Magnetic and electric properties of transition-metal doped wurtzite CdSe from first-principles calculations*

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The geometrical structures of $Cd_{0.75}TM_{0.25}Se$ (TM = Ti, V, Cr and Mn) are optimized, and then their electric and magnetic properties are investigated by performing first-principles calculations within the generalized gradient approximation for the exchange–correlation function based on density functional theory. $Cd_{0.75}TM_{0.25}Se$ (TM = Ti and V) are found to have high spin-polarization near 100% at the Fermi level. $Cd_{0.75}TM_{0.25}Se$ (TM = Cr and Mn) are half-metallic ferromagnets whose spin-polarization at the Fermi level is absolutely +100%. The supercell magnetic moments of $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$ are 4.00 and 5.00 μ_B, which arise mainly from Cr-ions and Mn-ions, respectively. The half-metallicity of $Cd_{0.75}Cr_{0.25}Se$ is more stable than that of $Cd_{0.75}Mn_{0.25}Se$. The electronic structures of Cr-ions and Mn-ions are Cr $e_g^2\uparrow t_{2g}^2\uparrow$ and Mn $e_g^2\uparrow t_{2g}^3\uparrow$, respectively.

Keywords: half-metallicity, electric and magnetic properties, supercell magnetic moments
PACC: 7115H, 7120H, 7170C

1. Introduction

Half-metallic ferromagnets (HMFs), whose spin-polarization is theoretically ±100% at the Fermi level, are very important spintronic materials.[1,2] Firstly, transmission of charges and spins of electrons can be simultaneously controlled in HMFs so that they are very important magnetoresistance materials.[1,2] Many spintronic devices based on the magnetoresistance effect, such as magnetoresistance random access memory (MRAM) and read–write magnetic-heads of computers, have been invented.[3−5] Secondly, realization of spintronic semiconductor devices requires highly spin-polarized current injected from magnetic electrodes to semiconductors.[2−6] HMFs have 100% spin-polarization, and their resistivity matches well with that of semiconductors so that they are the most magnetic electrode materials of spin semiconductors.[4−6] Therefore, HMFs have attracted much attention in the past few years. Recently, much attention has been paid to transition-metal doped or pure zinc blende semiconductor-type HMFs, such as CrAs, CrSb and doped ZnTe. Some of them have been prepared experimentally and found to have half-metallicity.[6−11] However, little attention has been paid to wurtzite HMFs. In this paper, some doped wurtzite HMFs are predicted and their electric and magnetic properties are investigated in detail based on density functional theory.

2. Technical

Generally, the experimental dopant concentration is from 5% to 30% for compounds with zinc blende or wurtzite structures.[7,11] Experiments on wurtzite TM-doped CdSe have not been found so far. Therefore, we used a hypothetic periodic 1×2×1 wurtzite supercell of CdSe which consists of eight ions including four Cd-ions and four Se-ions. Then one Cd-ion was substituted by transition-metal (TM) ions (TM = Ti, V, Cr and Mn) to achieve the possible experimental dopant concentration. The theoretic dopant concentration is 25.0% in this paper. The space group

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of the optimized supercell is $P1$.

The optimization of geometrical structures and calculations of the magnetic and electric properties of the wurtzite compounds were performed using the calculation module 'castep' of the software 'materials studio' based on density functional theory. During the optimization of geometric structures, the lattice constants of supercells were adjusted based on the variation of their energy by the software until the energy convergence was less than 2×10^{-6} eV/atom. Then the stable lattice constants were given and the magnetic and electric properties of these stable supercells were calculated.

In the self-correction optimization and calculation, the optimization and calculation quality 'fine' was elected, corresponding to the cutoff energy 340 eV and the k-point set 9×4×5. The wave functions of the software are expanded with plane-wave pseudo-potentials, and the exchange correlation functions are the Perdew–Burke–Ernzerh functions (PBE) of three nonlocal gradient-corrected exchange–correlation functions (GGA). The calculated electronic structures of isolated atoms include Ti $3s^2 3p^6 3d^2 4s^2$, V $3s^2 3p^6 3d^3 4s^2$, Cr $3s^2 3p^6 3d^5 4s^1$, Mn $3d^5 4s^2$, Cd $4d^{10} 5s^2$ and Se $4s^2 4p^4$.

The geometrical structures of wurtzite ZnO, CrAs and CrTe were optimized and compared with experiments or calculated results of others in order to confirm our calculations. The lattice constants are shown in Table 1. From Table 1, our calculated lattice constants of CrAs ($a = 4.03$ Å (1 Å = 0.1 nm), $b = 8.06$ Å and $c = 6.54$ Å) and CrTe ($a = 4.47$ Å, $b = 8.94$ Å and $c = 7.25$ Å) accord well with those calculated by Xie and Zhang, respectively.[12–14] Furthermore, the calculated lattice constants of ZnO ($a = 3.29$ Å, $b = 6.58$ Å and $c = 5.31$ Å) also accord well with the experimental values in Ref. [15].

Table 1. Calculated and expermental geometrical structures of some wurtzite materials, including the lattice constants, volume, half-metallic charaters and half-matellic gaps.

compounds	a/Å	b/Å	c/Å	volume/Å^3	half-metalllic gap/eV	HMF
CrAs	4.03	8.06	6.54			Yes
CrAs[a]	4.00	8.00	6.53			
CrTe	4.47	8.94	7.25			Yes
CrTe[a,b]	4.46	8.92	7.23			
ZnO	3.29	6.58	5.31	224.81		No
ZnO[c]	3.28	6.56	5.32			No
ZnO[d]	3.25	6.50	5.32			No
CdSe	4.44	8.88	7.17	243.50		No
$Cd_{0.75}Ti_{0.25}Se$	4.35	8.72	7.03	230.76		No
$Cd_{0.75}V_{0.25}Se$	4.39	8.69	7.09	233.18		No
$Cd_{0.75}Cr_{0.25}Se$	4.33	8.61	7.09	229.00	0.57	Yes
$Cd_{0.75}Mn_{0.25}Se$	4.42	8.85	7.21	241.47	0.29	Yes

[a] Ref. [12], [b] Ref. [13], [c] Ref. [14], [d] Ref. [15].

3. Results and discussions

3.1. Total state densities of wurtzite $Cd_{0.75}TM_{0.25}Se$

Total spin-polarized densities of states (TDOS) of wurtzite $Cd_{0.75}TM_{0.25}Se$ (TM = Ti, V, Cr and Mn) are shown in Fig. 1, where the solid and dashed lines show the TDOS of up-spin and down-spin subbands, respectively. From Fig. 1, the spin polarization of $Cd_{0.75}Ti_{0.25}Se$ and $Cd_{0.75}V_{0.25}Se$ at the Fermi level is near to +100% so that they are highly spin-polarized materials. However, they are not really half-metallic ferromagnets. Generally, the half-metallicity of some highly polarized materials has been induced by exerting some external pressure on them.[16–18] Similarly, it is possible that the half-metallicity of $Cd_{0.75}Ti_{0.25}Se$ and $Cd_{0.75}V_{0.25}Se$ may be induced to have some promising application possibility. This is not discussed here due to the limited length of this paper. The discussion of the influence of the exter-

nal pressure on the half-metallicity of wurtzite compounds will be published separately. The spin polarization of $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$ at the Fermi level is absolutely +100% so that they are really half-metallic ferromagnets, which have a wider application foreground. From Fig. 1, $Cd_{0.75}TM_{0.25}Se$ (TM = Ti, V, Cr and Mn) have similar TDOS near the Fermi level. Furthermore, their TDOS whose energies vary from –73.5 to –7.5 eV are almost same, but are not plotted in Fig. 1, due to limited space. The main reason is perhaps that Ti, V, Cr and Mn have similar atomic orbit structures (3d4s). However, the Fermi levels of $Cd_{0.75}TM_{0.25}Se$ relatively move toward lower energy when the dopants vary from Ti to Mn. The reasons are perhaps that intra-ionic interactions including Coulomb repulsion and exchange interaction are stronger if supercells have more electrons. $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$ have more electrons than $Cd_{0.75}Ti_{0.25}Se$ and $Cd_{0.75}V_{0.25}Se$ evidently. Stronger intra-atomic interaction results in larger separation of their down-spin sub-bands and pushes the Fermi levels to move toward the lower energy.

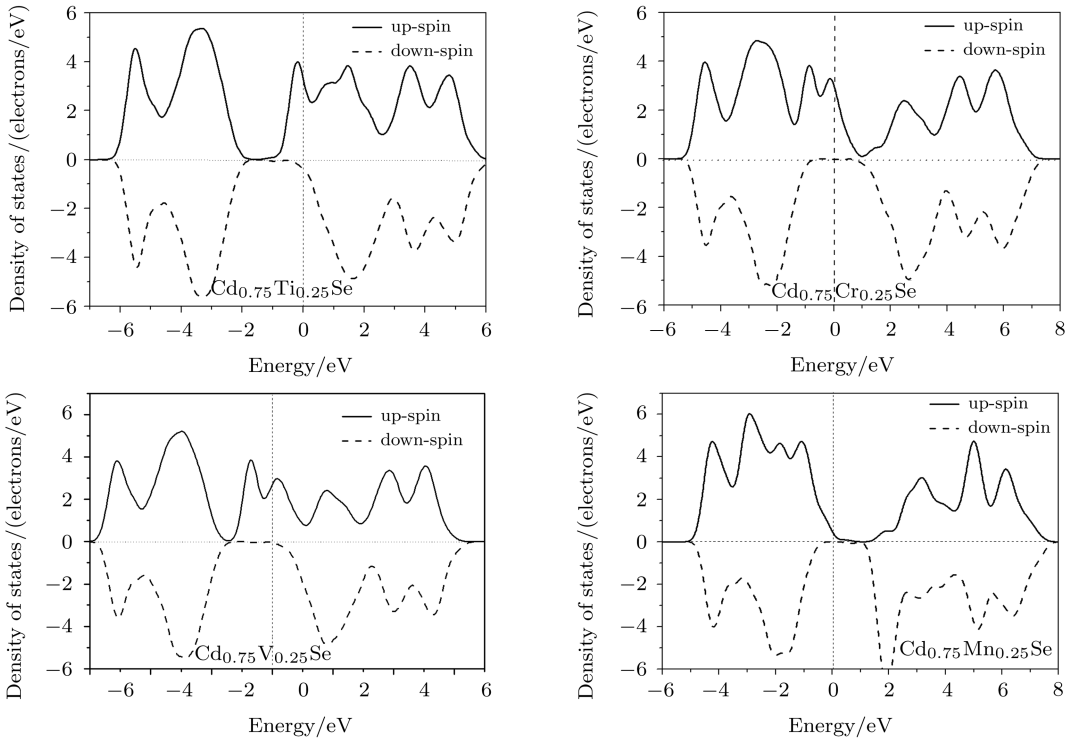


Fig. 1. Spin-polarized total state densities of wurtzite $Cd_{0.75}TM_{0.25}Se$ (TM = Ti, V, Cr and Mn).

From Fig. 1, the spin gap 1.07 eV of $Cd_{0.75}Cr_{0.25}Se$, defined as the energy distance from the maximum energy of down-spin valence sub-bands to the minimum energy of the down-spin conduction sub-bands, is a little lower than 1.24 eV of $Cd_{0.75}Mn_{0.25}Se$. However, the spin-flip gaps or half-metallic gaps, defined as the energy difference between the Fermi level of the metallic sub-bands and the valence band peak of the semiconducting sub-bands, are 0.57 and 0.29 eV for $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$, repectively. The front 0.57 eV is about two times the latter 0.29 eV. This shows that the half-metallicity of $Cd_{0.75}Cr_{0.25}Se$ is more stable than $Cd_{0.75}Mn_{0.25}Se$. It is also shown in Fig. 1 that the up-spin TDOS of $Cd_{0.75}Cr_{0.25}Se$ is 2.95 electrons/eV at the Fermi level, which is much larger than 0.45 electrons/eV of $Cd_{0.75}Mn_{0.25}Se$. This shows that there are many more conduction electrons in $Cd_{0.75}Cr_{0.25}Se$ than in $Cd_{0.75}Mn_{0.25}Se$ so that the conductivity of $Cd_{0.75}Cr_{0.25}Se$ is much higher than that of $Cd_{0.75}Mn_{0.25}Se$. On the other hand, $Cd_{0.75}Mn_{0.25}Se$ have some up-spin holes because the

maximum energy of its up-spin conduction sub-bands is a little higher than the Fermi level. However, $Cd_{0.75}Cr_{0.25}Se$ have no up-spin holes near the Fermi level. Therefore, the conductivity of $Cd_{0.75}Cr_{0.25}Se$ comes mainly from its conduction electrons at the Fermi level, but the conducitivity of $Cd_{0.75}Mn_{0.25}Se$ comes from both its conduction electrons and holes at the Fermi level.

3.2. Partial and local state densities of wurtzite $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$

The partial densities of states (PDOS) and local densities of states (LDOS) of $Cd_{0.75}Cr_{0.25}Se$ are shown in Figs. 2(a) and 2(b). Furthermore, PDOS and LDOS of $Cd_{0.75}Mn_{0.25}Se$ are shown in Figs. 2(c) and 2(d). From Figs. 2(a) to 2(d), curves above and below whose DOS are zero show the DOS of up-spin and down-spin sub-bands, respectively. The PDOS include the DOS of s, p and d-orbits and the LDOS include the DOS of one Cd-ion, one Cr-ion (or Mn-ion) and one Se-ion, respectively. In Figs. 2(a) and 2(c), the solid lines, the dots and the dashed lines show the PDOS of s, p and d-orbits, respectively. In Figs. 2(b) and 2(d), the solid lines, the dots and the dashed lines show the LDOS of one Cr (or Mn), Cd and Se-ion, respectively. Only the DOS near the Fermi level are plotted in Figs. 1 and 2 because the magnetic and electric properties of HMFs are mainly influenced by the DOS near the Fermi level. Their energy is from –5.0 eV to 7.5 eV.

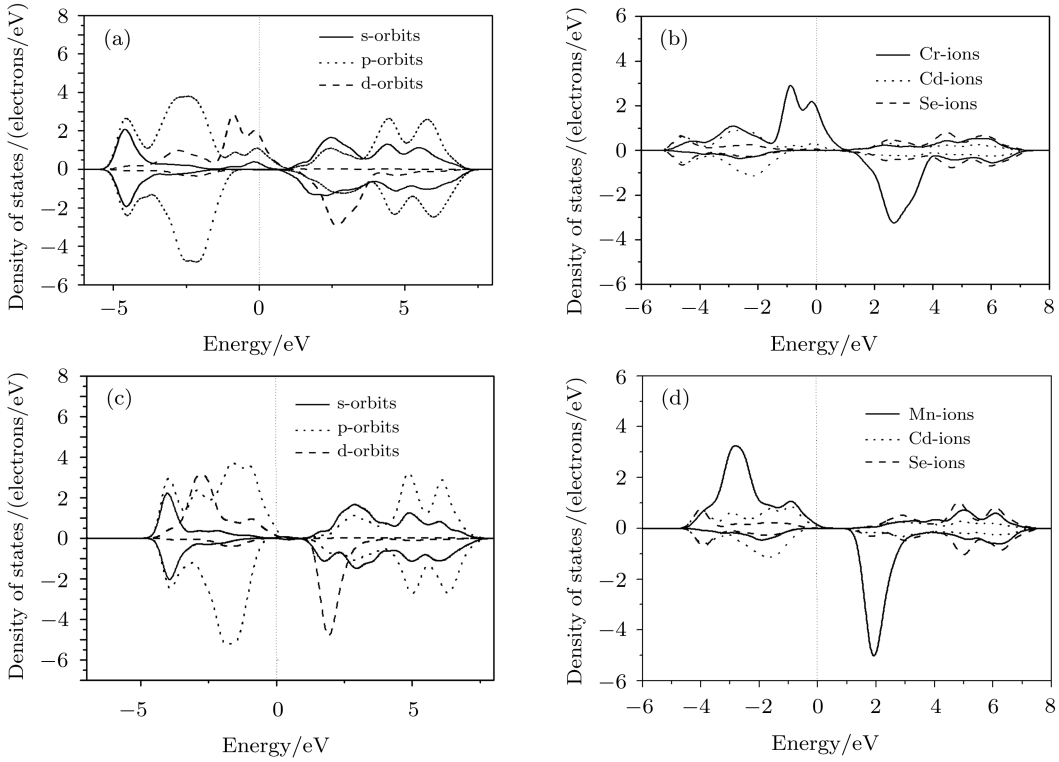


Fig. 2. Spin-polarized partial and local state densities of wurtzite $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$, where figures (a) and (b) show PDOS and LDOS of $Cd_{0.75}Cr_{0.25}Se$, respectively, and figures (c) and (d) show PDOS and LDOS of $Cd_{0.75}Mn_{0.25}Se$, respectively.

From Figs. 1 and 2(a), the TDOS of down-spin valence bands of $Cd_{0.75}Cr_{0.25}Se$ come mainly from p-orbits, and partially from s- and d-orbits. The PDOS of down-spin s-orbits whose energy is less than –1.25 eV are almost axially symmetrical with those of up-spin s-orbits so that they cause no influence on

the magnetic and electric properties of $Cd_{0.75}Cr_{0.25}Se$. However, the PDOS of down-spin p- and d-orbits whose energy is from –3.75 eV to –0.57 eV are not axially symmetrical with those of up-spin p- and d-orbits so that they cause some contribution on the supercell magnetic moments. There are only up-spin s-, p- and d-orbits through the Fermi level if the energy is larger than –0.57 eV so that they cause the main contribution on the supercell magnetic moments and the conductivity of $Cd_{0.75}Cr_{0.25}Se$. From Figs. 1 and 2(c), the TDOS of down-spin valence bands of $Cd_{0.75}Mn_{0.25}Se$ come mainly from p- and d-orbits, and partially from s-orbits. All s-, p- and d-orbits whose energy is from –4.6 eV to –0.29 eV cause a contribution on the supercell magnetic moments. However, the contribution of s- and p-orbits is much less than that of d-orbits evidently. There are only up-spin s-, p- and d-orbits through the Fermi level if the energy is larger than –0.29 eV so that they cause the main contribution on the conductivity of $Cd_{0.75}Cr_{0.25}Se$, but their contribution on the supercell magnetic moments is less than orbits whose energy is from –4.6 eV to –0.29 eV.

From Figs. 2(a) and 2(b), the TDOS of $Cd_{0.75}Cr_{0.25}Se$ at the Fermi level come mainly from 3d-orbits of Cr-ions, and then partially from 4p-orbits of Se-ions. The 4s-orbits of Cr-ions and 5s-orbits of Cd-ions also have a little contribution on the TDOS of $Cd_{0.75}Cr_{0.25}Se$. However, the contribution is much lower than that of 3d-orbits of Cr-ions and 4p-orbits of Se-ions. Similarly, the TDOS of $Cd_{0.75}Mn_{0.25}Se$ at the Fermi level come mainly from 3d-orbits of Mn-ions, and then partially from 4p-orbits of Se-ions from Figs. 2(c) and 2(d). The 4s-orbits of Mn-ions and 5s-orbits of Cd-ions also have a little contribution on the TDOS of $Cd_{0.75}Mn_{0.25}Se$. The main mechanism is that the energy of 3d-orbits of Cr or Mn-ions is near to that of 4p-orbits of Se-ions so that 3d-orbits and 4p-orbits are easily hybridized by the strong crystal field between the Cr-ions and Se-ions or between Mn-ions and Se-ions. Therefore there are p–d hybridized orbits in $Cd_{0.75}Mn_{0.25}Se$ and $Cd_{0.75}Cr_{0.25}Se$. On the other hand, the energy of 4s-orbits of Mn or Cr-ions and 5s-orbits of Cd-ions is far away from that of 3d-orbits of Mn or Cr-ions and 4p-orbits of Se-ions so that there is no s–d and s–p hybrization. However, the s-orbits are much wider than p and d-orbits so that s-orbits have a little contribution on the TDOS of both $Cd_{0.75}Mn_{0.25}Se$ and $Cd_{0.75}Cr_{0.25}Se$ at the Fermi level.

The ionic parameters of the $Cd_{0.75}Mn_{0.25}Se$ and $Cd_{0.75}Cr_{0.25}Se$ supercells are calculated and given in Tables 2 and 3, respectively, in order to know well their magnetic and electric properties. These parameters include the number of s-, p-, d- and total electrons, the charge and the ionic magnetic moments of all ions. From Tables 2 and 3, the ionic magnetic moments of one Cr-ion and one Mn-ion are 4.38 and 4.94 μ_B, respectively, which are much higher than those of Se-ions. On the other hand, those of Cd-ions are near zero. This also shows that there is a strong crystal field between the Cr-ions and Se-ions or between Mn-ions and Se-ions, which results in p–d hybridization. However, the p–d hybridization between Cr-ions and Se-ions is stronger than that between Mn-ions and Se-ions because the numerical values of the ionic magnetic moments of Se-ions in $Cd_{0.75}Cr_{0.25}Se$ are higher than in $Cd_{0.75}Mn_{0.25}Se$ in total.

Table 2. Calculated ionic parameters of wurtzite $Cd_{0.75}Cr_{0.25}Se$, including lattice constants, volume, half-metallic charaters and supercell magnetic moments.

ion	s	p	d	total	charge/e	spin/μ_B
Cr	2.64	6.76	4.70	14.10	–0.10	4.38
Se1	1.54	4.60	0.00	6.14	–0.14	–0.10
Se2	1.57	4.64	0.00	6.20	–0.20	0.02
Se3	1.52	4.55	0.00	6.07	–0.07	–0.22
Se4	1.53	4.61	0.00	6.14	–0.14	–0.08
Cd1	0.85	0.96	9.98	11.79	0.21	–0.02
Cd2	0.84	0.95	9.98	11.77	0.23	0.04
Cd3	0.85	0.96	9.98	11.79	0.21	0.02

Table 3. Calculated ionic parameters of wurtzite $Cd_{0.75}Mn_{0.25}Se$, including lattice constants, volume, half-metallic charaters and supercell magnetic moments.

ion	s	p	d	total	charge/e	spin/μ_B
Mn	0.63	0.75	5.36	6.74	0.26	4.94
Se1	1.56	4.66	0.00	6.22	–0.22	0.00
Se2	1.51	4.66	0.00	6.17	–0.17	0.02
Se3	1.56	4.67	0.00	6.23	–0.23	0.02
Se4	1.55	4.66	0.00	6.22	–0.22	0.00
Cd1	0.87	0.95	9.98	11.81	0.19	0.00
Cd2	0.87	0.96	9.98	11.81	0.19	0.02
Cd3	0.85	0.96	9.98	11.80	0.20	0.00

From the ligand field theory,[19–23] there are four Se-ligands around one TM-ion (TM = Cr and Mn) and one TM-ion and its ligands form the coordinate compound ML_4. There is a strong tetrahedral crystal field in ML_4, which results in 3d-orbits of TM-ions splitted into bonding orbits containing two e_g and three t_{2g}-orbits with lower energy, and their corresponding anti-bonding orbits containing two e_g^* and three t_{2g}^*-orbits

with higher energy. Furthermore, the energy of the e_g-orbits is lower than that of the t_{2g}-orbits. One Cr-ion has four 3d-electrons and they enter into two e_g-orbits and two t_{2g}-orbits, respectively, based on the lowest energy principle. On the other hand, the fifth 3d-electron enters into the Cr 4s-orbit with one 4s-electon because the energy of the 4s-orbit is lower than that of 3d-orbits. Therefore, the electronic structures of Cr-ions are Cr $e_g^2 \uparrow t_{2g}^2 \uparrow$. Similarly, five 3d-electrons of a Mn-ion enter into two e_g-orbits and three t_{2g}-orbits, respectively. Therefore, the electronic structures of Mn-ions are Mn $e_g^2 \uparrow t_{2g}^3 \uparrow$. From the electronic structures of Cr and Mn-ions, the magnetic moments of the supercell $Cd_{0.75}Mn_{0.25}Se$ and $Cd_{0.75}Cr_{0.25}Se$ are 4.00 and 5.00 μ_B, respectively.

On the other hand, all ionic magnetic moments of the supercell $Cd_{0.75}Mn_{0.25}Se$ and $Cd_{0.75}Cr_{0.25}Se$ are given in Tables 2 and 3. Adding up all ionic magnetic moments of a supercell, we can find that the supercell magentic moments of $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$ are 4.00 and 5.00 μ_B, respectively, and are consistent with the data based on the electronic structures of $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$. They both are just integral numbers. This shows that $Cd_{0.75}Cr_{0.25}Se$ and $Cd_{0.75}Mn_{0.25}Se$ are both half-metallic ferromagnets really.

4. Conclusions

In summary, we have explored the structural, electronic and magnetic properties of $Cd_{0.75}TM_{0.25}Se$ (TM = Ti, V, Cr and Mn) by performing first-principles calculations within the GGA-PBE for the exchange–correlation functional. $Cd_{0.75}TM_{0.25}Se$ (TM = Ti and V) are found to be highly spin-polarized materials and $Cd_{0.75}TM_{0.25}Se$ (TM = Cr and Mn) are half-metallic ferromagnets. The supercell magnetic moments of $Cd_{0.75}TM_{0.25}Se$ (TM = Cr and Mn) are 4.00 and 5.00 μ_B, respectively, which arise from Cr-ions and Mn-ions. The half-metallicity of $Cd_{0.75}Cr_{0.25}Se$ is more stable than that of $Cd_{0.75}Mn_{0.25}Se$. The electronic structures of Cr-ions and Mn-ions are Cr $e_g^2 \uparrow t_{2g}^2 \uparrow$ and Mn $e_g^2 \uparrow t_{2g}^3 \uparrow$, respectively.

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