

Electronic structure and band alignments of ZnTe/CrTe(001), CdSe/CrTe(001) and CdTe/CrTe(001) interfaces

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Abstract. All-electron full potential calculations based on spin density functional theory were performed to study cubic zincblende (ZB) and hexagonal NiAs structures of bulk CrTe and ZnTe/CrTe(001), CdTe/CrTe(001) and CdSe/CrTe(001) interfaces. The lattice mismatch effect in ZB CrTe and magnetic properties of CrTe in the ideal ZB CrTe structure were investigated. The band alignment properties of the ZnTe/CrTe(001), CdTe/CrTe(001) and CdSe/CrTe(001) interfaces were computed and a rather large minority valence band offset of about 1.09 eV was observed in ZnTe/CrTe(001) heterojunction. Also in the CdTe/CrTe(001) and CdSe/CrTe(001) interfaces, the conduction band minimum of minority spin in CrTe was above the conduction band minimum of CdTe and CdSe and so the majority spin electrons could be directly injected to both semiconductors, indicating the possibility of highly efficient spin injection into the CdSe and CdTe semiconductors.

Keywords. Spintronics; half-metallicity; interface; magnetic properties; electronic properties.

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1. Introduction

Half-metallic (HM) materials, exhibiting complete spin polarization (100%) at the Fermi level, have attracted much attention because of their promising applications in the high-performance spintronic devices. After de Groot *et al* [1] who discovered the half-metallic property of the half-Heusler NiMnSb and PtMnSb alloys, several half-metallic ferromagnets such as rutile CrO₂ [2], double perovskite Sr₂FeMoO₆ [3], spinel Fe₃O₄ [4], pyrite-type CoS₂ [5,6] and Heusler alloys [7] have been theoretically predicted and/or experimentally synthesized. Recently, many theoretical and experimental attempts were done on the zincblende (ZB) compounds such as *MAs* and *MSb* (*M* is a transition metal element) [8–13] which are compatible with III–V and II–VI semiconductors. It has already been established theoretically that the ZB MnAs phase is a ‘near HM’ ferromagnet because

its HM gap is zero [14,15] and the ZB CrAs [10,16], the ZB MnSb and ZB MnBi phases [17] are true HM ferromagnets with finite HM gaps. So far only three ZB phases were fabricated successfully: ZB MnAs in nanodots [9], ZB CrAs in thin films and multilayers [10,11] and ZB CrSb in thin films [12]. Recently, Sreenivasan *et al* attempted to grow ZB CrTe thin films on GaAs(001) using ZnTe buffer layer [18,19]. The lattice parameter of ZB CrTe is calculated to be equal to 6.29 Å [20] which is negligibly different from the experimental lattice parameters of ZnTe (6.10 Å), CdTe (6.49 Å) and CdSe (6.05 Å) semiconductors. Therefore, the ZB CrTe can be grown on ZB semiconductors such as ZnTe, CdTe and CdSe. But it is important to know, for practical applications, whether or not the half-metallic materials preserve the half-metallicity at the interfaces. In this paper, we have theoretically investigated the half-metallic behaviours of the ZnTe/CrTe(001), CdTe/CrTe(001) and CdSe/CrTe(001) interfaces.

2. Computational method

We used the FPLAPW+lo method implemented in the WIEN2K package [21] within the spin-polarized DFT, in which the exchange-correlation energy of electrons is described in the generalized gradient approximation (GGA) [22]. Relativistic effects were taken into account within the scalar approximation, neglecting the spin-orbit coupling. Basis functions, charge density and potential were expanded inside the muffin-tin spheres in combination with spherical harmonic functions with a cut-off $l_{\max} = 10$, and in Fourier series in the interstitial region. Moreover, we used a parameter $R_{\text{MT}} \cdot K_{\max} = 8$, to determine the matrix size (convergence), where K_{\max} is the plane-wave cut-off and R_{MT} is the smallest of all atomic sphere radii. For all atoms, R_{MT} was chosen as 2.2 a.u. In all calculations we used an $8 \times 8 \times 1$ mesh for k-points in the Brillouin zone integration. The self-consistent calculations are considered to be converged only when the integrated charge difference per formula unit, $\int |\rho_n - \rho_{n-1}| dr$, between the input charge density $[\rho_{n-1}(r)]$ and the output charge density $[\rho_n(r)]$ is less than 0.00001.

3. Results and discussion

3.1 Bulk properties

The ground state properties of ZB and NiAs structures of CrTe with ferromagnetic (FM), antiferromagnetic (AFM) and nonmagnetic (NM) states were obtained by calculating the total energy of these systems as a function of volume and then fitting the calculated values by the Murnaghan equation of state [23]. Our results showed that at low volumes, the NiAs phase was more stable than the ZB phase in the FM, AFM and NM states whereas increasing volume favoured the stability of the ZB structure. According to our results, although bulk ZB CrTe shows half-metallic behaviour, but like some other half-metals, surface or interface effects may destroy half-metallicity and substantially reduce the Fermi level spin polarization from the ideal 100% value. The interface effects originate from the lattice and chemical mismatches at the junction of the two compounds. To decrease the interface effects and also to obtain an epitaxial interface, the alloy should be grown on a substrate having a close lattice constant to the alloy. The calculated lattice parameters of

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ZnTe (6.18 Å), CdSe (6.19 Å) and CdTe(6.62 Å) semiconductors are close to the lattice parameter of CrTe (6.26 Å), indicating the suitability of these ZB semiconductors to be used as a substrate for growing ZB CrTe thin films. It explains why Sreenivasan *et al* used a ZnTe buffer layer on GaAs(001) to grow thin ZB CrTe layers [18]. To verify the lattice mismatch effect, we studied the tetragonally distorted ZB structure of CrTe by fixing the in-plane lattice constants of CrTe to that of ZnTe and relaxing the vertical lattice constant of CrTe in the growth direction. The relaxed value of c in the tetragonal structure was found to be about 6.43 Å. The band structures of the tetragonally distorted and equilibrium ZB CrTe is shown in figure 1. By comparing the band structure of the equilibrium and distorted ZB structures, we observed that in the $\Gamma \rightarrow M$ direction and in Γ point, tetragonal distortion

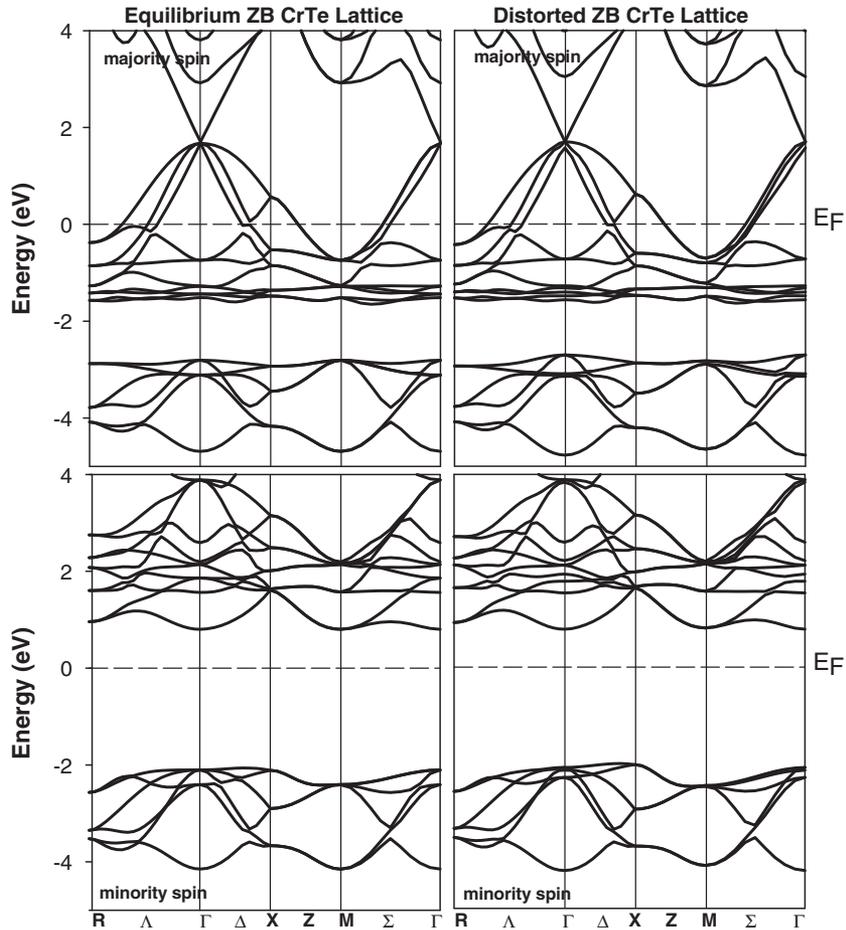


Figure 1. The spin-polarized electronic band structure of bulk CrTe in the tetragonal representation of the equilibrium ZB (left column) and tetragonally deformed ZB (right column) structures. The Fermi energy is set to zero.

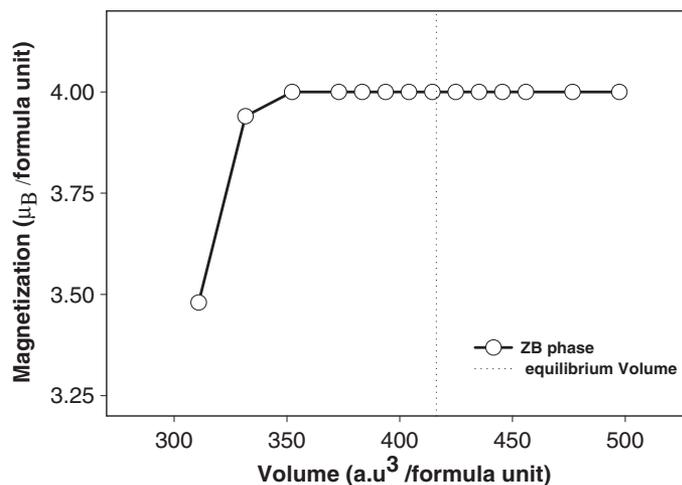


Figure 2. The variation of the total magnetic moment as a function of primitive cell volume in the ZB structure of the bulk CrTe. The equilibrium volume is shown by vertical dotted line.

removed the degeneracy of some bands and slightly split them. This is because the tetragonal distortion distinguishes the z -axis from the x - and y -axes and reduces symmetry of the crystal. The same behaviour was observed in the tetragonal ZB CrSb structure [24]. It is evident from figure 1 that the half-metallic property is preserved in the tetragonal structure of CrTe. We also calculated and plotted in figure 2 the magnetic moment of CrTe in the ideal ZB structure at different unit cell volumes. It is observed that the magnetic moment is fixed at $4 \mu_B$ in a wide range of volumes, pointing the half-metallicity of the system. The existence of a band gap at the Fermi level of the spin minority states leads to an integer number of spin-down electrons in the system. Consequently, the spin magnetic moment is also an integer number in a half-metal. This leads to a simple ‘rule of 8’ [25]:

$$M_{\text{tot}} = (Z_{\text{tot}} - 8) \mu_B, \quad (1)$$

where eight electrons contribute to bonding p-d bands and Z_{tot} is the total number of valence electrons. CrTe has 12 valence electrons in formula unit and so the total magnetic moment (M_{tot}) according to eq. (1) should be $4 \mu_B$. Reduction of the magnetic moment from integer value of 4 at low volumes indicates that the half-metallicity will be destroyed under high pressure.

3.2 Interface properties

3.2.1 Electronic properties. As already mentioned, ZnTe, CdTe and CdSe are appropriate substrates for growing very thin films of ZB CrTe. To establish the interface between CrTe and each of the three semiconductors, we used the supercell approach; in particular, tests performed as a function of the cell dimensions have shown that the bulk conditions on both sides of the interface were well recovered by using interface slabs composed of eight CrTe and eight semiconductor monolayers. In each heterojunction, the Cr atoms continue the fcc

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Zn and Cd sublattices (in ZnTe, CdTe and CdSe) of the substrate. All structural parameters of the interface supercell, including interlayer and interface distances and atomic positions were accurately relaxed and optimized. The results are similar in three interfaces and so we have presented the electronic properties of only CdSe/CrTe(001) interface. For investigating the electronic structure of the CdSe/CrTe(001) interface, the atomic partial density of

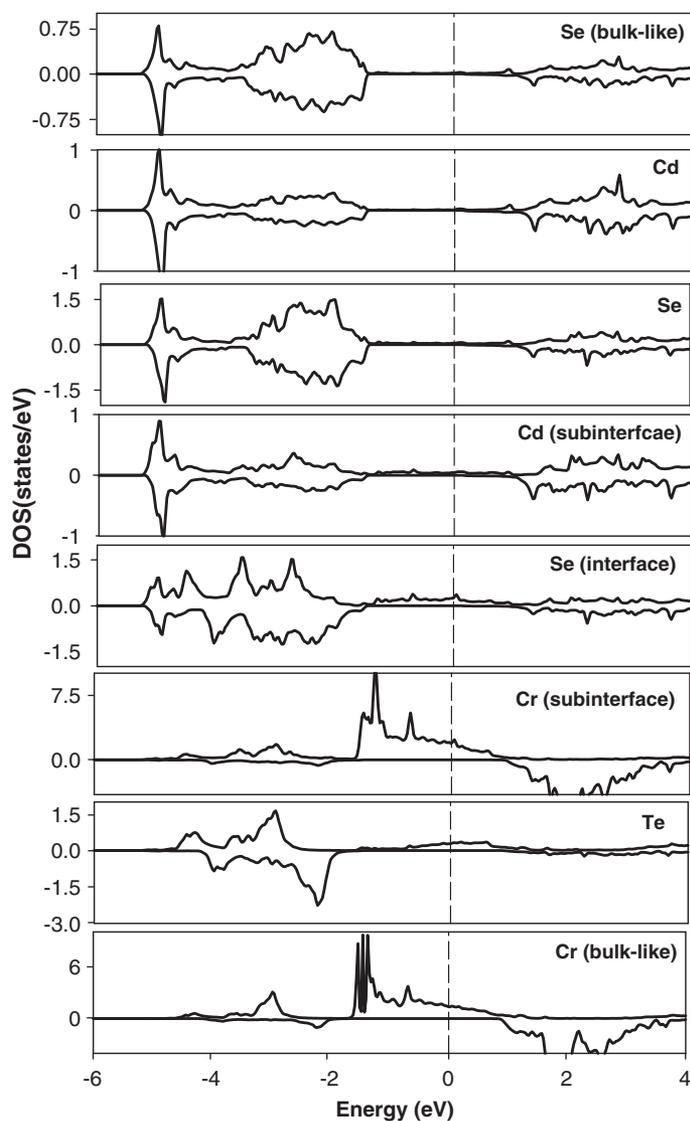


Figure 3. The spin-polarized atomic resolved DOS of various layers of the CdSe/CrTe(001) interface supercell. Negative DOS corresponds to minority spin. The Fermi energy is set to zero.

states (PDOS) of several layers from the centre of the CdSe substrate toward the centre of the CrTe film were calculated and presented in figure 3. We observed that the CdSe central layers have a bulk CdSe-like nonmagnetic DOS with a clear band gap at the Fermi level. On approaching the interface, the nonmagnetic partial DOS continuously changed towards the ferromagnetic half-metallic behaviour in such a way that the interface Se atom exhibited a moderate exchange splitting. This atom connected the nonmagnetic CdSe slab to the ferromagnetic CrTe layers. The p-d hybridization between Se and Cr enhanced exchange interactions in Se while the s-p hybridization between Se and Cd weakened this interaction. We observed that the central CrTe layers revealed a bulk CrTe-like half-metallic behaviour. Notably, it was seen that the partial DOS of the interface Se and subinterface Cr were more broadened than the central Se and Cr partial DOS, providing evidence for stronger Cr–Se interaction at the interface. The behaviour of the interface Se atom is similar to the interface Se atom in CrSe(00 1)/ZnSe(00 1) [26]. For further consideration of the interface

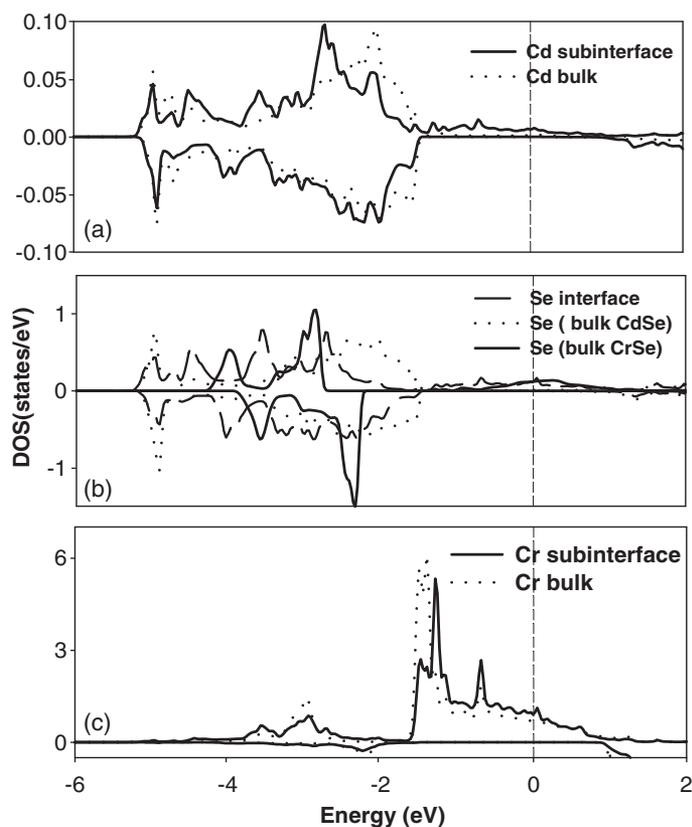


Figure 4. The spin-polarized orbital partial DOS of (a) the subinterface Cd, (b) the interface Se and (c) the subinterface Cr atoms. The bulk DOS are given for comparison. The interface Se p partial DOS is compared with both Se atoms in bulk CdSe and CrSe compounds. Negative DOS corresponds to minority spin. The Fermi energy is set to zero.

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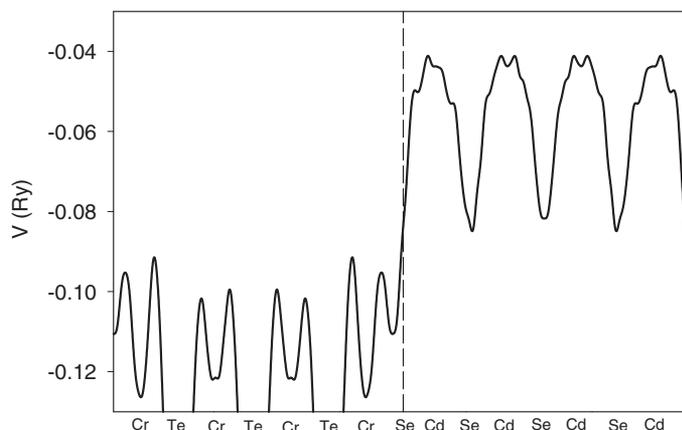


Figure 5. The total electrostatic potential profile at CdSe/CrTe(00 1) heterojunction. The interface Se layer is shown by the dashed line.

effects on electronic structure, we calculated and presented the orbital partial DOS of the interface Se and subinterface Cd and Cr atoms in figure 4. It is visible that the interface Cd partial DOS in both majority and minority channels are shifted away from the Fermi level compared to the bulk-like Cd states because of the electrostatic potential difference between the semiconductor and metal sides of the interface, which is clearly visible in the calculated and presented electrostatic potential diagram in figure 5. According to figure 5, the electrostatic potential increases from metal towards semiconductor side. Therefore, there is an electrostatic field at the interface of two slabs that affects the electronic states of atoms around the interface and shifts them. As is seen, the electrostatic potential is higher in semiconductor side than in metal side and so the electronic states of Cd atom are shifted away from Fermi level. This potential difference effect is also detectable in the PDOS of the interface Se (figure 4b) and subinterface Cr (figure 4c) atoms. The interface Se PDOS, compared to Se atom in bulk CdSe, is shifted away from the Fermi level while, compared to Se atom in bulk CrSe, is shifted towards the Fermi level. A slight shift towards the Fermi level is also visible in the subinterface Cr PDOS.

3.2.2 Magnetic properties. In table 1 we have listed the magnetic moments of different atomic species in the three junctions. Notably, sufficiently far from the junction, the bulk magnetic moments are recovered. The bulk values for Cr and Te atoms in the strained CrTe compound are 3.62 and $-0.14 \mu_B$ whereas ZnTe, CdTe and CdSe are nonmagnetic semiconductors with zero atomic magnetic moments. In the ZnTe/CrTe(00 1) junction, the magnetic moment of the interface Te atom is equal to the average of the corresponding bulk values on two sides of the interface, consistent with the intermediate character of the interface Te atom observed in the DOS plots (not shown here). On approaching the interface, the magnetic moment of Cr decreases while that of Zn atom slightly increases. Obviously, this behaviour is due to the hybridization of the ferromagnetic CrTe layers with nonmagnetic ZnTe layers at the interface. Similar behaviours are seen in the CdSe/CrTe(00 1) and CdTe/CrTe(00 1) interfaces.

Table 1. The spin magnetic moments in μ_B for subinterface and atoms at ZnTe/CrTe(00 1), CdSe/CrTe(00 1) and CdTe/CrTe(00 1) heterojunctions. The bulk-like values are given for comparison (SC: substrate centre; IL: intermediate layer; SI: subinterface layer; I: interface; FC: film centre).

Heterojunction	Bulk-like (SC)	IL	SI	I	SI	IL	Bulk-like (FC)		
ZnTe/CrTe(00 1)	Te 0	Zn 0	Te 0	Zn 0.02	Te -0.07	Cr 3.58	Te -0.14	Cr 3.61	Te -0.14
CdTe/CrTe(00 1)	Te 0	Cd 0	Te 0	Cd 0.01	Te -0.07	Cr 3.60	Te -0.15	Cr 3.62	Te -0.14
CdSe/CrTe(00 1)	Se 0	Cd 0	Se 0	Cd 0.01	Se -0.06	Cr 3.49	Te -0.13	Cr 3.53	Te -0.13

3.2.3 *Band alignment.* The spin-resolved band alignment parameters are technologically relevant in the electronic transport properties of layered devices. Generally, a half-metal/semiconductor heterojunction for the majority spin resembles a metal/semiconductor contact with a p- or n-type Schottky barrier (Φ_p, Φ_n) while in the minority channel this interface acts as a semiconductor/semiconductor heterojunction and the band discontinuities are defined as the valence and conduction band offsets (VBO, CBO).

These band discontinuities arise from the bulk properties of the compounds, which form the interface, and physical effects of the interface. So we should use a combination of the bulk and interface calculations to evaluate interface band parameters. The important point is that reference energy in bulk compounds is different and interface calculations should be applied to align these energies.

To calculate the band alignment parameters, we follow the well-established ‘bulk plus line up’ procedure presented by Peressi *et al* [27], in which the bulk band structures are combined with a potential line-up parameter (ΔV) obtained from the interface slab calculations. According to this method the band alignment parameters are defined as

$$\Phi_p = \Delta E_p + \Delta V \tag{2}$$

$$\Phi_n = \Delta E_n + \Delta V \tag{3}$$

$$\text{VBO} = \Delta E_v + \Delta V \tag{4}$$

$$\text{CBO} = \Delta E_c + \Delta V. \tag{5}$$

ΔE_p (ΔE_n) are defined as the difference between semiconductor valence band maximum (VBM), conduction band minimum (CBM) and metal Fermi level while ΔE_v (ΔE_c) is the difference between minority half-metal VBM (CBM) and semiconductor VBM (CBM).

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To calculate ΔV at each heterojunction we followed the procedure of Massidda *et al* [28], which was determined by comparing the electronic structure of the core electrons in the bulk and interface central layers. The $1s$ core electrons were selected for this purpose as they are well shielded from the interface effects. The potential line-up parameter is defined as $\Delta V = \Delta E_s^{\text{bulk}} - \Delta E_s^{\text{slab}}$ where ΔE_s^{bulk} and ΔE_s^{slab} are the energy difference of

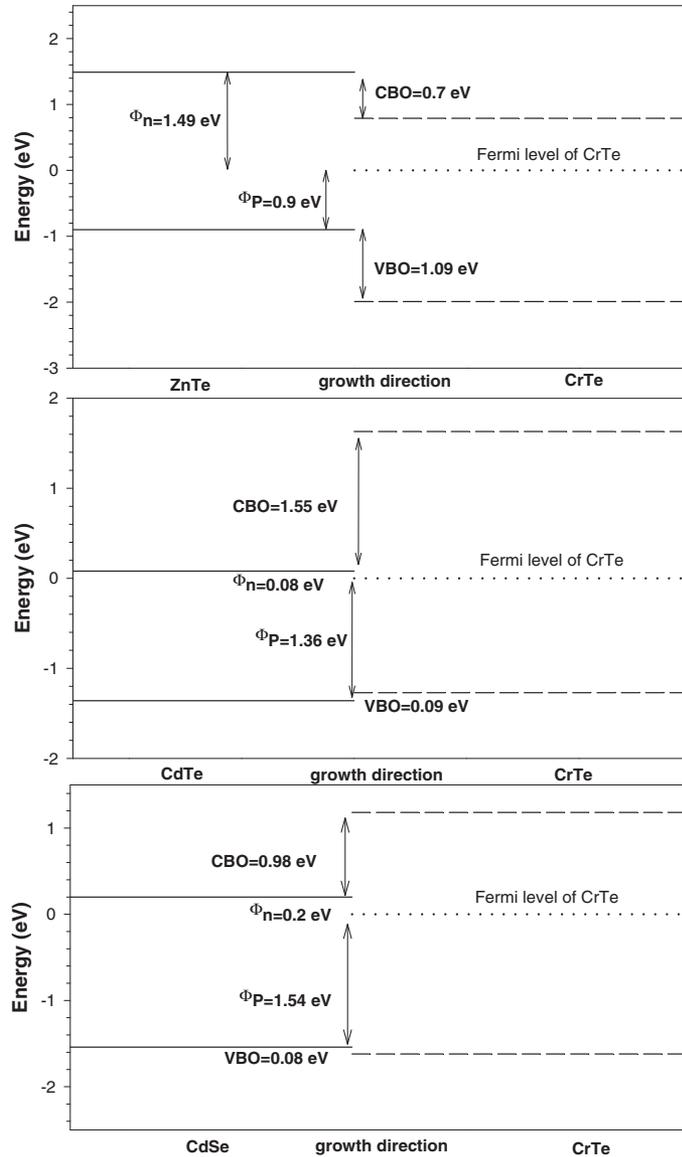


Figure 6. The schematic band diagram at ZnTe/CrTe(001), CdTe/CrTe(001) and CdSe/CrTe(001) heterojunctions. The CrTe Fermi energy is set to zero.

Cr 1s and Zn 1s (or Cd 1s) core electrons in the bulk compounds and slab central layers, respectively. In this way potential line-ups of about 0.16, 0.64 and 0.4 eV were obtained for the ZnTe/CrTe(00 1), CdTe(00 1)/CrTe(00 1) and CdSe(00 1)/CrTe(00 1) interfaces, respectively. By applying these potential line-ups, we aligned and matched the separately calculated bulk band structures of CrTe with ZnTe, CdTe and CdSe to determine the band diagrams of ZnTe/CrTe(00 1), CdTe(00 1)/CrTe(00 1) and CdSe(00 1)/CrTe(00 1) heterojunctions (figure 6). Following Peressi *et al* [27], we emphasize the necessity of many-body corrections to the single-particle eigenvalues obtained from the LDA/GGA calculations and used to evaluate the bulk band structures and the interface line-ups. Since these corrections are normally much less important for the valence bands than they are for the conduction bands in semiconductors, many-body corrections mainly influence the CBO and Φ_n parameters. To improve the reliability of these parameters, we shifted up the CBM of semiconductors to recover the experimental band gap values (2.39, 1.44 and 1.74 eV for ZnTe, CdTe and CdSe, respectively). The minority band gap of ZB CrTe is calculated, since we are not aware of any experimental measurement and many-body corrections in this system. The final estimate of band alignment parameters in three interfaces are listed in table 2 accompanied by the corresponding reported data for other interfaces. Notably, ZnTe/CrTe(00 1) interface, similar to ZnSe/CrSe(00 1) and GaAs/VAs(00 1) interfaces, has a higher minority VBO compared to Heusler alloys. It may be an evidence for lower contribution of minority electrons in the injected currents and so more efficient spin injection into semiconductors. Moreover, the n-type Schottky barrier height of CdTe/CrTe(00 1) interface is smaller than that of the other interfaces, suggesting higher rate of majority electrons injecting into semiconductor in CdTe/CrTe(00 1) junction. In the CdTe/CrTe(00 1) and CdSe/CrTe(00 1) interfaces the conduction band minimum of minority spin in the CrTe lies above the conduction band minimum of CdTe and CdSe and so the majority spin electrons can be directly injected into both semiconductors with less

Table 2. The majority Schottky barriers (eV) and minority band offsets (eV) at CrTe/ZnTe(00 1), CrTe/CdSe(00 1) and CrTe/CdTe(00 1) heterojunctions. Our results are compared with the band alignment parameters of some other half-metal/semiconductor heterojunction.

Heterojunction	Φ_n	Φ_p	VBO	CBO
ZnTe/CrTe(00 1) (present work)	1.49	0.90	1.09	0.70
CrTe/CdTe (present work)	0.08	1.36	0.09	1.55
CrTe/CdSe (present work)	0.20	1.54	0.08	0.98
CrSe/ZnSe ^a	1.84	0.88	1.94	1.28
VAs/GaAs ^b	1.19	0.23	1.03	0.93
Co ₂ MnSi/GaAs ^c	1.20	0.18	0.03	0.50
Co ₂ Cr _{0.5} Fe _{0.5} Al/GaAs ^d	2.20	-0.78	0.32	1.93

^aRef. [26].

^bRef. [28].

^cRef. [29].

^dRef. [30].

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probability of being flipped to the conduction bands of the minority spin. This suggests the possibility of highly efficient spin injection into the CdSe and CdTe semiconductors.

4. Conclusions

Density functional computations were employed to investigate the electronic and magnetic properties of bulk CrTe in ZB and NiAs structures and ZnTe/CrTe(0 0 1), CdTe/CrTe(0 0 1) and CdSe/CrTe(0 0 1) interfaces. It was found that the FM NiAs structure is the stable state of bulk CrTe. Results of our calculations confirmed that CrTe remained half-metallic at the ZnTe/CrTe(0 0 1), CdTe/CrTe(0 0 1) and CdSe/CrTe(0 0 1) interfaces. The interface band alignment parameters were determined and it was found that the ZnTe/CrTe(0 0 1) heterojunction had a substantially higher minority valence band offset compared to the other two heterojunctions. Also in the CdTe/CrTe(0 0 1) and CdSe/CrTe(0 0 1) interfaces the conduction band minimum of minority spin in the CrTe was above the conduction band minimum of CdTe and CdSe semiconductors. So these heterojunctions are suitable candidates in the field of spintronics.

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