{hh}^{001}} \right), \quad (3)$$

$$\gamma_3^L = \frac{1}{4} \left(\frac{1}{m_{lh}^{001}} + \frac{1}{m_{hh}^{001}} - \frac{2}{m_{hh}^{111}} \right). \quad (4)$$

Energies and momentum matrix elements are given in eV, and effective masses are given in unit of the electron rest mass m_0 throughout the paper. All the calculations have been performed for two values of the lattice constants: (i) determined experimentally (to be called experimental lattice constant hereafter), and (ii) determined by a search of the total energy minimum (to be called theoretical lattice constant hereafter).

3. Results

3.1. Lattice constants

It will become clear that the band structure depends critically upon such parameters as the lattice constant, among others. By a search of the total-energy minimum, lattice constants have been found (Table 1) which for the A^{III}B^V compounds and A^{II}B^{VI} semiconductors with d -electrons included into the valence complex differ from those determined experimentally by < 3 and $< 1.5\%$, respectively. However, if the d -electrons of group-II atoms are included into the core, then the calculated lattice constants for the A^{II}B^{VI} compounds differ from experimentally determined ones significantly ($> 7\%$). It should be noted that experimentally determined lattice constants for A^{II}B^{VI} compounds given in handbooks differ from each other. For example, in Ref. [37], the lattice constant for CdSe is $a = 6.052$ Å while in another handbook, Ref. [38], $a = 6.084$ Å. Our calculated lattice

constant is in between the two experimental values. Since for all other semiconductors considered in this work, the calculated lattice constant is always smaller than the experimentally determined one, we used $a = 6.084$ Å for CdSe from Ref. [38] for band-structure calculations using the experimental lattice constant. For other A^{II}B^{VI} compounds, we used the experimental lattice constants given in Ref. [37].

3.2. Eigenvalues

Self-consistent and non-consistent band-structure calculations have been performed using both calculated and experimentally determined lattice constants. Since we neglected spin-orbit coupling, the valence band maximum at Γ point is triple degenerated for all compounds considered. For A^{III}B^V and A^{II}B^{VI} compounds, eigenvalues at Γ , X and L are given in Table 2, and they are in general agreement with previous calculations [9,13,14,24–26,29,41–43]. Band gaps (E_g) for AIP, AlAs, AlSb and GaP are indirect with valence band maximum at Γ point and conduction band minimum at X point, while those for other A^{III}B^V compounds are direct. As expected, band gaps for AIP, AlAs, AlSb, GaP, GaAs, GaSb calculated using both of the lattice constants are underestimated, while those for InP, InAs and InSb are overestimated for calculated lattice constant and underestimated for experimentally determined lattice constant. The overestimate can be related to the small gap and the neglect of the spin-orbit coupling; similar results were obtained by Huang and Ching [14]. One can also see that LDA calculations of different authors differ significantly. For example, the direct band gap of GaAs, GaSb, InAs and InSb calculated by Geller et al. [10] within LDA by the full-potential linearized augmented plane-wave (FLAPW) method is 0.25, -0.3 , -0.53 , -0.57 eV respectively, while that of AlAs, GaAs and GaSb calculated by Wei and Zunger [41] within LDA are 1.84, 0.15 and -0.165 eV, respectively. Our calculated band gaps of A^{III}B^V compounds are similar to those of Ref. [8,9,15].

It should also be noted that the direct band gaps calculated in this work using the calculated lattice constant

Table 2. Eigenvalues (eV) at Γ , X , and L for the zinc-blende $A^{III}B^V$ and $A^{II}B^{VI}$ compounds calculated using the theoretical (a_0, ad_0) and experimental (a_e, ad_e) lattice constants including the d -electrons of group-II atoms into the core (a_0, a_e) and into valence complex (ad_0, ad_e). The results have been compared to experimental data [39,40] and theoretical calculations within $\mathbf{k} \cdot \mathbf{p}$ theory [2], LDA and GW [25]

		AIP	AlAs	AlSb	GaP	GaAs	GaSb	InP	InAs	InSb
Γ_1^c	a_0	3.3457	2.1517	1.6488	2.5982	1.1885	0.5885	1.3831	0.4131	0.2986
	a_e	3.0929	1.9979	1.4354	1.7736	0.5337	0.0000	0.7205	0.0000	0.0000
X_1^c	a_0	1.4194	1.3127	1.1291	1.4058	1.2861	0.8275	1.5522	1.3821	1.2050
	a_e	1.4739	1.3437	1.1766	1.5872	1.4245	0.9086	1.7198	1.5340	1.3487
L_1^c	a_0	2.7809	2.1399	1.3611	1.9424	1.2413	0.5738	1.8019	1.2331	0.7186
	a_e	2.6692	2.0680	1.2806	1.6262	0.9888	0.3868	1.4918	0.9624	0.5300
Experiment [39]		3.6200	3.1400	2.2190	2.7800	1.4240	0.7500	1.3400	0.4180	0.1800
	$\mathbf{k} \cdot \mathbf{p}$ [2]	5.1200	3.0600		2.8700	1.5200	0.8100	1.4200	0.4200	0.2370

		ZnS	ZnSe	ZnTe	CdS	CdSe	CdTe
Γ_1^c	a_0	5.325	3.908	2.971	3.646	2.780	2.186
	a_e	2.933	1.968	1.587	2.155	1.513	1.217
	ad_0	2.004	1.180	1.077	0.913	0.394	0.499
	ad_e	1.868	1.076	0.901	0.901	0.371	0.420
X_1^c	a_0	2.953	2.594	1.971	3.379	2.932	2.329
	a_e	3.618	3.171	2.451	3.757	3.322	-1.263
	ad_0	3.132	2.764	2.125	3.301	2.923	2.364
	ad_e	3.242	2.820	2.167	3.311	2.943	2.427
L_1^c	a_0	5.159	4.073	2.621	-0.487	4.003	2.750
	a_e	3.985	3.107	2.117	3.908	3.186	-0.462
	ad_0	3.128	2.395	1.610	2.770	2.193	1.605
	ad_e	3.084	2.351	1.563	2.761	2.179	1.581
Experiment [40]		3.680	2.700	2.280	2.500	1.900	1.490
	$\mathbf{k} \cdot \mathbf{p}$ [2]	3.800	2.820	2.390	2.560	1.840	1.600
LDA [25]		2.370	1.450	1.330	1.370	0.760	0.800
GW [25]		3.980	2.840	2.570	2.830	2.010	1.760

is bigger than those found using the experimentally determined lattice constants. This can be attributed, in part, to the direct gap increase with compression (equivalent to small a). In the latter case, the band gaps are even zero for GaSb, InAs and InSb. Also, the band gaps for AIP, GaP, GaAs, GaSb, InP, InAs and InSb calculated using the calculated lattice constants are much closer to the experimental band gaps.

For the $A^{II}B^{VI}$ compounds, the calculated eigenenergies are in general agreement with previous calculations [24–26]. If the d -electrons of the atoms of group-II are included into the core with nonlinear core corrections and theoretical lattice constants are used in band-structure calculations, then the band gaps of all the $A^{II}B^{VI}$ compounds (except CdSe and CdTe) become indirect with the valence-band maximum at the Γ point and the conduction-band minimum at the X point (see Table 2 and Fig. 1), which contradicts the experimental data [37,38,40]. This error is because of the big difference of the LDA lattice constants from the experimentally determined ones (see Table 1). If the experimental lattice constants are used in the band-structure calculations, then eigenenergies (Table 2 and Fig. 1) agree much better with LDA [25,26] and GW [25] calculations.

It is well known that the inclusion of d -electrons of atoms of group-II into the valence complex causes strong $p-d$ coupling of the upper valence band with the d -states, which results in the repulsion of the former upward and reduces the band gap [24–26,29]. Our results in Table 2 and Fig. 2 are consistent with this statement. Furthermore, energy levels of the d -electrons (Γ_{12}^d and Γ_{15}^d) fall in between the s and p valence bands, which are in good agreement with calculations of Wang and Klein [13] for ZnS and ZnSe using the linear combination of Gaussian orbitals method with LDA. However, energies of the bands are much higher than the experimentally determined ones [30], which indicates overestimation of the $p-d$ coupling by LDA in agreement with calculations in Ref. [13,24–26,29]. The Γ_{12}^d and Γ_{15}^d bands are almost dispersionless with very narrow widths. It indicates that these states are well localized. So, the above-mentioned overestimation is consistent with statement of Wang and Klen [13]: „... the more these lower states are localized (narrower bands), the larger is the disagreement...“. Comparing Fig. 1 with Fig. 2, one can see that, due to involvement of the d -electrons into the valence shell, band gaps are reduced significantly for the $A^{II}B^{VI}$ compounds considered. Note that the difference

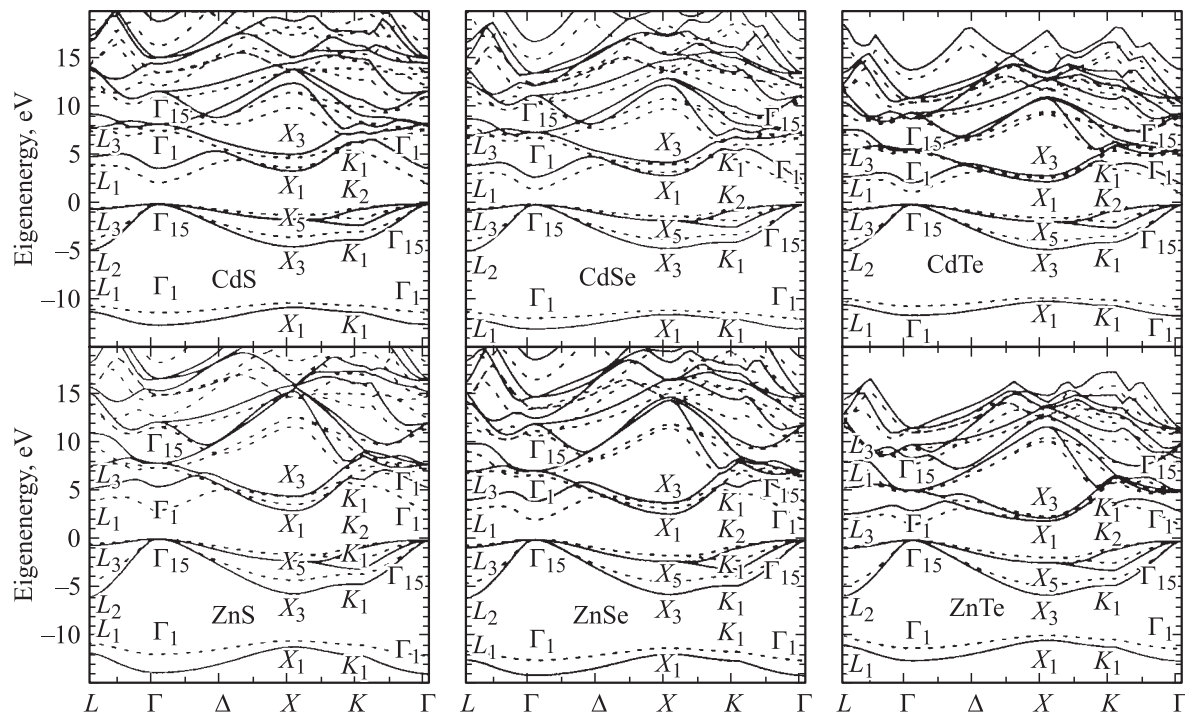


Figure 1. Results of the band-structure calculations. Solid curves are calculated with theoretical lattice constants (a_0) and dashed curves with experimental ones (a_e).

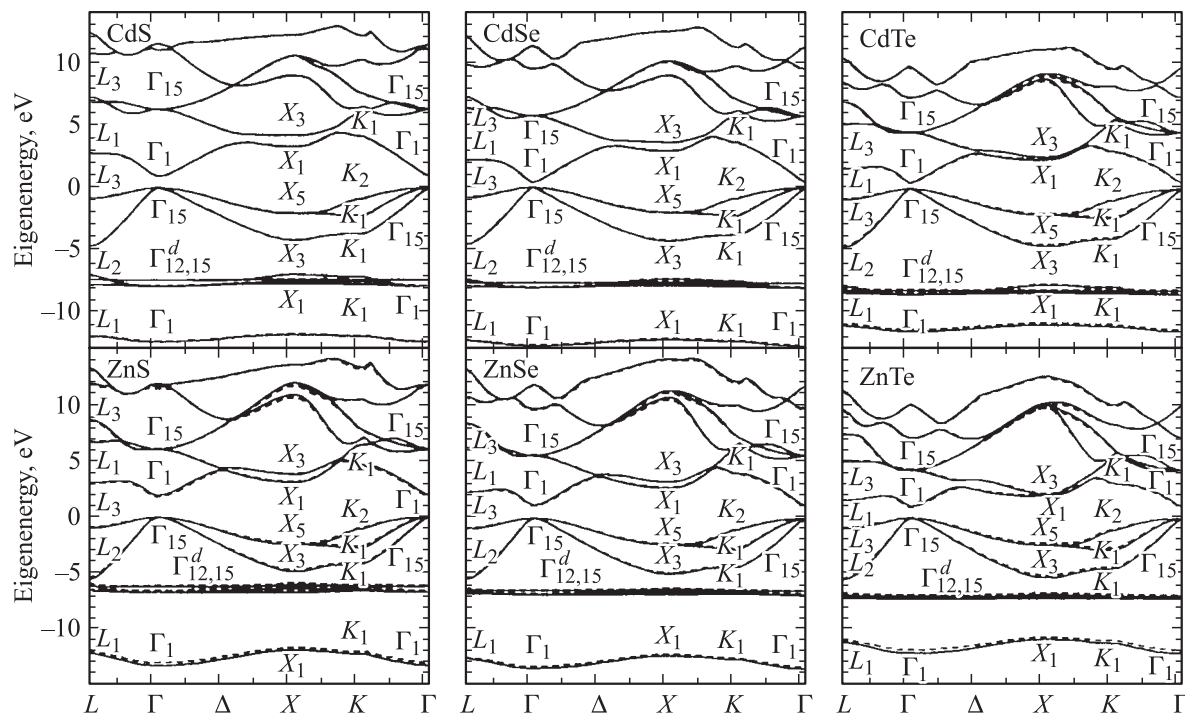


Figure 2. Results of the band-structure calculations with the inclusion of d -electrons of atoms of group-II into the valence complex. Solid curves are calculated with theoretical lattice constants (ad_0) and dashed curves with experimental ones (ad_e).

between eigenenergies calculated using the theoretical and the experimental lattice constants in Fig. 2 are smaller compared to that in Fig. 1. Such small difference for the former is because the LDA and experimental lattice constants are close to each other.

Analysis of Table 2 (also Fig. 1 and Fig. 2) shows that the band gaps calculated in this work using the experimental lattice constant and including the d -electrons into the core are much bigger than those of previous ones calculated by LDA [25] and smaller than those determined by the

Table 3. Momentum matrix elements (eV) and Luttinger parameters for zinc-blende A^{III}B^V compounds using the theoretical (a_0) and the experimental (a_e) lattice constants

		E_p	E'_p	γ_1^L	γ_2^L	γ_3^L
AlP	a_0	17.183	0.015	3.696	0.826	1.454
	a_e	16.807	0.036	3.750	0.893	1.494
	$\mathbf{k} \cdot \mathbf{p}$ [2]	17.700		3.470	0.060	1.150
AlAs	a_0	15.678	0.144	5.203	1.526	2.179
	a_e	15.437	0.172	5.355	1.628	2.263
	[39]	21.100		3.45,3.25	0.68,0.64	1.29,1.21
AlSb	$\mathbf{k} \cdot \mathbf{p}$ [2]	21.100		4.040	0.780	1.570
	a_0	14.548	0.592	5.810	1.659	2.401
	a_e	14.206	0.634	6.180	1.898	2.604
GaP	$\mathbf{k} \cdot \mathbf{p}$ [2]	18.700		4.150	1.010	1.750
	a_0	18.758	0.150	5.729	1.222	2.289
	a_e	17.496	0.366	6.517	1.872	2.672
GaAs	[39]	22.200		4.050	0.490	1.250
	$\mathbf{k} \cdot \mathbf{p}$ [2]	22.200		4.200	0.980	1.660
	a_0	17.189	0.440	10.336	3.526	4.479
GaSb	a_e	16.136	0.634	18.198	7.674	8.493
	[39]	25.700		6.80–7.20	2.10–2.50	1.00–2.90
	$\mathbf{k} \cdot \mathbf{p}$ [2]	25.700		7.650	2.410	3.280
GaSb	$\mathbf{k} \cdot \mathbf{p}$, TB [45]	22.500	0.025	7.070	2.400	3.050
	Experiment [17]	22.53–28.9	3.55–6.0	5.64–7.21	1.35–2.49	2.49–3.09
	Experiment [18]	27.860	2.36	4.80–8.56	1.22–2.90	1.85–3.74
GaSb	LDA [15]	15.820	2.27	9.270	3.120	4.010
	a_0	15.726	0.997	16.291	6.305	7.371
	a_e	0.000	8.540	115.200	56.033	56.933
InP	$\mathbf{k} \cdot \mathbf{p}$ [2]	22.400		11.800	4.030	5.260
	[39]	25.00,26.1		13.10,13.30	4.40,4.50	5.70,6.00
	a_0	15.456	0.048	6.638	3.033	2.760
InP	a_e	14.314	0.205	9.768	3.836	4.423
	[39]	17.000		4.95–5.15	0.94–1.65	1.62–2.35
	$\mathbf{k} \cdot \mathbf{p}$ [2]	20.400		6.280	2.080	2.760
InAs	a_0	14.427	0.169	19.481	8.428	9.171
	a_e	0.000	7.132	33.807	15.819	16.427
	$\mathbf{k} \cdot \mathbf{p}$ [2]	22.200		19.670	8.370	9.290
InSb	a_0	13.866	0.454	24.259	10.681	11.504
	a_e	0.000	7.152	23.493	10.545	11.220
	[39]	21.200		33.50,40.10	14.50,18.10	15.70,19.20
	$\mathbf{k} \cdot \mathbf{p}$, TB [45]	23.100		35.080	15.640	16.910

GW [25] approach and using experimental lattice constants. Our calculated band gap for ZnS is also smaller than 3.55 eV [26]. However, our calculated band gaps obtained with the d -electrons included in the valence complex are in good agreement with 1.02 eV for ZnTe and 0.47 eV for CdTe [24] and 1.84 eV for ZnS [26], which are too small compared to the experimental data.

The eigenvalues at some special k -points for some of the compounds considered is in general agreement with other LDA calculations (e.g. with those by Huang and Ching [14] using a minimal basis semi-*ab initio* approach and by Wang and Klein [13] using the LDA). However, the agreement is not systematic. Note that the discrepancies between the theoretical band gaps of different authors can be related to the accuracy of the LDA calculations, different parameters used to generate the pseudopotentials of the

atoms of group-II, III, V and VI, and different values of the E_{cut} and lattice constant values.

The other important conclusions which can be derived from the comparative analysis is that the band gaps (E_g) are underestimated and the energies of the semicore states are overestimated systematically. However, this error, as discussed in Section 1, is not an artifact of numerical band-structure approximations, but rather is a failure of DFT.

3.3. Momentum matrix elements and Luttinger parameters

Momentum matrix elements, are the key parameters for discussing the optical properties of semiconductors. So, to study the problem using *ab initio* band structure calculations

Table 4. Momentum matrix elements (eV) and Luttinger parameters for A^{II}B^{VI} semiconductors for *d*-electrons of group-II atoms included into the core (a_0, a_e) and into the valence complex (ad_0, ad_e) using the theoretical (a_0, ad_0) and the experimental (a_e, ad_e) lattice constants. The results have been compared to calculations within other methods such as TBLMTO [5] and $\mathbf{k} \cdot \mathbf{p}$ [2,23]

		E_p	E'_p	γ_1^L	γ_2^L	γ_3^L
ZnS	a_0	19.649	0.008	3.158	0.746	1.262
	a_e	14.735	0.279	2.981	0.973	1.278
	ad_0	12.262	0.232	4.113	1.160	1.641
	ad_e	12.013	0.301	4.143	1.241	1.686
	TBLMTO [5]	24.882	20.998	2.120	0.510	1.560
	TBLMTO [5]	15.295	6.708	1.280	0.090	1.140
	$\mathbf{k} \cdot \mathbf{p}$ [2]	20.400		2.540	0.750	1.090
ZnSe	a_0	16.961	0.048	3.954	1.079	1.635
	a_e	12.843	0.545	4.238	1.542	1.882
	ad_0	11.358	0.484	6.465	2.371	2.831
	ad_e	11.146	0.544	6.817	2.530	3.008
	[37]			4.300	1.140	1.840
	$\mathbf{k} \cdot \mathbf{p}$ [23]	23.000				
	TBLMTO [5]	16.230	9.835	3.210	0.750	2.000
ZnTe	a_0	16.075	0.507	4.327	1.132	1.759
	a_e	12.758	1.062	4.835	1.721	2.131
	ad_0	12.272	0.907	7.215	2.511	3.123
	ad_e	11.820	1.020	7.790	2.897	3.451
	TBLMTO [5]	19.667	0.837	3.440	0.590	2.030
	[37]			3.900	0.600	0.900
	[37]			3.900	0.830	1.300
CdS	a_0	15.356	0.000	2.721	0.841	1.152
	a_e	11.631	0.195	2.647	0.975	1.181
	ad_0	9.301	0.219	5.101	1.880	2.224
	ad_e	9.273	0.228	5.121	1.897	2.238
	TBLMTO [5]			3.440	0.970	2.150
	TBLMTO [5]			2.200	0.350	1.530
	$\mathbf{k} \cdot \mathbf{p}$ [23]	21.000				
CdSe	a_0	13.563	0.036	3.265	1.162	1.443
	a_e	10.125	0.374	3.806	1.515	1.735
	ad_0	8.670	0.384	11.694	5.144	5.511
	ad_e	8.600	0.405	12.160	5.394	5.752
	TBLMTO [5]			4.400	1.600	2.680
	$\mathbf{k} \cdot \mathbf{p}$ [23]	20.000				
	CdTe	a_0	13.600	0.256	3.862	1.258
a_e		10.732	0.663	4.353	1.709	1.982
ad_0		9.735	0.628	10.072	4.207	4.652
ad_e		9.488	0.697	11.208	4.831	5.245
TBLMTO [5]		21.066	5.098	4.340	1.600	2.660
[37]				5.300	1.700	2.000
[37]				4.110	1.080	1.950
	$\mathbf{k} \cdot \mathbf{p}$ [23]	18.500				
	$\mathbf{k} \cdot \mathbf{p}$ [2]	20.700		5.290	1.890	2.460

is an important problem. Our calculated results for E_p , E'_p and Luttinger parameters γ_1^L , γ_2^L , γ_3^L are given in Table 3 and Table 4 for the A^{III}B^V and A^{II}B^{VI} compounds, respectively.

Analysis of Table 3 and Table 4 shows that momentum matrix elements calculated in this work are much

smaller than those found from $\mathbf{k} \cdot \mathbf{p}$ theory for all the semiconductors considered except AlP, ZnS and ZnSe for which good agreement was achieved. The small values of E_p can be related to the underestimation of the coupling of the valence-band maximum [20]. For InP our result agrees

Table 5. Effective masses (in units of the free-electron mass m_0) for zinc-blende $A^{III}B^V$ compounds calculated using the theoretical (a_0) and experimentally determined (a_e) lattice constants. The results have been compared to those calculated within pseudopotential [46], $\mathbf{k} \cdot \mathbf{p}$ [17,18,45] and semi-*ab initio* [14] theories, and to experimental data [17,18,45,46]

		m_c^{001}	m_c^{011}	m_c^{111}	m_{hh}^{001}	m_{hh}^{011}	m_{hh}^{111}	m_{lh}^{001}	m_{lh}^{011}	m_{lh}^{111}
AlP	a_0	0.176	0.176	0.176	0.489	6.272,0.490	1.270	0.187	0.139	0.128
	a_e [14]	0.170	0.170	0.170	0.509 0.513	6.138,0.509	1.310 1.372	0.181 0.211	0.137	0.126 0.145
AlAs	a_0	0.115	0.115	0.115	0.465	5.199,0.465	1.183	0.121	0.098	0.092
	a_e [14]	0.110	0.110	0.110	0.476 0.409	5.142,0.476	1.206 1.022	0.116 0.153	0.095	0.090 0.109
	[46]	0.152			0.457		1.087	0.200		0.161
	Experiment [46]	0.150			0.478		1.149	0.208		0.166
	LDA [9] Experiment [9]		0.122 0.124			0.480 0.491			0.129 0.153	
AlSb	a_0	0.110	0.110	0.110	0.401	3.746,0.401	0.992	0.110	0.088	0.083
	a_e [14]	0.100	0.100	0.100	0.419 0.336	3.769,0.419	1.029 0.872	0.100 0.123	0.083	0.078 0.091
GaP	a_0	0.128	0.128	0.128	0.305	2.444,0.305	0.731	0.122	0.090	0.083
	a_e [14]	0.100	0.100	0.100	0.361 0.419	2.687,0.361	0.853 0.997	0.097 0.160	0.079	0.074 0.113
GaAs	a_0	0.058	0.058	0.058	0.304	2.353,0.305	0.726	0.058	0.049	0.047
	a_e [14]	0.030	0.030	0.030	0.351 0.395	2.551,0.351	0.826 0.934	0.030 0.089	0.028	0.027 0.072
	[45]	0.067			0.460		0.950	0.085		0.077
	Experiment [17] $\mathbf{k} \cdot \mathbf{p}$ [18]				0.340–0.475 0.340–0.800		0.450–1.030 0.520–4.000	0.082–0.120 0.082–0.142		0.070–0.082 0.075–0.120
GaSb	a_0	0.035	0.035	0.036	0.272	2.074,0.272	0.646	0.035	0.031	0.030
	a_e [14]	0.004	0.006	0.008	0.219 0.231	2.274,0.319	0.747 0.551	0.004 0.052	0.006	0.008 0.047
InP	a_0	0.095	0.095	0.095	0.389	2.570,0.389	0.895	0.093	0.078	0.074
	a_e LDA [42]	0.058	0.058	0.058	0.477 0.430	2.979,0.477	1.084 0.970	0.057 0.057	0.052	0.051
	SLDA [42]	0.060			0.400		0.900	0.057		
	SEPM [42]	0.095			0.470		1.030	0.097		
	Experiment [42]	0.079,0.081			0.520,0.610		0.630,0.950	0.104,0.118		
InAs	a_0	0.028	0.028	0.028	0.381	2.524,0.381	0.878	0.028	0.026	0.026
	a_e EPM [47]	0.015	0.017	0.018	0.461 0.480	2.885,0.461	1.048	0.015 0.040	0.016	0.017
	LDA [10]	0.094		0.112	0.353			0.046		
	sX [10]	0.022		0.021	0.388			0.025		
	Experiment [10]	0.023			0.410			0.026		
	$\mathbf{k} \cdot \mathbf{p}$ [2] Experiment [2]	0.023 0.024			0.410 0.410			0.026 0.026		
InSb	a_0	0.022	0.023	0.023	0.345	2.333,0.345	0.799	0.022	0.021	0.021
	a_e	0.023	0.024	0.025	0.416	2.638,0.416	0.949	0.022	0.023	0.024

well with that of Fu, Wang and Zunger [21,44] calculated by direct diagonalization method. Also, $E_p' < E_p$ for the semiconductors except GaSb, InAs and InSb with zero band gaps in the LDA calculations using experimentally determined lattice constants.

Momentum matrix elements calculated keeping the d -electrons of group-II atoms in the core are bigger than those found for the d -electrons included into the valence complex. It indicates that the d -electrons result in underestimation of the coupling between the conduction band minimum and valence band maximum. The former

approach gives better agreement with tight-binding and LMTO calculations [5] for ZnS, ZnSe and ZnTe, and with $\mathbf{k} \cdot \mathbf{p}$ calculations [2] for ZnS. However, for all $A^{II}B^{VI}$ compounds considered except ZnTe, the value of E_p' is much smaller than that calculated in Ref. 5, which found that the value of E_p' is comparable with that of E_p . Note, that momentum matrix element between the semicore Γ_{15}^d states and conduction band minimum (not shown in Table 4) is in between 1 and 3 eV, which is smaller than E_p , but about 10 times is bigger than those between the other remote bands for all the $A^{II}B^{VI}$ compounds considered. It can

Table 6. Effective masses (in units of the free-electron mass m_0) for A^{II}B^{VI} semiconductors including the d -electrons of atoms of group-II into the core (a_0, a_e) and into the valence complex (ad_0, ad_e), and using the LDS (a_0, ad_0) and experimentally determined (a_e, ad_e) lattice constants. In Refs. [2,37] all effective masses (except CdTe and m_c^{011} for ZnS, Ref. [37]) are given without specific directions and determined experimentally [37]

		m_c^{001}	m_c^{011}	m_c^{111}	m_{hh}^{001}	m_{hh}^{011}	m_{hh}^{111}	m_{lh}^{001}	m_{lh}^{011}	m_{lh}^{111}
ZnS	a_0	0.193	0.193	0.193	0.601	8.463,0.601	1.578	0.215	0.161	0.149
	a_e	0.183	0.183	0.183	0.966	8.938,0.961	2.350	0.203	0.171	0.162
	ad_0	0.145	0.145	0.145	0.557	2.884,0.556	1.203	0.155	0.127	0.119
	ad_e	0.142	0.141	0.141	0.602	3.071,0.602	1.297	0.151	0.126	0.119
	Experiment [37]	0.340	0.184			1.760,1.121			0.230	0.169
ZnSe	$\mathbf{k} \cdot \mathbf{p}$ [2]		0.280							
	a_0	0.146	0.146	0.146	0.557	7.505,0.561	1.462	0.164	0.129	0.120
	a_e	0.126	0.126	0.126	0.866	7.550,0.867	2.113	0.137	0.120	0.115
	ad_0	0.083	0.084	0.084	0.581	3.651,0.559	1.246	0.089	0.078	0.075
	ad_e	0.081	0.081	0.081	0.569	3.078,0.571	1.248	0.084	0.075	0.073
ZnTe	Experiment [37]	0.142	0.147	0.160						
	Experiment [40]	0.130	0.170	0.570	0.750					
	$\mathbf{k} \cdot \mathbf{p}$ [2]		0.140							
	[14]				1.814		0.784	0.191		0.147
	a_0	0.146	0.147	0.147	0.485	5.501,0.484	1.236	0.152	0.118	0.110
CdS	a_e	0.118	0.118	0.118	0.717	5.975,0.719	1.742	0.121	0.105	0.101
	ad_0	0.081	0.081	0.081	0.456	2.800,0.456	1.032	0.082	0.071	0.068
	ad_e	0.073	0.073	0.073	0.501	2.988,0.501	1.126	0.074	0.066	0.063
	Experiment [37]	0.122	0.128	0.130						
	Experiment [40]	0.130			0.600					
CdSe	$\mathbf{k} \cdot \mathbf{p}$ [2]		0.180							
	[14]				0.541		1.354	0.155		0.119
	a_0	0.196	0.197	0.197	0.962	12.800,0.953	2.400	0.227	0.184	0.173
	a_e	0.191	0.190	0.190	1.433	12.621,1.433	3.499	0.218	0.192	0.184
	ad_0	0.108	0.108	0.108	0.745	3.249,0.745	1.532	0.113	0.101	0.097
CdTe	ad_e	0.107	0.107	0.107	0.754	3.285,0.754	1.551	0.112	0.101	0.097
	Experiment [40]		0.140		0.510					
	[14]				0.929		1.935	0.201		0.161
	a_0	0.079	0.104	0.116	1.063	46.105,0.943	2.643	0.179	0.147	0.139
	a_e	0.134	0.133	0.133	1.289	8.295,1.309	2.982	0.146	0.133	0.129
CdTe	ad_0	0.045	0.045	0.045	0.711	3.282,0.712	1.491	0.045	0.043	0.043
	ad_e	0.043	0.043	0.043	0.729	3.355,0.729	1.524	0.044	0.042	0.041
	Experiment [37]	0.11								
	Experiment [40]		0.110		0.44					
	a_0	0.145	0.146	0.146	0.743	7.910,0.742	1.874	0.157	0.132	0.125
CdTe	a_e	0.122	0.122	0.122	1.070	8.542,1.070	2.567	0.129	0.117	0.113
	ad_0	0.054	0.054	0.054	0.603	3.110,0.603	1.304	0.054	0.051	0.050
	ad_e	0.047	0.048	0.048	0.647	3.292,0.647	1.393	0.048	0.045	0.045
	Experiment [37]	0.094	0.096	0.095	0.720	0.810	0.840	0.130	0.120	0.120
	Experiment [37]	0.099								
CdTe	Experiment [40]		0.90		0.720	0.840	0.120			
	$\mathbf{k} \cdot \mathbf{p}$ [2]		0.096							
	[14]				0.478		1.114	0.125		0.095

be related to LDA overestimation of the influence of the valence band semicore d states. Matrix elements between the lowest conduction band Γ_1^c and valence band Γ_{12}^d , and remote conduction band states $\Gamma_1^c, \Gamma_{12}^c$ is zero, which is related to symmetry properties of the crystal.

Luttinger parameters calculated in this work for A^{III}B^V compounds in Table 3 are much smaller than those found by $\mathbf{k} \cdot \mathbf{p}$ theory and experiment, though the order of magnitude is the same. For A^{II}B^{VI} semiconductors, we

found that involvement of d -electrons into the core reduces the Luttinger parameters significantly compared to those with d -electrons in the valence complex (see Table 4). However, the former approach gives better agreement with $\mathbf{k} \cdot \mathbf{p}$ theory [2] and tight-binding and linear muffin-tin-orbital (TBLMTO) calculations [5]. This analysis indicates that, from LDA calculations, one can sometimes get the correct momentum matrix elements and Luttinger parameters, but it is not systematic.

3.4. Effective masses

Carrier effective masses are one of the important parameters in discussion of transport phenomena, exciton effects, electron-hole liquids etc in semiconductors. They are usually determined by cyclotron resonance, electroreflectance measurements or from analysis of transport data. In this section we present the results of our calculations of electron effective masses at the conduction band minimum and hole effective masses at valence band maximum. The results are given in Table 5 and Table 6 for A^{III}B^V and A^{II}B^{VI} compounds, respectively. For indirect gap semiconductors AlP, AlAs, AlSb and GaP m_c is usually discussed for conduction band minimum at Γ and other than Γ (say X or L) points. In this work, we consider all effective masses only for Γ point.

Analysis of the Table 5 and 6 shows that the effective masses of conduction band electrons are isotropic, while those of holes are anisotropic. The effective masses for heavy-holes (m_{hh}) and light-holes (m_{lh}) correspond to splitting of the Γ_{15}^v state into a double and single degenerate bands, respectively. Since we have neglected spin-orbit coupling, the split-off mass band is not discussed. Analysis of the Table 5 shows that conduction-band effective masses for AlP, AlSb, GaP, GaSb and InSb are much smaller than $m_c = 0.25, 0.18, 0.17, 0.22, 0.13$ calculated by $\mathbf{k} \cdot \mathbf{p}$ theory [2]. One can also see that conduction-band effective masses calculated using the LDA lattice constant are closer to experimental data than those calculated using the experimental lattice constant. Note that all the effective masses for AlP, AlAs, AlSb and InSb using the theoretical and experimentally determined lattice constants do not differ from each other so much, while the difference is significant for the other A^{III}B^V semiconductors studied.

Analysis of the Table 5 shows that the values of $m_{hh}^{001}, m_{hh}^{111}$ for AlAs, GaAs, InP, and InAs calculated in this work agree well with previous calculations and experimental data, while such an agreement was not achieved for $m_{lh}^{001}, m_{lh}^{111}$. Due to the lack of experimental or calculated data, we could not make such a comparison for other semiconductors and for effective masses along other directions. Note that for InP, InAs and InSb not only band gaps, but also conduction-band effective masses are overestimated. It indicates that there is a correlation between changes of the band gap and the conduction-band effective mass, which is qualitatively consistent with the $\mathbf{k} \cdot \mathbf{p}$ theory (see e.g. Ref. [2]). Also, distinct from Fiorentini and Baldereschi [8,9], none of the conduction-band effective masses for A^{III}B^V compounds except AlAs agree with experimental data.

Analysis of Table 6 shows that the effective masses of all A^{II}B^{VI} compounds calculated keeping the d -electrons in the core is bigger than those found when including the d -electrons into the valence complex. It indicates that the semicore d -electrons results in underestimation of not only band and coupling between the valence band maximum and conduction band minimum, but also change the dispersion around the Γ point. Our calculated values of the light-

hole effective masses (m_{lh}) are in good agreement with experimental data for ZnS and CdTe. Due to the lack of theoretical or experimental data we could not make such a comparison for the other A^{II}B^{VI} compounds. Calculated heavy-hole effective masses (m_{hh}) differ significantly from those of Refs. [2,37,40] for all the A^{II}B^{VI} compounds considered except CdTe. For the latter good agreement is achieved if the theoretical lattice constant is used.

The effective masses for all the compounds considered somewhat agree with those calculated by Huang and Ching [14] using a minimal basis semi-*ab initio* approach and by Wang and Klein [13] using LDA, but the agreement is not systematic. Based on the above analysis, one can say that by LDA calculations one can sometimes get the correct values of conduction or valence-band effective masses along some of the specific directions. However, it is not systematic.

4. Conclusion

In summary, band-structure calculations have been performed for A^{III}B^V and A^{II}B^{VI} semiconductors with zinc-blende structure. By a search of the total energy minimum lattice constants have been found which differ from the experimentally determined ones by $< 3\%$ for A^{III}B^V compounds, and by 1.5 and 7% for the A^{II}B^{VI} semiconductors with d -electrons of group-II atoms included into the valence shell and into the core, respectively.

Band parameters calculated within the LDA show the correct tendency to be smaller than those determined experimentally or calculated theoretically within the $\mathbf{k} \cdot \mathbf{p}$, tight-binding or semi-empirical methods. From this point our results are in general agreement with those obtained using the other *ab initio* codes.

Difference of the calculated direct band gaps for A^{III}B^V compounds are in the range from 6.5 to 66% for theoretical lattice constants and from 15 to 100% for experimental lattice constants. The difference for the A^{II}B^{VI} semiconductors with d -electrons of group-II atoms included into the core is in the range from 30 to 47% for theoretical lattice constant and from 14 to 28% for experimental lattice constant. If the d -electrons are included into the valence complex, then the error in calculation of the band gap becomes significant due to p - d repulsion.

Momentum matrix elements E_p calculated in this work are smaller compared with those obtained within the $\mathbf{k} \cdot \mathbf{p}$ theory [2], since the latter is known to be closer to experimental data. For A^{III}B^V compounds difference of the values of E_p obtained within the two theories is in the range from 2.9 to 35% for theoretical lattice constant and from 21 to 38% for experimentally determined lattice constants. For A^{II}B^{VI} compounds with d -electrons of group-II atoms included into the core the difference is in the range from 3.7 to 34.3% for theoretical lattice constant and from 27.8 to 48.1% for experimentally determined lattice constant. Involvement of the d -electrons into the valence complex increased the error in calculation of E_p .

The effective masses of conduction band electrons are found to be isotropic, while those of holes are anisotropic. Calculated m_c for the A^{III}B^V semiconductors differs from experimentally determined ones from 13 to 23% for theoretical lattice constant and from 26 to 55% for experimental lattice constant. For A^{II}B^{VI} compounds with d -electrons of group-II atoms included into the core the difference of the calculated m_c from experimentally determined one is in the range from 8 to 54% for theoretical lattice constant, while that for experimental lattice constant is in the range from 2 to 46%. We found that the effective masses of all A^{II}B^{VI} compounds calculated keeping the d -electrons in the core is bigger than those found when including the d -electrons into the valence complex. It indicates that the semicore d -electrons result in underestimation of not only band gaps and coupling between the valence band maximum and conduction band minimum, but also change the dispersion around the Γ point. Also, conduction-band effective masses calculated using the LDA lattice constant are closer to experimental data than those calculated using the experimental lattice constant. The effective masses for all the compounds considered somewhat agree with those calculated by Huang and Ching [14] using a minimal basis semi-*ab initio* approach and by Wang and Klein [13], but the agreement is not systematic.

We found that correctness of the LDA band parameters for all the compounds considered is not systematic. Comparing the LDA band parameters calculated using LDA and using experimental lattice constants, we conclude that the latter is more preferable to use for LDA band-structure calculation. We have shown that consideration of the d -electrons of group-II atoms in the core can give more correct band parameters for A^{II}B^{VI} compounds. We found that involvement of the d -electrons of group-II atoms into the valence shell in the LDA band-structure calculations results in decrease of band gaps, increase of lattice constants, decrease of momentum matrix elements, increase of Luttinger parameters, and decrease of electron, heavy-hole and light-hole effective masses along all directions. In this case, only equilibrium lattice constant can be determined with high accuracy, while all the other band parameters are inaccurate.

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