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Half-metallic ferromagnetism in $Cd_{1-x}TM_xSe$ (TM = Cr, V and Mn) semiconductors

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Abstract

Electronic structures and magnetic properties of transition-metal-doped ternary systems based on zinc-blende CdSe compound are systematically explored using first-principles full-potential lineralized augmented plane-wave method. From the analysis of the spin-dependent density of states, band structure and magnetic moments, half-metallic ferromagnetism is obtained in the Cr- and V-doped systems with an integer value of $3\mu_B$ and $4\mu_B$ per unit cell for μ/x ratio, whereas Mn-doped systems show magnetic semiconducting character with a magnetic moment $5\mu_B$ per unit cell. Half-metallic ferromagnetism comes mainly from spin-polarization of electrons in TM-d orbitals. It is also noted that the half-metallic gaps are increased with increasing TM (TM = Cr, V and Mn) concentrations, which make these materials possible candidates for spin injection in spintronic devices.

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Keywords: Electronic structure; Half-metallic ferromagnetism; First-principles calculation

Ferromagnetic magnetic semiconductors have attracted great interest from researchers due to their potential applications in the field of spintronics [1–6]. In ferromagnetic semiconductors spins can be switched in addition to charges, allowing magnetic or electric control over transport properties. One method of making a semiconductor magnetic is to dope it with 3d transitional metals (TM). So far, most of the works have focused on (Ga, Mn)As or (In, Mn)As semiconductors [7], with transition temperatures up to 160 K. However, the solubility of 3d transition metals in III–V semiconductors is so low (<7–8%) that high Curie temperatures seem to be difficult to realize with current synthesis techniques. On the other hand, although the Curie temperatures are dramatically low in the II–VI semiconductors, the large solubility of 3d elements in them [8] and the opportunity to independently control the localized spin makes them particularly attractive for fundamental studies and also as magneto-optical materials [9–11]. Therefore, it is highly desirable to explore new half-metallic (HM) ferromagnetic materials, which are compatible with important II–VI semiconductors. To our knowledge, the most published *ab initio* studies performed for TM-doped II–VI compounds have been focused on the research of new ferromagnetic semiconductors having high T_C [12–14], such as Zn-, Co-, Fe-, Cr, V-, Mn-doped compounds based on BeTe and ZnSe, and CdTe-doped with Cr, V, and Mn, as well as ZnO-based DMS doped with Fe, Co, and Ni. However, no investigations have been reported concerned as CdSe compounds doped with V, Cr, and Mn. In this paper we aim to give a detailed description of the electronic and magnetic properties using density-functional calculation. It is reasonably hoped that some HM ferromagnetism will be achieved when CdSe semiconductor are doped with some of 3d transitional metals.

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In this paper, the doped ternary $Cd_{1-x}TM_xSe$ (TM = Cr, V, Mn) systems in ZB structure, where x takes values of 0.25, 0.5, and 0.75 to simulate doped from 0.0 to 1.0, have been investigated systematically using first-principles functional calculation. In order to find the ground state properties of $Cd_{1-x}TM_xSe$ (M = Cr, V, Mn) systems, we compute the total energies as a function of the volume per formula unit and fit them with the empirical Murnaghan equation of state. The obtained equilibrium lattice constant, the magnetic moments, and the band gap of the ferromagnetic $Cd_{1-x}TM_xSe$ (M = Cr, V, Mn) systems are listed in Table 1. Note that consistent with the integer value for the total magnetic moment, half-metallicity is obtained for Cr- and V-doped systems, whereas the Mn-doped systems are semiconductor. Compared to the parent compound CdSe, we also find that the equilibrium lattice for Cr- and V-doped systems increases with the TM concentration, whereas decreases for Mn-doped system.

Computations are performed with the all-electron full-potential linearized augmented plane wave method [15] within the framework of density-functional theory [16], where the potential and charge density are treated with no shape approximation. The relativistic effect is taken into account in the scalar style, but the spin–orbital coupling was neglected because it has little effect on the main results. The muffin-tin sphere radii R used are both 2.2 a.u. and 2.0 a.u. for TM (Cd) and Se, respectively. An angular momentum expansion up to $l_{max} = 10$ for the potential and charge density representations is used in the calculations. The Brillouin-zone integration is done with a modified tetrahedron method [17] and we use 1000 k-points in the first irreducible Brillouin zone. The density plane-wave cutoff is $RK_{max} = 8.0$. The self-consistency is better than 10^{-4} e/a.u.^{3} for charge density and spin density, and the stability is better than 10^{-5} Ry for the total energy per formula unit.

As a representative for all doped ternary systems, due to the similarity of the electronic structure of $Cd_xTM_{1-x}Se$ (TM = Cr, V, Mn), we mainly focus on the computational band structure of the doped ternary $Cd_{0.75}TM_{0.25}Se$ (TM = Cr, V, Mn) systems at its optimized equilibrium lattice constant. Figs. 1–3 present the band structures corresponding to spin-up (left panel) and spin-down (right panel) alignments for each compound. It is clear that the bottom of the conduction bands and the top of the valence bands at Γ point in the Brillouin zone is similar with ones in parent binary CdSe. Due to the exchange splitting and the hybridization of p–d, the doped effects of TM lead to the increase in energy for the majority-spin bands, resulting in the conducting band, whereas the decrease in energy for

Table 1
The calculated equilibrium lattice constant, band gap, magnetic moment (μ_B) per unit cell and per TM atom in the TM-doped $Cd_{1-x}TM_xSe$ (TM = Cr, V and Mn) systems

Compound	a (Å)	μ (tot)	μ/x	μ (TM)	μ (Cd)	μ (Se)	Band gap
$Cd_{0.75}Cr_{0.25}Se$	6.1571	1	4	3.55	0.01	−0.05	0.39
$Cd_{0.5}Cr_{0.5}Se$	5.9776	2	4	3.75	0.02	−0.17	0.42
$Cd_{0.25}Cr_{0.75}Se$	5.9975	3	4	3.52	0.03	−0.10	0.58
$Cd_{0.75}V_{0.25}Se$	6.1629	0.75	3	2.44	0.01	−0.04	0.44
$Cd_{0.5}V_{0.5}Se$	5.9429	1.5	3	2.90	0.03	−0.16	0.46
$Cd_{0.25}V_{0.75}Se$	5.8573	2.25	3	2.42	0.04	−0.07	0.58
$Cd_{0.75}Mn_{0.25}Se$	6.1724	1.25	5	4.28	0.01	0.03	0.11
$Cd_{0.5}Mn_{0.5}Se$	6.2253	2.5	5	4.34	0.03	0.06	0.14
$Cd_{0.25}Mn_{0.75}Se$	6.3282	3.75	5	4.67	0.01	0.01	0.19

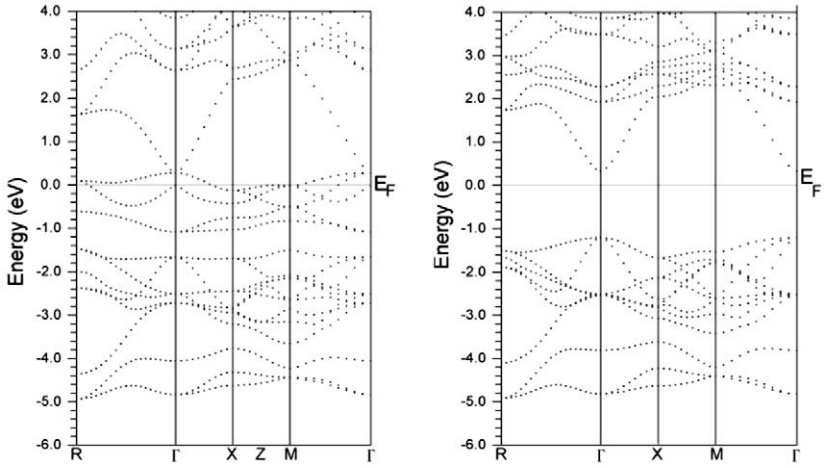

Fig. 1. Spin-dependent band structure of $Cd_{0.75}Cr_{0.25}Se$. The left and right panels are spin-up and spin-down components, respectively.