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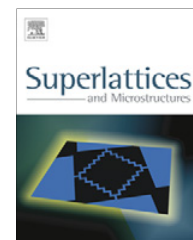
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First principles calculations of Cd and Zn chalcogenides with modified Becke–Johnson density potential

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ABSTRACT

In this work, we present first principles calculations based on a full potential linear augmented plane-wave method (FP-LAPW) to calculate structural and electronic properties of CdX and ZnX (X = S, Se, Te) based II–VI chalcogenides. First principles calculations using the local density approximation (LDA) and the related generalized gradient approximation (GGA) lead to a severe underestimate of the band gap. The proposed model uses various exchange–correlation potentials (LSDA, GGA and MBJLDA) to determine band gaps and structural properties of semiconductors. We show that using modified Becke–Johnson (MBJLDA) density potential leads to a better agreement with experimental data for band gaps of Cd and Zn based semiconductors.

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1. Introduction

Cadmium and Zinc based semiconductor compounds have attracted considerable theoretical and experimental interest in the last decades since they have a potential to be employed as base materials for light-emitting and laser diodes, infrared detectors, photovoltaic devices, and quantum dots applications [1]. Most of the theoretical calculations has been performed by using density functional theory (DFT) for II–VI chalcogenides. DFT calculations give satisfactory ground state properties such as total

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energies and also lattice constant [27]. On the other hand, the calculations performed by using conventional DFT give unsatisfactory electronic properties such as band gaps and effective masses. Calculated band gaps are much smaller than those of experimental and theoretical data [2]. Using different approaches such as GW approximation or hybrid functionals overcomes the band gap problem. However, even GW and hybrid functionals can result in band gap error on the order of 10–20% compared to experimental data [2]. Accurate modeling of electronic properties of semiconductors allows a better prediction of their material properties in utilizing them for high performance electronic and optical device applications. Our main goal is that to describe the electronic properties such as band gap, correctly. Tran and Blaha [3] proposed a new potential called MBJLDA that combines modified Becke–Johnson exchange potential and the LDA correlation potential to get better band gap results compared to experiment [2,4,25,26]. MBJLDA is a XC-potential, not a XC-energy functional, thus E_{xc} is taken from LDA. We emphasize that since there is no exchange functional E_x such that $V_{x,\sigma}^{MBJ} = \delta E_x / \delta \rho_\sigma$. Therefore it cannot be used to calculate total energy. It is recommended to use a GGA or LDA based functional for structural properties, and then to use MBJLDA potential for the calculation of electronic properties [3]. MBJLDA has similar computational cost with LDA and GGA. Beside that, MBJLDA results can be compared with the more expensive methods like GW and hybrid functionals for band gaps. According to our present calculations, the modified Becke–Johnson density potential performs well for describing the band properties. It can be used to model the electronic properties of semiconductors.

In this work, we present a full potential linear augmented plane wave method within DFT to calculate structural properties and electronic band structure of zinc-blende CdX and ZnX (X = S, Se, Te) semiconductors. The present calculations are compared with other methods and available experimental data. We found that the proposed model accurately reproduces band gaps and band dispersion curves at high symmetry points at the edge of Brillouin zone.

2. Method of calculation

The WIEN2k [5] package is used for calculating structural and electronic band properties of Cd and Zn compounds. The total energy calculations were performed using local spin density approximation (LSDA) as parameterized by Perdew and Wang [23], the generalized gradient approximation (GGA) as parameterized by Perdew, Burke and Ernzerhof [24], and the modified Becke–Johnson LDA (MBJLDA) [3].

CdX and ZnX (X = S, Se, Te) have a zinc-blende structure (space group F-43m No:216) in which the Cd/Zn atoms are located at (000) and S (or Se and Te) at (0.25 0.25 0.25). A converged results are obtained using 10,000 k points in the first Brillouin zone with $R_{MT}K_{max} = 8.50$ where R_{MT} represents the smallest muffin-tin radius and K_{max} is the maximum size of reciprocal lattice vectors. LSDA, GGA and MBJLDA as implemented in the WIEN2k code are used for exchange and correlation potentials during the calculations. SCF iterations are repeated until total energy converges to a point less than 10^{-4} Ryd.

3. Result and discussion

3.1. Structural properties

The lattice constant (a_0) was obtained by fitting the total energy as a function of volume to Murnaghan's [6] equation of state. We obtained the lattice constant (a_0), bulk modulus (B_0), and its pressure derivative (B_0') from this numerical fitting procedure. These calculated structural parameters for LSDA, GGA and MBJLDA are given in Table 1.

It is reported that IIIA–VA compounds (zinc blende structure), LDA underestimates a_0 slightly (less than –1%) while PBE overestimates a_0 significantly (up to 2%) [27].

We can see that in Table 1 for all II–VI compounds, the trends are similar as for the elements of group IIIA–VA. For CdX (X = S, Se, Te) LDA (PW) underestimates a_0 (for CdSe and CdTe $\sim -1\%$ and for CdS $\sim 2\%$) GGA (PBE) overestimates a_0 (for CdSe, CdTe and CdS $\sim 2\%$). For ZnX (X = S, Se, Te) LDA (PW) underestimates a_0 (for ZnS and ZnSe more than –1.5% and for ZnTe less than 1.5%) GGA (PBE) overestimates a_0 (for ZnS less than 1% and for ZnSe and ZnTe more than 1%).

Table 1

Calculated lattice constant (a_0), bulk modulus (B_0), and its pressure derivative (B'_0) for CdX (X = S, Se, Te) and ZnX (X = S, Se, Te). PW stands for Perdew Wang [23], PBE stands for Perdew, Burke and Ernzerhof [24], PZ stands for Perdew, Zunger [15].

Compound	Reference	$a_0(\text{\AA})$	B^0 (GPa)	B'
CdS	Present (LSDA (PW))	5.722	73.337	5.129
	Present (MBJLDA)	5.779	68.765	4.375
	Present (GGA (PBE))	5.948	53.838	4.72
	Theory (LDA(PW), GGA(PBE)) ^h	5.839, 6.006	66.01, 51.54	
	Theory (LDA(PZ)) ^b	5.810	72.42	4.31
	Experiment ^a	5.830	64.3, 62	
CdSe	Present (LSDA (PW))	6.017	57.866	4.977
	Present (MBJLDA)	5.994	53.799	2.364
	Present (GGA (PBE))	6.201	54.948	1.584
	Theory (LDA(PW), GGA(PBE)) ^h	6.088, 6.276	56.59, 44.11	
	Theory (LDA(PZ)) ^b	6.05	65.12	4.20
	Experiment ^a	6.084	55, 53	
CdTe	Present (LSDA (PW))	6.420	44.472	3.799
	Present (MBJLDA)	6.425	47.778	5.200
	Present (GGA (PBE))	6.624	37.440	3.873
	Theory (LDA(PW), GGA(PBE)) ^h	6.500, 6.706	46.76, 34.91	
	Theory (LDA(PZ))	6.480 ^b	48.94 ^b , 46.7 ^d	4.47 ^b , 3.00 ^d
	Experiment ^a	6.480	44.5	
ZnS	Present (GGA (PBE))	5.460	73.761	2.17
	Present (MBJLDA)	5.301	77.344	4.455
	Present (LSDA (PW))	5.311	87.835	4.84
	Theory (LDA(PW), GGA(PBE)) ^h	5.460, 5.581	91.71, 74.97	
	Theory (LDA (PZ))	5.302 ^e	77.3 ^f	5.0 ^g
	Experiment ^a	5.411	76.9	
ZnSe	Present (GGA (PBE))	5.746	57.046	4.359
	Present (MBJLDA)	5.554	82.379	3.646
	Present (LSDA (PW))	5.580	72.494	4.844
	Theory (LDA(PW), GGA(PBE)) ^h	5.690, 5.834	73.91, 58.08	
	Theory (LDA (PZ)) ^g	5.608	74	5.0
	Experiment ^a	5.669	62.5	
ZnTe	Present (GGA (PBE))	6.194	43.607	4.381
	Present (MBJLDA)	5.985	54.038	4.290
	Present (LSDA (PW))	6.011	55.446	4.988
	Theory (LDA(PW), GGA(PBE)) ^h	6.039, 6.218	55.56, 44.45	5.1
	Theory (LDA (PZ)) ^g	6.030	55.900	
	Experiment ^a	6.089	50.9	

^a Ref. [9].

^b Ref. [10].

^c Ref. [11].

^d Ref. [12].

^e Ref. [13].

^f Ref. [14].

^g Ref. [15].

^h Ref. [1].

MBJLDA potential is not a functional derivative of a functional. Therefore it cannot be used to calculate the total energy so we don't include MBJLDA lattice results in this examination given above. In Table 1, MBJLDA results where in fact obtained by plugging the MBJLDA electron density into the LDA functional. It is expected that MBJLDA lattice parameters close to LDA results. The only difference comes from the MBJ density. It can be seen how MBJ density affects the lattice parameters in Table 1. It is a well-known fact that the GGA lattice parameters are always larger than those of LDA. Our present calculations also support this condition.

There are several functionals that were designed to obtain better lattice constants [27]. In some cases, the difference between present results and cited values are rather big. Our present calculated

Table 2

Calculated band gap, spin–orbit splitting and effective mass for CdX (X = S, Se, Te) and ZnX (X = S, Se, Te). PW stands for Perdew Wang [23], PBE stands for Perdew, Burke and Ernzerhof [24].

Compound	Reference	E_g (eV)	Δ_{so} (meV)	m^* (m_e)	Relative error in E_g (%)
CdS	Present (MBJLDA)	2.66	33	0.158	4.31
	Theory (LSDA(PW)) ^a	0.85			–66.67
	Theory (LSDA(PW)+ ΔE) ^a	2.60			1.96
	Theory (GW, G'W') ^b	2.11, 2.47			–17.25, –3.14
	Theory (LDA (PW))	1.20 ^c			–52.94
	Theory(GGA(PBE))	1.43 ^c	42.7 ^c , 50 ^d	0.080 ^c	–43.92
	Experiment ^e	2.55	62	0.12	
CdSe	Present (MBJLDA)	1.89	314	0.118	3.85
	Theory (LSDA (PW)) ^a	0.32			–82.42
	Theory (LSDA (PW)+ ΔE) ^a	1.89			3.85
	Theory (GW, G'W') ^b	1.25, 1.56			–31.32, –14.29
	Theory (LDA (PW))	1.03 ^c			–43.41
	Theory (GGA(PBE))	1.11 ^c	345 ^c , 369 ^d	0.057 ^c	–39.01
	Experiment	1.82 ^f	390 ^g	0.20 ^e	
CdTe	Present (MBJLDA)	1.56	770	0.101	–2.50
	Theory (LSDA(PW)) ^a	0.49			–69.38
	Theory (LSDA (PW)+ ΔE) ^a	1.75			9.37
	Theory (GW, G'W') ^b	1.22, 1.47			–23.75, –8.13
	Theory (LDA (PW))	0.60 ^c			–62.50
	Theory (GGA(PBE))	0.52 ^c	796 ^c , 826 ^c	0.057 ^c	–67.50
	Experiment	1.60 ^f	800 ⁱ	0.096 ^h	
ZnS	Present (MBJLDA)	3.66	43	0.172	–4.19
	Theory (GGA(PBE)) ^a	2.07			–45.81
	Theory (GGA(PBE)+ ΔE) ^a	3.82			0.00
	Theory (GW, G'W') ^b	3.38, 3.80			–11.52, –0.52
	Theory (LDA (PW))	1.95 ^c			–48.95
	Theory (GGA(PBE))	1.94 ^c	54 ^c , 65 ^e	0.107 ^c	–49.21
	Experiment	3.82 ^f	86 ⁱ	0.184 ^j , 0.340 ^j	
ZnSe	Present (MBJLDA)	2.67	331	0.133	–5.32
	Theory (GGA(PBE)) ^a	1.26			–55.32
	Theory (GGA(PBE)+ ΔE) ^a	2.82			0.00
	Theory (GW, G'W') ^b	2.24, 2.58			–20.57, –8.51
	Theory (LDA (PW))	1.50 ^c			–46.81
	Theory (GGA(PBE))	1.47 ^c	360 ^c , 395 ^c	0.080 ^c	–47.87
	Experiment ^c	2.82 ^e	400 ⁱ	0.17 ^j , 0.13 ^j	
ZnTe	Present (MBJLDA)	2.22	814	0.118	–7.11
	Theory (GGA(PBE)) ^a	1.16			–51.46
	Theory (GGA(PBE)+ ΔE)	2.41			0.84
	Theory (GW, G'W') ^b	1.98, 2.26			–17.15, –5.44
	Theory (LDA (PW)) ^c	2.20			–7.95
	Theory (GGA(PBE)) ^c	1.94	775 ^c , 888 ^c	0.100 ^c	–18.83
	Experiment	2.39 ^e	910 ⁱ	0.13 ^j	

^a Ref. [8].

^b Ref. [22].

^c Ref. [1].

^d Ref. [16].

^e Ref. [9].

^f Ref. [17].

^g Ref. [18].

^h Ref. [19].

ⁱ Ref. [20].

^j Ref. [21].

lattice constants differ from experiment up to 2%. According to DFT modeling this is a well-known issue [10,27] and calculated values are in acceptable ranges. Moreover, calculated bulk modulus and its pressure derivative have similar trends with available experimental and theoretical data.

Table 3

Calculated energies (in eV) at symmetry points for the CdS, CdSe, and CdTe.

	Reference	Γ_{1v}	Γ_{15v}	Γ_{1c}	Γ_{15c}	L_{1v}	L_{1v}	L_{3v}	L_{1c}	L_{3c}	X_{1v}	X_{3v}	X_{5v}	X_{1c}	X_{3c}
CdS	Present (MBJLDA)	–12.21	0.00	2.66	7.20	–11.85	–3.89	–0.66	4.28	7.74	–11.75	–3.48	–1.68	4.71	5.35
	Theory (LSDA (PW)) ^a	–12.39	0.00	0.85	6.34	–11.94	–4.53	–0.77	2.76	7.22	–11.80	–4.08	–1.93	3.32	4.17
	Theory (LDA (CA)) ^b	–12.92	0.00	1.45	6.60	–12.39	–4.46	–0.78	3.42	7.30	–12.29	–3.88	–1.98	3.72	5.09
CdSe	Present (MBJLDA)	–12.31	0.00	1.89	6.72	–11.99	–4.01	–0.67	3.40	7.10	–11.89	–3.73	–1.70	4.04	4.50
	Theory (LSDA (PW)) ^a	–12.69	0.00	0.32	5.80	–12.30	–4.48	–0.77	2.16	7.18	–12.18	–4.17	–1.89	2.96	3.61
	Theory (LDA (CA)) ^b	–12.09	0.00	1.08	6.08	–11.74	–4.47	–0.79	2.79	7.15	–11.63	–4.03	–1.97	3.53	5.30
CdTe	Present (MBJLDA)	–11.11	0.00	1.56	4.99	–10.81	–4.30	–0.72	2.36	7.75	–10.72	–4.18	–1.79	3.03	3.10
	Theory (LSDA (PW)) ^a	–11.29	0.00	0.49	4.52	–10.88	–4.50	–0.79	1.63	6.86	–10.75	–4.39	–1.89	2.46	2.56
	Theory (LDA (CA)) ^b	–13.60	0.00	1.88	4.81	–12.53	–4.37	–0.79	2.58	5.59	–12.27	–4.16	–1.92	3.18	3.20

^a Ref. [8].^b Ref. [10].**Table 4**

Calculated energies (in eV) at symmetry points for the ZnS, ZnSe, and ZnTe.

	Reference	Γ_{1v}	Γ_{15v}	Γ_{1c}	Γ_{15c}	L_{1v}	L_{1v}	L_{3v}	L_{1c}	L_{3c}	X_{1v}	X_{3v}	X_{5v}	X_{1c}	X_{3c}
ZnS	Present (MBJLDA)	–12.97	0.00	3.66	7.15	–12.14	–5.97	–0.79	4.48	7.62	–11.87	–4.05	–2.01	4.42	5.09
	Theory (GGA (PBE)) ^a	–13.13	0.00	2.07	6.36	–12.20	–5.28	–0.86	3.29	6.93	–11.90	–4.57	–2.21	3.42	4.08
	Theory & Exp. ^b	–13.51	0.00	3.72	6.49	–12.43	–5.75	–0.96	3.31	–	–12.05	–4.87	–2.46	3.18	4.02
ZnSe	Present (MBJLDA)	–13.02	0.00	2.67	6.50	–12.28	–4.85	–0.79	3.61	6.91	–12.02	–4.38	–2.03	3.78	4.25
	Theory (GGA (PBE)) ^a	–13.27	0.00	1.26	5.79	–12.49	–5.23	–0.87	2.52	6.40	–12.21	–4.77	–2.19	3.00	3.47
	Theory & Exp. ^b	–13.49	0.00	2.84	7.67	–12.44	–5.23	–0.81	4.14	8.18	–12.07	–5.03	–2.08	4.41	5.01
ZnTe	Present (MBJLDA)	–11.78	0.00	2.22	4.75	–10.96	–5.05	–0.86	2.45	8.19	–10.67	–4.86	–2.11	2.71	2.82
	Theory (GGA (PBE))	–11.87	0.00	1.16	4.35	–10.99	–5.24	–0.91	1.70	7.38	–10.67	–5.07	–2.21	2.19	2.27
	Theory & Exp. ^b	–12.07	0.00	2.57	5.91	–10.95	–5.31	–0.88	3.07	6.52	–10.52	–5.27	–2.16	3.47	3.53

^a Ref. [8].^b Ref. [20].

3.2. Electronic band properties

In the conventional DFT calculations for electronic properties of semiconductors, as suggested by Fiorentini and Balderschi [7], the exchange–correlation potential contribution to the DFT band gap was shifted by using a scissor operator. The difference between the LDA and experimental band gaps, ΔE , scales with the electronic part of the dielectric constant ϵ_{∞} as $\Delta E \sim 9.1/\epsilon_{\infty}$. Our previous [8] LSDA or GGA band gap calculations were shifted by using the scissor operator. In the present calculations using MBJLDA, we obtained satisfactory band gap values according to the experimental data and there is no need to shift or correct the calculated band gaps. We compared present band gap calculations with GW (RPA-type screening of the electron–electron interaction) and G'W' (GW-RPA with G and W recalculated by updating the eigenvalues.) results. According to our calculations MBJLDA brings an improvement over LDA and GGA for band gaps. In most cases, except ZnS, MBJLDA is a better agreement with experiment than GW and G'W'. It can be easily seen that in Table 2, MBJLDA underestimates band gap between –2.50% and –7% for CdTe, ZnS, ZnSe, ZnTe and overestimates up to ~4% for CdS and CdSe. Calculated band gaps, spin–orbit splitting, effective masses and theoretical and

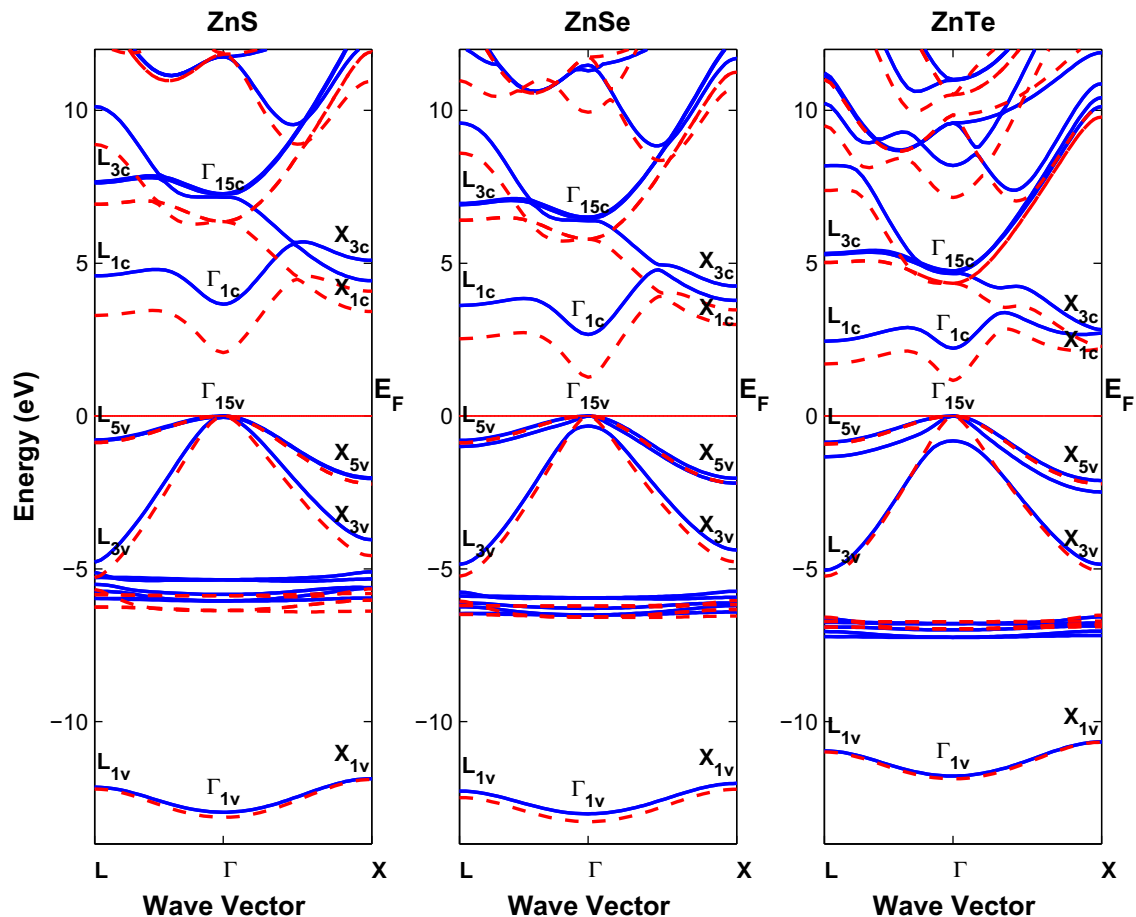


Fig. 1. (a–c): Energy band structure of ZnS (a), ZnSe (b) and ZnTe (c) bulk semiconductors, obtained by using program package WIEN2k [15] with MBJLDA (solid line) and GGA (dash line).

experimental data are shown in Table 2. Calculated energies at L , Γ and X high symmetry points are shown in Table 3 for CdX and in Table 4 for ZnX. We also compared our present results with available theoretical and experimental data. For CdS, CdSe and CdTe, we compared MBJLDA band energies with our previous uncorrected LSDA results [8] and other LDA results as parameterized by Perdew and Zunger [10]. We observed similar band energies for valance bands. On the other hand, for conduction bands and band gaps MBJLDA results are more satisfactory than LSDA results. Due to the band gap problem in DFT using different parameterized schemes (LSDA, GGA, MBJLDA) results in different values. We compared the different methods with available theoretical and experimental data in Table 1–4 since we aim to show how different methods affect to band gap and band properties.

Figs. 1 and 2(a–c) demonstrate that the electronic band structure of ZnS, ZnSe, ZnTe and CdS, CdSe, CdTe calculated with the package WIEN2k. In Figs. 1 and 2, we compared MBJLDA band structures with LSDA band structures for CdX ($X = S, Se, Te$) and GGA band structures for ZnX ($X = S, Se, Te$). As shown in Table 2, DFT calculations with MBJLDA are in good agreement with the experimental data in terms of band gaps. Accurate modeling of band structure properties have a key role in the design of cadmium and zinc chalcogenides based device applications. According to current calculations MBJLDA performed better than other conventional DFT functionals and GW approximations to calculate band structure. For this reason, MBJLDA is a very effective method and it can be used for a wide range of semiconductors.

The spin–orbit splitting at the top of the valance band is an important parameter for determination of optical transitions [1] in the II–VI chalcogenides. We calculated spin–orbit splitting value for Cd and Zn based chalcogenides. Our calculated spin–orbit splitting parameter is underestimated by MBJLDA. The same trend of Ref. [1] for spin orbit splitting is also valid for MBJLDA spin orbit parameter results. It means that the SO splitting increases as the anion atomic number increases from S, Se to Te. However, SO splitting decreases as the cation atomic number increases from Zn to Cd. This fact comes

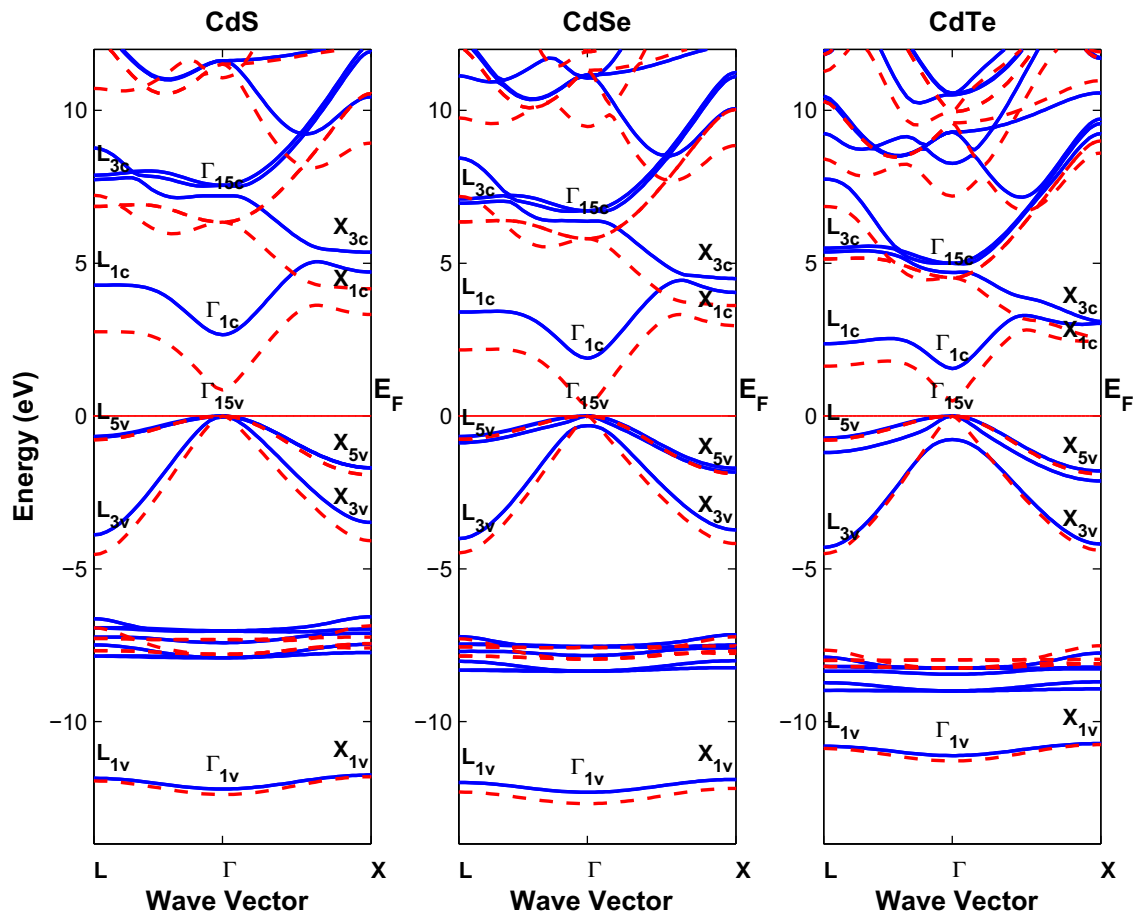


Fig. 2. Energy band structure of CdS (a), CdSe (b) and CdTe (c) bulk semiconductors, obtained by using program package WIEN2k [15] with MBJLDA (solid line) and LSDA (dash line).

from a large anion p characteristic of valence band maximum. SO splitting of anion valence p states increases with the atomic number [1].

The electron effective masses are calculated by fitting the dispersion curves around Γ gamma point along the direction (Γ to X) [100]. The calculated effective masses are almost in a good agreement with the available experimental data. Moreover, conduction band effective masses decrease with an increasing atomic number of anion S, Se to Te for CdX and ZnX [1].

4. Conclusion

We have presented a full potential linear augmented plane wave method within density functional theory (DFT) with modified Becke–Johnson potential to determine structural properties and electronic band structure of cadmium and zinc based binary semiconductors. In the meaning of calculation of lattice constants and band gaps, unfortunately, there is no functional which is sufficiently accurate for all solids. We reported lattice parameters and band properties by using various functionals for CdX and ZnX ($X = S, Se, Te$) based materials. These results may serve as guidelines, which functional should give accurate structural and electronic properties for II–VI based compounds. Present calculations reproduce the band dispersion curves near high symmetry points of Brillouin zone of semiconductors. The model shows a good agreement with the available experimental data for band gaps, lattice constants and effective masses.

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