Journal of Alloys and Compounds 508 (2010) 245–250

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jallcom

First-principles study of spin-polarized electronic band structures in ferromagnetic $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni)

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ARTICLE INFO

Article history:
Received 13 June 2010
Received in revised form 19 August 2010
Accepted 24 August 2010
Available online 22 September 2010

Keywords:
Half-metallic ferromagnetism
FPLAPW
Structural
Electronic and magnetic properties

ABSTRACT

We report a first-principles study of structural, electronic and magnetic properties of crystalline alloys $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) at $x = 0.25$. Structural properties are computed from the total ground state energy convergence and it is found that the cohesive energies of $Zn_{1-x}TM_xS$ are greater than that of zincblende ZnS. We also study the spin-polarized electronic band structures, total and partial density of states and the effect of TM 3*d* states. Our results exhibit that $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ are half-metallic ferromagnetic with a magnetic moment of $4\mu_B$, $3\mu_B$ and $2\mu_B$, respectively. Furthermore, we calculate the TM 3*d* spin-exchange-splitting energies $\Delta_x(d)$, $\Delta_x(x{-}d)$, exchange constants $N_0\alpha$ and $N_0\beta$, crystal field splitting ($\Delta E_{cryst} \equiv E_{t_{2g}} - E_{e_g}$), and find that *p*–*d* hybridization reduces the local magnetic moment of TM from its free space charge value. Moreover, robustness of $Zn_{1-x}TM_xS$ with respect to the variation of lattice constants is also discussed.

1. Introduction

In recent years, diluted magnetic semiconductors (DMSs) have gained a lot of interest and are being studied due to the possibility of having magnetic properties in semiconductors. In order to control the electron spin currents and charge spin currents for increasing data processing speeds, reducing power consumption and the hardware dimensions, ferromagnetic DMSs are considered to be of fundamental importance in spintronic devices [1]. DMSs are compounds in which fractions of the cation sites are randomly and partially occupied by transition-metal ions (such as Cr, Mn, Fe, Co or Ni) or rare earth metals. The optical properties of DMSs, which are obtained by doping II–VI semiconductors with transition-metal (TM) ions have received great attention in the past few years [2–4].

Half-metallic ferromagnetic (HMF) materials have been studied widely in the field of spintronics due to their potential applications. Much attention has been paid to the study of Cr doped II–VI systems of ferromagnetic materials with a high Curie temperature [5]. HMF is also found in magnetic Heusler compounds such as NiMnSb [6] and various HM ferromagnets have been predicted theoretically, while a number of them such as CoMnSb and CoVSb, have been verified experimentally [7]. Wide-band DMSs such as GaMnN and ZnMnO having Curie temperature above room temperature were predicted by Dietl et al. [8]. There are, however, several HMF whose Curie temperature is relatively low ($T_c < 160$ K) and it is highly desirable to investigate these new HMF materials, which are suitable for their application above room temperature and are compatible with II–VI semiconductors [9]. The studies so far indicate that most of the DMSs either cannot obtain ferromagnetism or they have very low Curie temperature; this is the reason that, presently, intensive research studies are being undertaken to understand the ferromagnetic mechanism and for searching high T_c ferromagnetism in DMSs [10]. Also doped II–VI transition metals crystals are of particular interest due to the possibility of their use as optical limiters and nonlinear absorber for passive laser modulation [11,12].

Recently, Fe, Co and Ni based wide-band gaps HM diluted magnetic semiconductors such as $Zn_{1-x}Fe_xO$ [13], $Zn_{1-x}Fe_xS$ ($0.05 < x < 0.26$) [2,14], ZnFeS thin film [3], $Zn_{1-x}Fe_xS$ ($0.18 < x < 0.40$) [15], $Zn_{1-x}Co_xS$ [16–23], ZnO:Ni [24], ZnS:Ni [25] have become the burning spot of scientific research, and it is reasonably hoped that some HM ferromagnetism will be attained when ZnS semiconductors are doped with some of 3*d* transition metals. To the best of our knowledge, no theoretical investigation so far has been reported that is based on ZnS compounds doped with Fe, Co and Ni. ZnS occurs in cubic ZB and hexagonal wurtzite (in tetrahedral bonded Zn^{2+}) structure and has a band gap of 3.7 eV (cubic phase) at room temperature. It can be used as light emitting diode in the blue to UV spectral region, as a reflector due to high refractive index and it is

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doi:10.1016/j.jallcom.2010.08.079

appropriate material as a dielectric filter for applications because of high transmittance in the visible range [15]. In this paper, we have attempted to do a comprehensive study of the structural, electronic and magnetic properties of TM compounds based on ZB-ZnS semiconductors. To the best of our knowledge, there are no previous experimental and theoretical data available to compare these properties for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) at $x = 0.25$. The knowledge of electronic and magnetic properties of these crystalline alloys may give insight related to their performance in field of spintronics application.

2. Computational details

First principles calculations for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) at $x = 0.25$ are performed using the full potential linearized augmented plane wave plus local orbitals (FP-LAPW + lo) method based on spin-polarized density functional theory (SDFT), as implemented in the Wien2k code [26] which has proven to be one of the accurate methods [27,28] for the computation of the electronic structure of solids within a framework of density functional theory (DFT). We used the new generalized gradient approximation as presented by Wu and Cohen for the exchange-correlation potential [29]. Relativistic effects are taken into account for the core states and the scalar approximation is used for the valence electrons by neglecting the spin–orbit (SO) coupling because it has a little affect on the ferromagnetism of the system [30]. Also, from the two different spin-up and spin-down densities, spin-polarized calculations are performed and two sets of Kohn-Sham single particle equations are solved self consistently. In these calculations, FP-LAPW + lo basis set consists of $3d^{10}$, $4s^2$ states of Zn, $3d^6$, $4s^2$ of Fe, $3d^7$, $4s^2$ of Co, $3d^8$, $4s^2$ of Ni and $3S^2$, $3p^4$ states of S.

The unit cell is divided into two regions, the spherical harmonic expansion is used inside the non-overlapping spheres of muffin-tin radius (R_{MT}) and the plane wave basis set is chosen in the interstitial region (IR) of the unit cell. The R_{MT} for Zn, Fe, Co, Ni and S are chosen in such a way that the spheres do not overlap. In order to get the total energy convergence, the basis function in the IR is expanded up to $R_{mt} \times K_{max} = 8.0$ (where K_{max} is the plane wave cut-off and R_{mt} is the smallest of all MT sphere radii) and inside the atomic spheres for the wave function the maximum value of l is taken as l_{max} 0, while the charge density is Fourier expanded up to $G_{max} = 24$. We use 72 **k**-points in the irreducible Brillouin zone for our calculations. The stability of ferromagnetic state is also determined by the total energy difference between the antiferromagnetic (AFM) and ferromagnetic (FM) state ($\Delta E = E_{AFM} - E_{FM}$) of the supercell ($1 \times 1 \times 2$) in order to get even number of TM element for switching spin state up and down. If ΔE is positive then FM state is stable and if ΔE turns outs to be negative, the AFM state is more stable.

Table 1
Calculated lattice constants a_0 (Å), bulk modulus B_0 (GPa), derivative of bulk modulus B', total energy difference ΔE (meV) and cohesive energy ΔE_{coh} (eV) for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$.

Compound	a_0	B_0	B'	ΔE	ΔE_{coh}
ZnS	5.403, 5.410[a]	81.5, 78[b]	4.5	–	6.31, 6.33[b]
$Zn_{0.75}Fe_{0.25}S$	5.33	81.136	4.321	5.4	7.03
$Zn_{0.75}Co_{0.25}S$	5.25	85.343	4.176	8.5	7.25
$Zn_{0.75}Ni_{0.25}S$	5.21	88.282	4.045	9.8	7.41

[a] Ref. [34].
[b] Ref. [35].

3. Results and discussion

3.1. Structural properties

In order to study the structural properties of bulk $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni), first we calculate the total energy as a function of the cell volume for both FM and AFM states. The equilibrium lattice constant a_0, bulk modulus B, the derivative of the bulk modulus B', total energy difference ΔE between the FM and the AFM states and cohesive energies for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) are listed in Table 1. These results have been obtained by fitting the calculated total energies to the Birch equation of state [31]. It is found that for every TM concentration, the FM state is lower in energy than the AFM state, which indicates that the FM state is more stable than the AFM state. The cohesive energies of these compounds are also calculated from the difference between the total atomic energies of Zn, Fe, Co, Ni and S atoms and the minimum energy of bulk compounds, which are also displayed in Table 1. It is observed that the cohesive energy of ZnS is less than that of the ternary compounds

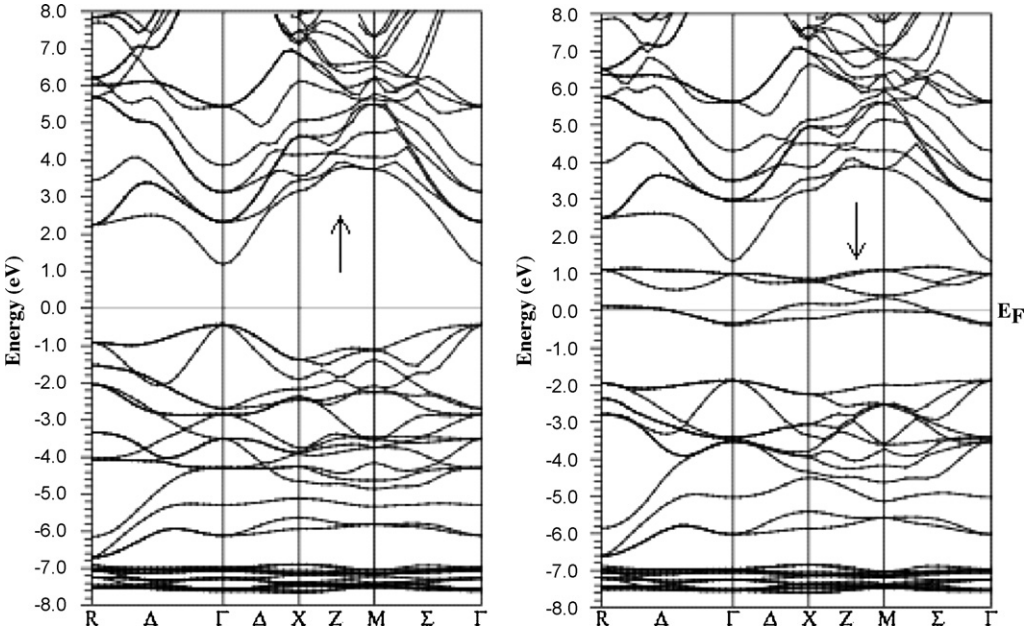

Fig. 1. Calculated spin-polarized band structures for $Zn_{0.75}Fe_{0.25}S$.

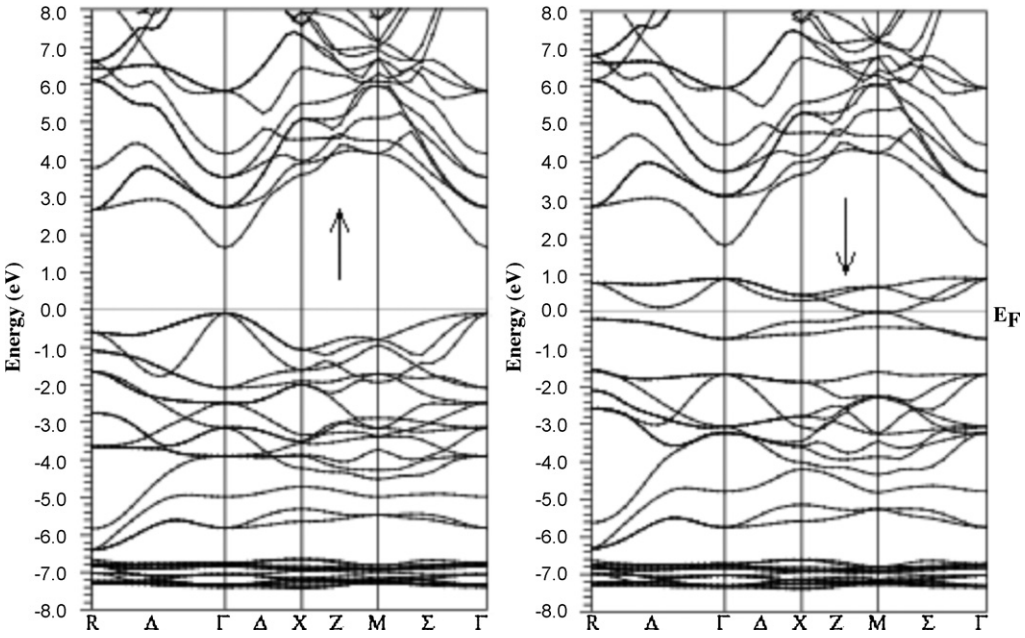

Fig. 2. Calculated spin-polarized band structures for $Zn_{0.75}Co_{0.25}S$.

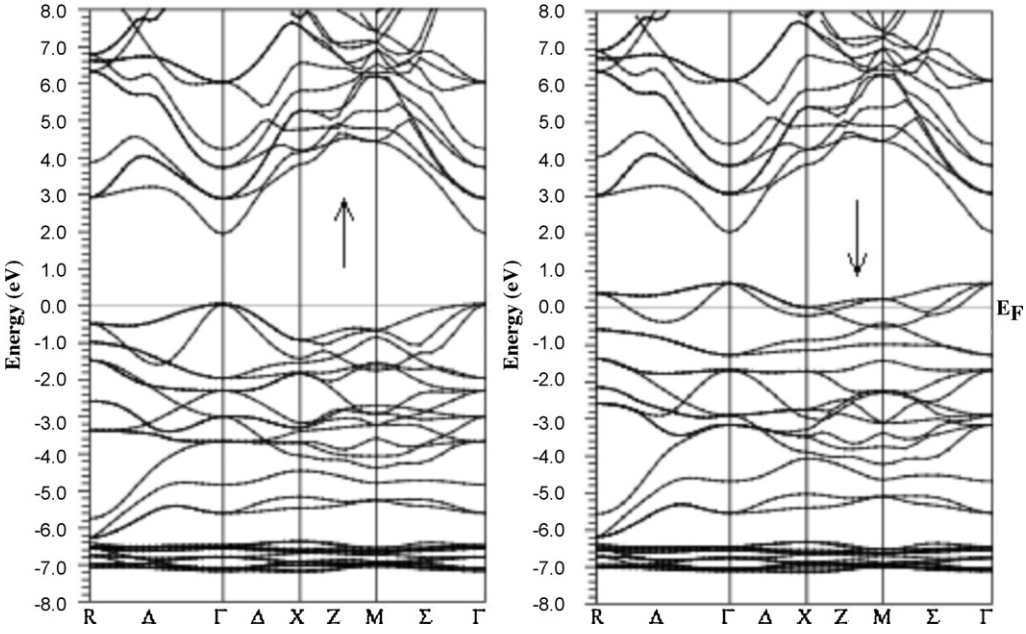

Fig. 3. Calculated spin-polarized band structures for $Zn_{0.75}Ni_{0.25}S$.

$Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$. As already explained in [32,33], this difference in the value of cohesive energy can be attributed to lower the spin-polarized energy ΔE_{SP} that can occur when a free atom having localized orbitals is transferred to the solid that obviously have less localized orbitals, and by the effect of 3*d* electrons of transition-metal atoms.

3.2. Electronic band structure and density of states

The spin-polarized electronic band structures of $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ for spin-up (majority-spin) and spin-down (minority-spin) configurations are shown in Figs. 1–3, respectively along the high symmetry directions in the first Brillouin zone. The Co doping generates only five majority-spin *d* states in the semiconductors $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ band gaps. When the Fermi level is operating through the impurity band, the $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ alloys are half metallic. Figs. 1–3 show that each of these compounds has a direct band gap at the Γ- point. The calculated energy band gap, $E_g^{\Gamma-\Gamma}$, values for spin-up structures are listed in Table 2. The half-metallic gap (G_{HM}) is calculated as the difference between

Table 2
Calculated direct band gaps $E_g^{\Gamma-\Gamma}$ (eV) and half-metallic gaps G_{HM} (*eV*) for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$.

Compound	$E_g^{\Gamma-\Gamma}$	G_{HM}
$Zn_{0.75}Fe_{0.25}S$	1.58	0.4
$Zn_{0.75}Co_{0.25}S$	1.63	0.1
$Zn_{0.75}Ni_{0.25}S$	1.85	0.0

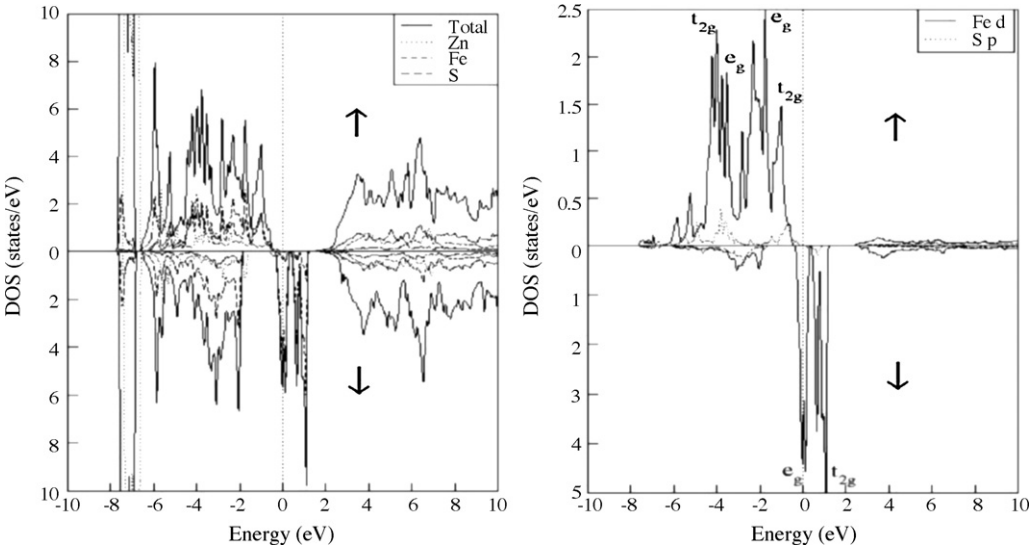

Fig. 4. Spin-dependent total and partial density of states for $Zn_{0.75}Fe_{0.25}S$ projected on three atoms.

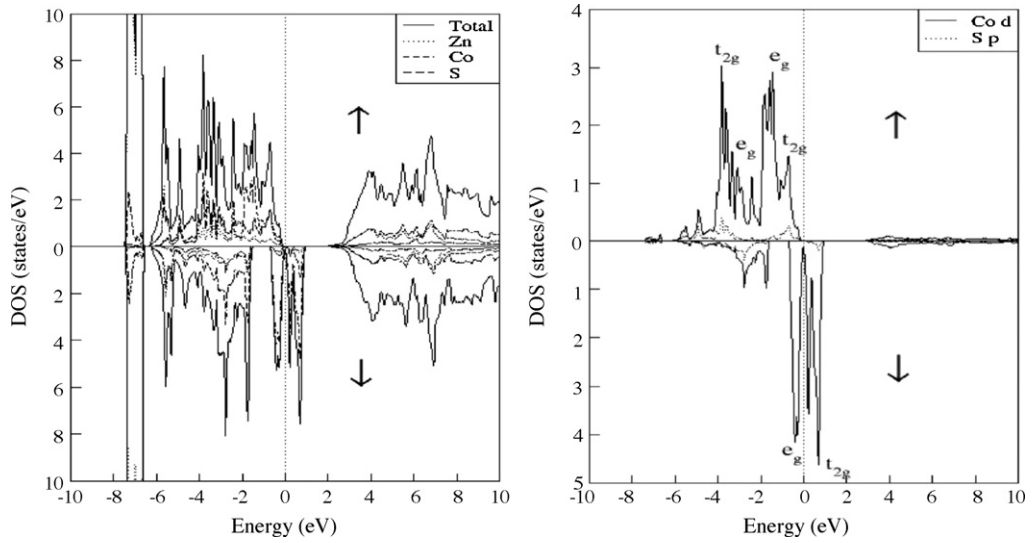

Fig. 5. Spin-dependent total and partial density of states for $Zn_{0.75}Co_{0.25}S$ projected on three atoms.

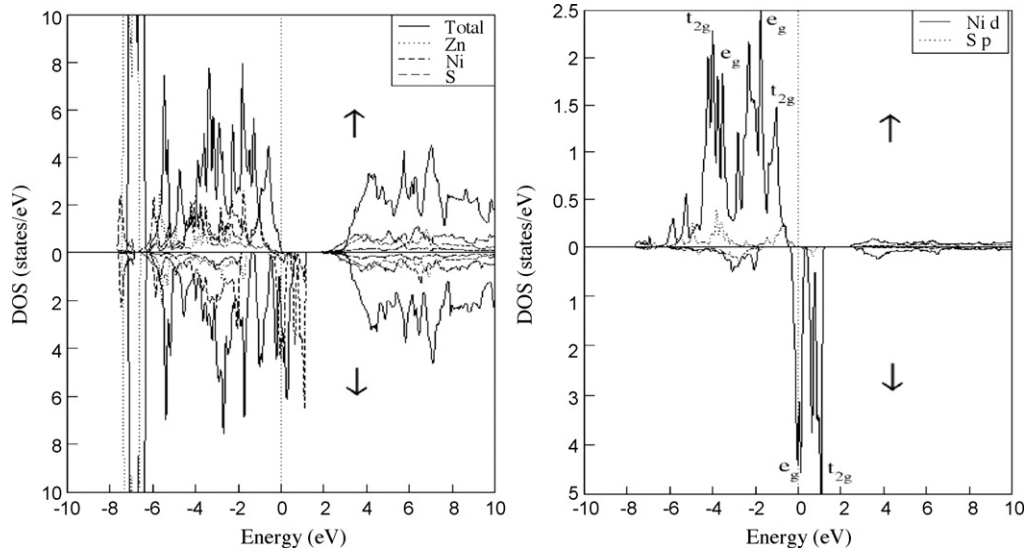

Fig. 6. Spin-dependent total and partial density of states for $Zn_{0.75}Ni_{0.25}S$ projected on three atoms.

Table 3
Calculated total magnetic moments M^{Tot} (μ_B) and the local magnetic moments m (μ_B) of several sites for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$.

Site	$Zn_{0.75}Fe_{0.25}S$	$Zn_{0.75}Co_{0.25}S$	$Zn_{0.75}Ni_{0.25}S$
M^{Tot}	4.000	3.000	2.000
m^{Fe}	3.23917	–	–
m^{Co}	–	2.20072	–
m^{Ni}	–	–	1.22587
m^{Zn}	0.02580	0.02394	0.02142
m^{S}	0.027726	0.09906	0.011514
$m^{interstitial}$	0.37476	0.33153	0.24952

the minimum energy point of the conduction band and maximum energy point of the valence band near the Fermi level for both the spin-up and spin-down cases and then taking the smaller of the two values. The values of G_{HM} for $Zn_{0.75}Fe_{0.25}S$ and $Zn_{0.75}Co_{0.25}S$ are 0.4 eV and 0.1 eV, respectively.

After substitution into a cation site, the degenerate Fe, Co and Ni 3*d* states split into the triply degenerate *p*–*d* bonding t_{2g} states and doubly degenerate non-bonding e_g states. The triply degenerate t_{2g} and doubly degenerate e_g states are separated due to strong *p*–*d* exchange interaction between Co *d* and anion *p* orbitals. We discuss only the spin-up band structures which have a large number of electrons. The bands in the range −7.51 to −4.53 eV for $Zn_{0.75}Fe_{0.25}S$, −7.45 to −4.42 eV for $Zn_{0.75}Co_{0.25}S$ and −7.32 to −4.23 eV for $Zn_{0.75}Ni_{0.25}S$ generally arise from Zn 3*d* states with a small contribution of S 3*s* states. The bands near the Fermi level mostly appear due to the Fe, Co and Ni 3*d* orbitals with a little contribution of anion *p* state. The conduction band of the spin-up electrons is totally dominated by S *p* state, while for the spin-down case conduction band crosses the Fermi level leading to the HM ferromagnetism.

In order to understand the effect of atomic relaxation on the electronic band structure, we calculate the total and partial density of states (DOS) for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) as shown in Figs. 4–6. The results of DOS show that these compounds exhibit HM behavior, which is semiconducting for the majority-spin and metallic for the minority-spin. It is seen that the upper part of the valence band has TM 3*d* and S *p* character that is different for majority-spin and minority-spin around the Fermi level. While the valence band of the spin-up band structure in the range −2.1 to 5.89 eV is mostly composed of S electrons, ferromagnetism is induced due to the exchange-splitting of S *p* and TM 3*d* hybridized bands,. For all the doped systems under study, the spin-up *d* bands are occupied for all TM (TM = Fe, Co, Ni), whereas the spin-down states are unoccupied. This trend is generally observed in most of the magnetic semiconductors [4,36]. Moreover, the exchange-splitting (∼.73, 2.08 and 1.86 eV for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$, respectively) between the spin-up and spin-down TM 3*d* states is larger than their respective crystal field splitting $\Delta E_{crystal} \equiv E_{t_{2g}} - E_{e_g}$ (∼1.85 1.54and 1.21 eV). We have also calculated the spin-exchange-splitting energy $\Delta_x(d)$, which is defined as the separation between the corresponding majority-spin and minority-spin peaks. The values of $\Delta_x(d)$ are 4.62, 4.45 and 4.23 eV for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$, respectively.

3.3. Magnetic properties and exchange constants

The calculated total and local magnetic moments per TM atom within the muffin-tin spheres as well as in the interstitial sites for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) are given in Table 3. Because of unoccupied TM 3*d* states, permanent local magnetic moments are produced in these materials and it is found that the TM magnetic moment decreases in going from Fe to Ni. The results show that the total magnetic moments generally come from the TM ions with a small contribution of Zn and S sites whose magnetic moments are parallel to the TM ions; this may be understood as the tunneling of spin-up impurity states into the neighboring atoms. It can be seen (Figs. 4-6) that there is hybridization between the anion *p* states and the TM 3*d* states and this *p*–*d* hybridization reduces the total magnetic moments of the TM atoms from its free space charge value and produces small local magnetic moments on the non-magnetic Zn and S sites.

Table 4
Calculated conduction and valance band-edge spin-splittings ΔE^c and ΔE^v and exchange constants for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$.

Compounds	ΔE^v	ΔE^c	$N_0\alpha$	$N_0\beta$
$Zn_{0.75}Fe_{0.25}S$	−0.27318	−3.8532	−3.8532	−0.2732
$Zn_{0.75}Co_{0.25}S$	−0.26513	−3.7324	−4.9765	−0.3535
$Zn_{0.75}Ni_{0.25}S$	−0.25314	−2.8456	−5.6912	−0.5063

The significant parameters which are computed from the magnetic properties of DMSs are the *s*–*d* exchange constant $N_0\alpha$ and the *p*–*d* exchange constant $N_0\beta$ where N_0 denotes the concentration of cations. $N_0\alpha$ describes the exchange interactions between the conduction electron carriers and the TM spin, whereas $N_0\beta$ is due to the exchange interaction between the holes and the TM *d* states. From the conduction and valence band edges the exchange constants can be calculated as given in Ref. [37] and the calculated values of $N_0\alpha$ and $N_0\beta$ for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ are displayed in Table 4. We find that $N_0\alpha$ is much smaller than $N_0\beta$, which means that the interaction between the cation *s* and the TM *d* states at the conduction band minimum is much weaker than the *p*–*d* interaction at the valence band maximum; this result indicates ferromagnetic behavior of these materials.

3.4. Robustness

It is important to investigate the robustness of half-metallicity with respect to the variation of lattice constants for spintronic device applications. Fig. 7 shows the total magnetic moments for $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) as a function of the lattice constants. It is found that the total magnetic moment for all the above compounds remains an integer with the change of lattice constants until they are compressed to the critical values of 5.0102, 5.04 and 5.1058 Å for $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$, respectively. The half-metallicity of $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ is, therefore, maintained up to the reduction of the lattice constants by 6%, 4% and 2%, respectively.

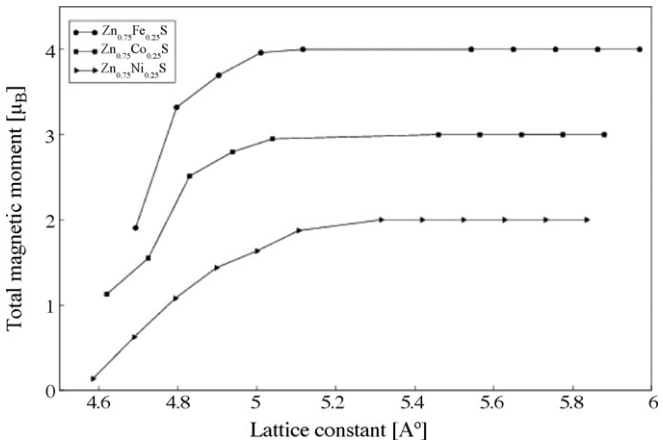

Fig. 7. Total magnetic moments as a function of lattice constant for $Zn_{1-x}TM_xS$ (TM = Fe, Co, Ni) at $x = 0.25$.

4. Conclusions

In the present study, we have performed the first principles calculations of structural, electronic and magnetic properties of $Zn_{1-x}TM_xS$ (TM = Fe, Co and Ni) at $x = 0.25$ by using FP-LAPW + lo method based on spin-polarized density functional theory (SDFT). Structural parameters have been computed and it is shown that the cohesive energy of $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ is greater than ZnS – a result which can originate from the TM 3*d* states and from the loss of spin-polarized energy. Ferromagnetic state is found to be more favorable in energy than the antiferromagnetic state. The results of electronic band structures and density of states for these compounds reveal that they are HM ferromagnets, while the half-metallicity is robust with respect to lattice contraction and is maintained up to compression of the lattice constants of $Zn_{0.75}Fe_{0.25}S$, $Zn_{0.75}Co_{0.25}S$ and $Zn_{0.75}Ni_{0.25}S$ by 6%, 4% and 2%, respectively. Additionally, values of the exchange-splitting energies, crystal field splitting, exchange constants $N_0\alpha$ and $N_0\beta$ have been calculated and the total magnetic moments of these DMSs analyzed. It is also found that *p*–*d* hybridization of TM 3*d* (t_{2g}) and S*p* states reduced the magnetic moments of TM ions from its free space charge value and produced the local magnetic moments on the non-magnetic Zn and S sites.

Acknowledgements

For A. H. Reshak and Y. Saeed the work was supported from the institutional research concept of the Institute of Physical Biology, UFB (No. MSM6007665808), the Program RDI of the Czech Republic, the project CENAKVA (No. CZ.1.05/2.1.00/01.0024), grant no. 152/2010/Z of the Grant Agency of the University of South Bohemia. The Institute of Nano Electronic Engineering, University Malaysia Perlis, 01000 Kangar, Perlis, Malaysia.

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