บทความวิจัย

การศึกษาอิทธิพลของการเจือโลหะทรานซิชันในสารกึ่งตัวนำเจอร์เมเนียมเทลลูไรด์เพื่อการประยุกต์ทางสปินทรอนิกส์ด้วยทฤษฎีฟังก์ชันนอลความหนาแน่น

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บทคัดย่อ

สมบัติทางโครงสร้าง อิเล็กทรอนิคและแม่เหล็กของสารกึ่งตัวนำเจอร์เมเนียมเทลลูไรด์ที่เจือด้วยโลหะทรานซิชันได้รับการศึกษาโดยวิธีทฤษฎีฟังก์ชันนอลความหนาแน่น จากการคำนวณพลังงานก่อเกิด (Ge, Cr)Te มีสภาพเสถียรที่สุด เมื่อเจือโลหะทรานซิชันทำให้ค่าคงที่แลชทิชและปริมาตรลดลง สมบัติทางแม่เหล็กเกิดจากโลหะทรานซิชัน เทลลูเรียม และเจอร์เมเนียม ตามลำดับ โดยสมบัติทางแม่เหล็กเกิดจากไฮบริไดเซชันแบบพี-ดีเอ็กเชงค์ (Ge, Mn)Te เป็นสารกึ่งตัวนำที่มีช่องว่างพลังงานลดลง เมื่อเจือ Co Ni และ Cu เข้าไปทำให้สารเหล่านี้เป็นโลหะ เมื่อเจือ V Cr และ Fe เข้าไปทำให้สารเหล่านี้มีสภาพครึ่งโลหะสุดท้าย งานวิจัยนี้ให้ความเข้าใจเกี่ยวกับผลกระทบของการเจือโลหะทรานซิชันเพื่อการประยุกต์ทางสปินทรอนิกส์

คำสำคัญ: ความเป็นแม่เหล็ก โลหะทรานซิชัน เจอร์เมเนียมเทลลูไรด์ การคำนวณฟังก์ชันนอลความหนาแน่น

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Research Article

Insight into the role of transition metals doping in GeTe for spintronic application: Spin density functional study

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Abstract

The structural, electronic and magnetic properties of GeTe semiconductors doped with several transition metals are determined by the spin density functional theory. Due to the formation energies, (Ge, Cr)Te is the most stable among all doped systems. The incorporation of transition metals convinces the reduction of lattice parameters and volumes. The total magnetization is mainly contributed from transition metal, Te and Ge atoms, respectively. The p-d exchange hybridization gives rise to the magnetism. (Ge, Mn)Te is the semiconductor with a reduced band gap. Co, Ni and Cu impurities convert semiconductor to metal. Possibility of p-type half metallicity in V-, Cr- and Fe-substituted GeTe is achieved. Finally, the theoretical work delivers the valuable clues for improving the understanding of transition-metal doping impacts and sheds some light on the exploration of spintronic materials based on transition-metal doped GeTe.

Keywords: Magnetism, transition metal, GeTe, density functional calculations

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Introduction

Diluted magnetic semiconductors have been investigated in the recent years because of their outstanding prospective in the spintronic applications (Dietl, 2007; Dietl, 2007; Ohno et al., 2002; Wolf et al., 2006). For the utilization in the spintronic applications, it is highly necessary to find new half-metallic materials well-suited with semiconductors (Dietl et al., 2014). This efficiency is triggered by the mixture of semiconductor band gap manipulation and tunable magnetic properties into a single semiconductor system. At the moment, there are three main groups of diluted magnetic semiconductors such as II-VI, III-V and IV-VI semiconductor group. II-VI and III-V semiconductor groups have been in an expansive focus of the interest, while so far less discovered materials are IV-VI compounds. Since the introduction of manganese (Mn) in the GeTe host successfully transformed it into the dilute magnetic semiconductor (Rodot et al., 1966; Cochrane et al., 1974). GeTe semiconductors doped with 3d transition metals have been paid the substantial attention in term of theoretical and experimental viewpoints. In term of theoretical study, Zhao et al. (2006) implemented the density functional method to investigate various ternary transition-metal GeTe semiconductors in rock-salt phase. The half-metallic ferromagnetic performance was found in Cr- and V-substituted GeTe compounds. (Ciucivara et al. (2007) determined the magnetization of the Mn and hole densities using GGA+U technique. The total magnetization approximately increased up to x of 0.5 and then dropped beyond that. The magnetic properties of GeTe in both rock-salt and zinc-blende phase doped with V, Cr, and Mn were conveyed using density functional study by Liu et al. (2012) Some of the studied compounds were half metallic. Aside from the theoretical study, there is a large body of experimental research. For example, Fukuma et al. (2007) fabricated the $Ge_{1-x}Cr_xTe$ ferromagnetic semiconductor with Curie temperature close to 180 K using molecular-beam epitaxy. J. D. Liu et al. (Liu et al., 2013) studied the magnetic and transport performances of $Ge_{0.98}Fe_{0.02}Te$ thin film. The relatively high Curie temperature with 160 K was obtained. For Mn doping in GeTe semiconductor, there have been various experimental works. Fukuma et al. (2008) tried to grow the $Ge_{1-x}Mn_xTe$ diluted magnetic semiconductor by means of molecular beam epitaxy. The ferromagnetic order and Curie temperature of 100 K were gained. Zvereva et al. (2010) investigated the magnetic properties and electron spin resonance of $Ge_{1-x}Mn_xTe$ diluted magnetic semiconductors with x ranging from 0.07 to 0.44. The Curie temperatures were amplified with increasing Mn contents with the high value of 90 K. Exhausting the molecular beam epitaxy, $Ge_{1-x}Mn_xTe$ with Mn content ($x\approx0.5$) was grown by Lechner et al. (2010) The phase separation was induced. Lim et al. (2011) and Lim et al. (2011) presented the magnetotransport studies of $Ge_{1-x}Mn_xTe$ ferromagnetic semiconductor in the presence of the hydrostatic pressures. The natural properties of $Ge_{1-x}Mn_xTe$ ferromagnetic semiconductor were mainly sensitive with the applied pressures.

All of the above-mentioned studies activate my interests to explore for more transition metals doping in GeTe semiconductors, especially in the hardly studied transition metal cases. In view of the large body of obtainable experimental work, we embark on a systematic theoretical study of the GeTe semiconductors doped with several transition metals (V, Cr, Mn, Fe, Co, Ni and Cu) in order to discover the emergence of half-metallic behavior. Utilizing the generalized gradient approximation (GGA) with exchange functional proposed by the Perdew, Burke and Ernzerhof (PBE) (Perdew et al., 1996) in the CASTEP package (Clark et al., 2005; Segall et al., 2002), these atomistic properties of GeTe semiconductors doped with different transition metals are declared and analyzed. The remaining part of this manuscript is outlined as follows. In Section 2, we concisely describe the structures and elucidate the first-principle calculations. The main results of each configuration including the lattice parameters, volumes, formation energies, band gaps, magnetizations, electronic band structures, density of states and partial density of states are presented in Section 3. The mechanism for the half metallic emergence in these compounds is analyzed. These calculations open the gate for further utilization of these materials for the spintronic applications. Finally, a conclusion is successfully presented.

Theory and Methodology

The observed structural, electronic and magnetic properties of GeTe semiconductors doped with several transition metals are discussed in the theoretical context. This scenario is determined by the spin density functional theory with the help of CASTEP package for all calculations. In this manuscript, the exchange-correlation potentials are utilized under the generalized gradient approximation (GGA) proposed by Perdew et al. (1996) The extension of the plane wave function basis up to 520 eV is used throughout these calculations. Using MonkhorstePack method, the Brillouin zone incorporation is performed over the $4\times4\times4$ grid. GeTe crystallizes in rock-salt phase at the equilibrium condition. (Fukuma et al., 2007; Fukuma et al., 2008; Fukuma et al., 2001) Hence, rock-salt GeTe semiconductor with a space group of $Fm\bar{3}m$ is a modelling structure. Taking all these parameters into the consideration, the calculations of bulk GeTe semiconductor are used to primarily verify the precision of the computational method. The lattice constant of GeTe is 6.009 Å which agrees well with the literatures (6.016 Å (Liu et al., 2016), 5.996 Å (Tung et al., 1969), 5.862 Å (Okoye, 2002), 5.995 Å (Okoye, 2002) and 5.996 Å (Seddon et al., 1976)). In addition, the band gap of GeTe with 0.346 eV consents with the previous data (0.23 eV (Lewis, 1973), 0.20 eV (Chang et al., 1966; Tsu et al., 1968), 0.244 eV (Okoye, 2002) and 0.201 eV (Okoye, 2002)). Consequently, this employed technique is appropriate to further study the electronic and magnetic properties of GeTe semiconductor with Ge replacement by transition metals like V, Cr, Mn, Fe, Co, Ni and Cu. For the inquiries, the substitutional method is used to define the doped systems. A $2\times1\times1$ pure GeTe supercell containing 16 atoms is generated as exemplified in Figure 1. Latter, one of Ge atoms in the supercell is substituted by transition metal to set the transition-metal doped GeTe. All transition-metal doped GeTe are fully minimized by the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm (Broyden, 1970; Fletcher, 1970; Goldfarb, 1970; Shanno, 1970). The convergence benchmark of the total energy, maximum force, the maximum stress and maximum displacement are 2.0×10^{-6} eV/atom, 1.0×10^{-5} eV/$\mathring{A}$, 0.05 GPa and 0.001 Å, respectively. For the analysis, the electronic and magnetic properties consisting of lattice parameters, volumes, formation energies, band gaps, magnetizations, spin-polarized band structures, density of states and partial density of states are calculated for the equilibrium lattice parameters. Gaussian smearing technique with a smearing value of 0.1 eV is used to evaluate the total and partial density of states.

Results and discussions

This work systematically presents the results for the structural, electronic and magnetic properties of GeTe doped with several transition metals like V, Cr, Mn, Fe, Co, Ni and Cu from the perspective of spintronics. Here, we shed light on the problem of transition-metal doped GeTe compounds using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange functional. In general, the doping can simultaneously affect the electronic and magnetic properties of the studied materials. First, the formation energies of GeTe with Ge substitution by transition metal are itemized in Table I. The formation energies of GeTe with Ge substitution by transition metals (TM) are calculated from this relation, $E^{f}(TM) = E_{Dope}(TM) - E_{pure} - (\mu_{TM} - \mu_{Ge})$. Here, $E^{f}(TM)$ is the formation energy of GeTe doped with the studied transition metal. $E_{Dope}(TM)$ is the total energy of the doped GeTe and E_{pure} is the total energy of the pure GeTe. μ_{TM} is the chemical potential of transition metal and μ_{Ge} is the chemical potential of Ge atom. The chemical potential (μ) is computed from the free atom energy. For the calculations, the free atom is placed in the center of a very huge empty cubic box with lattice constant of 30 atomic units. As can be seen from the formation energies, (Ge, Cr)Te is the most stable among all doped structures. To perceive the change in the structural properties by different transition metals, Table II lists the lattice parameters and volumes. The incorporation of transition metals causes significant decreases of lattice parameters and volumes. This is due to the fact that radius of host (143 pm) is greater than one of the impurities as itemized

in Table II. In addition, the band gaps of GeTe semiconductors doped with different transition metals are itemized in Table II. Mn doping in GeTe remains a semiconductor with a decreased band gap, whereas the others are metallic. The insight on the magnetic properties is gained by analyzing the magnetic moments of each element as exposed in Table II. The key contributions to the total magnetization are mainly from transition metal, Te and Ge atoms, respectively. The high-to-low net magnetic moments are observed in (Ge, Mn)Te, (Ge, Cr)Te, (Ge, Fe)Te, (Ge, V)Te, (Ge, Co)Te, (Ge, Ni)Te and (Ge, Cu)Te, correspondingly. A schematic diagram of the spin-polarized band structure of pure GeTe semiconductor is illustrated in Figure 2 under different spin channels along the symmetry paths in the irreducible Brillouin zone. The symmetry between the alpha and beta spin channel reflects the semiconducting behaviour. The insight on the effect of the transition metal dopants on the spin-resolved band structures is achieved in Figure 3 computed along the high symmetric paths in the first Brillouin zone. GeTe with the substitution of transition metals demonstrate the spin-polarized band structures, exhibiting the magnetism. (Ge, Mn)Te is categorized as semiconductor. V, Cr and Fe doping in GeTe semiconductor are half metallic. In (Ge, V)Te and (Ge, Cr)Te, alpha spin channel is metal but beta spin channel is semiconductor. In (Ge, Fe)Te, alpha spin channel remains semiconductor but beta spin channel is metal. (Ge, Co)Te, (Ge, Ni)Te and (Ge, Cu)Te are characterized as metal because the Fermi level is crossing through the conduction and valence bands. Hence, V, Cr and Fe doping in GeTe semiconductor are the promising dilute magnetic semiconductors which are appropriate for spintronic applications.

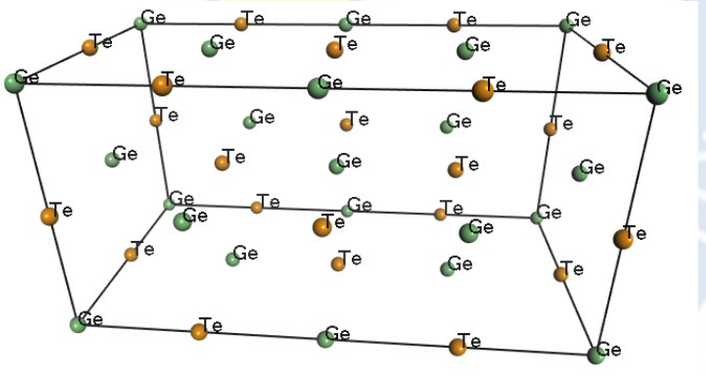

Figure 1: The $2\times1\times1$ GeTe supercell in zinc-blende phase.

Table 1: The formation energies of GeTe with Ge substitution by V, Cr, Mn, Fe, Co, Ni and Cu.

Ge substitute	Formation energy (eV)
(Ge, V)Te	-3.840
(Ge, Cr)Te	-6.481
(Ge, Mn)Te	-3.866
(Ge, Fe)Te	-5.346
(Ge, Co)Te	-3.867
(Ge, Ni)Te	-0.484
(Ge, Cu)Te	1.120

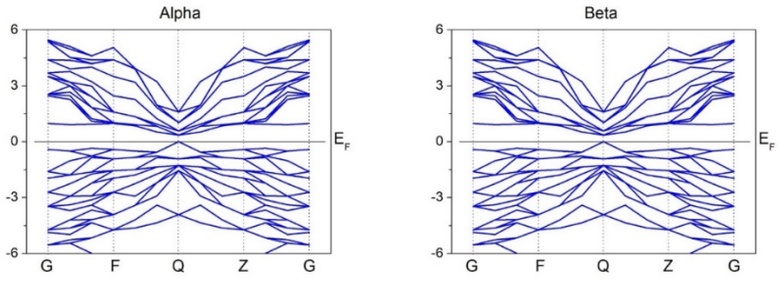

Figure 2: Spin-polarized band structures of GeTe.

Table 2: The calculated lattice parameters, volumes, band gaps and magnetic moments of GeTe with Ge substitution by the transition metals (TM = V, Cr, Mn, Fe, Co, Ni and Cu).

parameters	GeTe	(Ge, V)Te	(Ge, Cr)Te	(Ge, Mn)Te	(Ge, Fe)Te	(Ge, Co)Te	(Ge, Ni)Te	(Ge, Cu)Te
a ($\mathring{A}$)	12.017	11.943	11.938	11.963	11.874	11.854	11.821	11.868
b ($\mathring{A}$)	6.009	5.946	5.947	5.969	5.945	5.925	5.917	5.928
c ($\mathring{A}$)	6.009	5.945	5.947	5.971	5.941	5.921	5.917	5.937
Volume ($\mathring{A}^3$)	433.855	422.135	422.228	426.345	419.405	415.862	413.874	417.651
Radius of the dopant (pm)	-	132	125	124	124	125	125	128
Band gap (eV)	0.346	0.000	0.000	0.143	0.000	0.000	0.000	0.000
$M_{total}(\mu_B)$	0.000	3.741	5.191	5.058	4.051	3.030	2.013	1.007
$M_{Ge}(\mu_B)$	0.000	0.110	0.120	0.020	0.090	0.090	0.070	0.030
$M_{Te}(\mu_B)$	0.000	0.160	0.220	0.020	0.100	0.130	0.150	0.140
$M_{TM}(\mu_B)$	-	3.120	4.450	4.840	3.530	2.250	1.030	0.170

To explore the intrinsic origins of magnetism, it is necessary to understand the orbital contributions localized in these compounds. Here, we shed light on this task by means of total and partial density of states. For the demonstration, the total and partial density of states of undoped GeTe and transition-metal doped GeTe are plotted in Figure 4. The alpha spin and beta spin channel of GeTe are symmetric and display the semiconductor. The conduction bands close up to the band edge are mainly derived from Ge-p states. In the region with the energy greater 2.0 eV, the conduction bands are generated from the couple of Ge-p and Te-p states. The valence bands are mainly initiated from Te-p states. The mixture of Ge-p and Te-p states are also dominated in the valence bands with the energy lower than -2.0 eV. When incorporating GeTe with transition metals, both spin channels are not symmetric. V, Cr, Fe, Co, Ni and Cu induce the d orbital across or nearby the Fermi level. Mn introduces the d orbital close to the conduction band edges, thus responsibility to reduce the band gap. The existence of the exchange hybridization between d states of the transition metal and Te-p states gives rise to the magnetism, called p-d exchange hybridization. Both spin channels of (Ge, Mn)Te are fully occupied, making it the semiconductor with a reduced band gap. (Ge, Co)Te, (Ge, Ni)Te and (Ge, Cu)Te become metallic because both spin channels are partially filled. In (Ge, V)Te and (Ge, Cr)Te, alpha spin channel is partially occupied but beta spin channel is fully occupied. In (Ge, Fe)Te, alpha spin channel remains fully filled but beta spin channel is partly filled. Hence, V, Cr and Fe doping transform the semiconducting to half metallic performance. The hybridization of d states of V, Cr and Fe with Te-p states

provides a gap with spin polarization of 100% at Fermi level. The p-type carrier is additionally demonstrated in V-, Cr- and Fe-doped GeTe semiconductor because of the strong p-d exchange hybridization nearby the Fermi level. Finally, this work demonstrates the numerical results with the aim to provide some theoretical guidance to experimentalists attempting to fabricate the transition-metal doped GeTe materials indeed appropriate for spintronic devices.

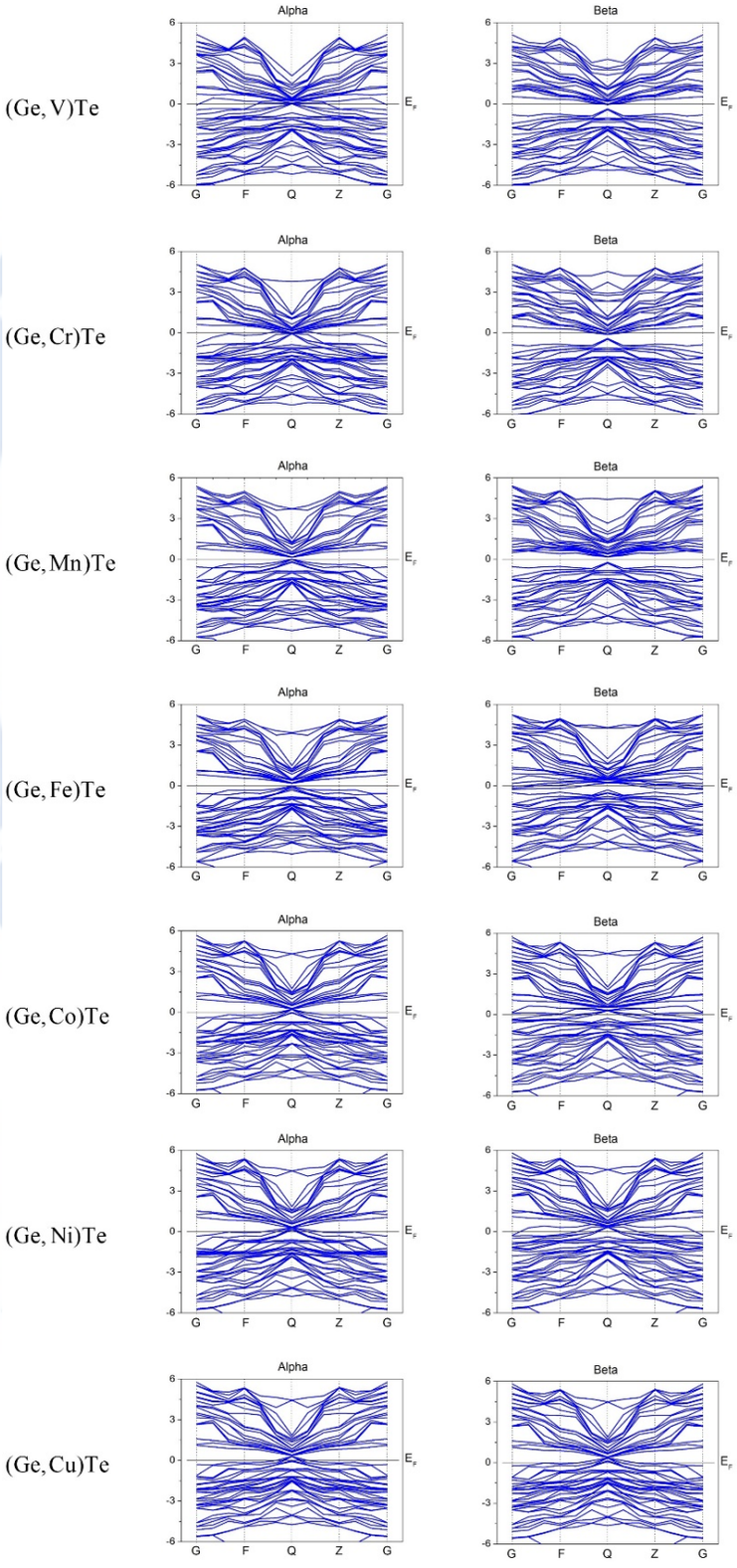

Figure 3: Spin-polarized band structures of (Ge, V)Te, (Ge, Cr)Te, (Ge, Mn)Te, (Ge, Fe)Te, (Ge, Co)Te, (Ge, Ni)Te and (Ge, Cu)Te.

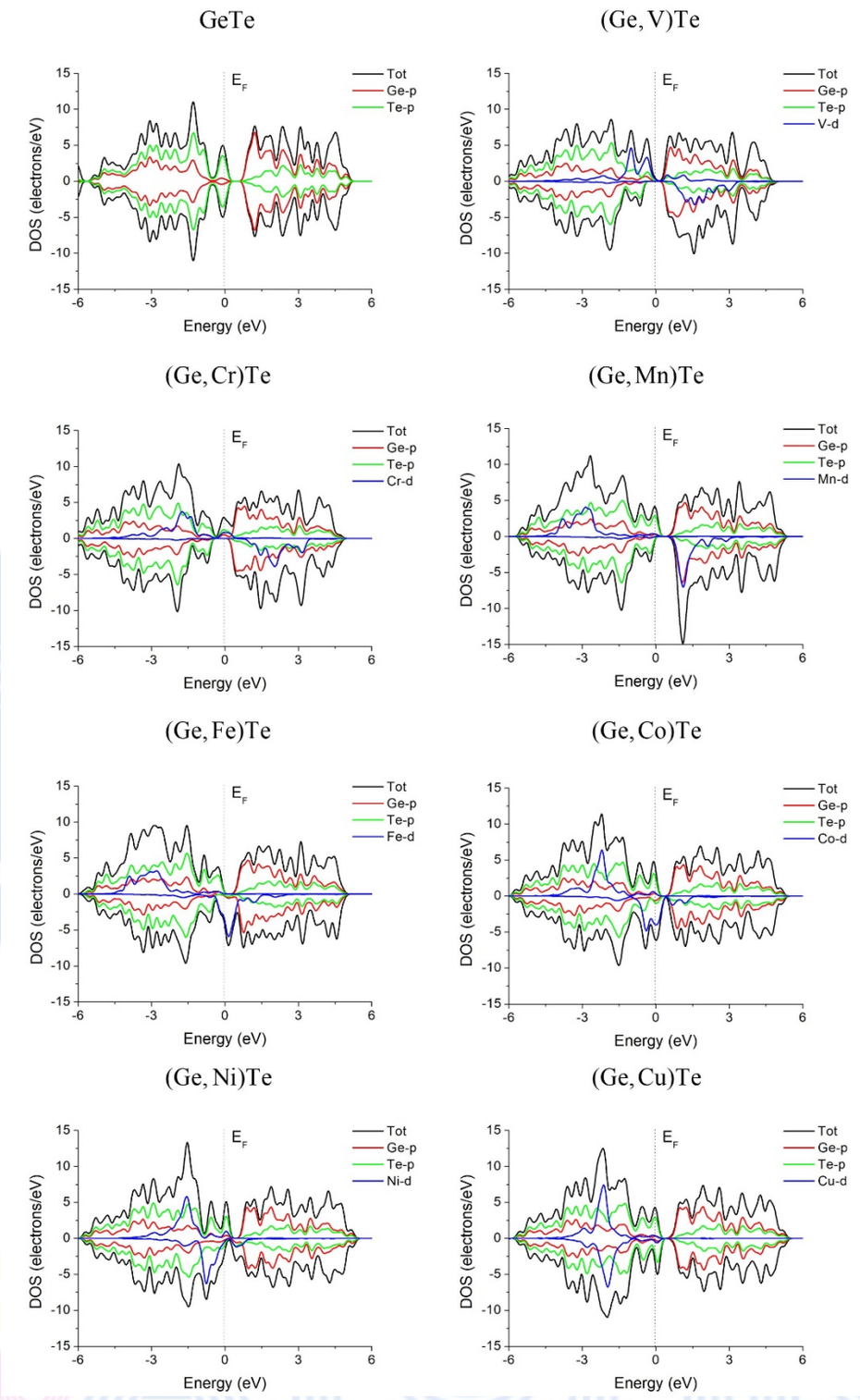

Figure 4: The total and partial density of states of GeTe, (Ge, V)Te, (Ge, Cr)Te, (Ge, Mn)Te, (Ge, Fe)Te, (Ge, Co)Te, (Ge, Ni)Te and (Ge, Cu)Te.

Conclusion

By means of spin density functional calculations, we reveal that the transition metals play a strategic role in tuning the structural, electronic and magnetic properties of rock-salt GeTe semiconductors doped with various transition metals. Through the formation energies, (Ge, Cr)Te is the most stable among all doped systems. The introduction of transition metals decreases the lattice parameters and volumes because the radius of host is larger than one of the impurities. In addition, the source of the net magnetic

moment is correspondingly donated from transition metal, Te and Ge. In the presence of the transition-metal dopants, the spin polarization of the electronic band structures is illuminated. Using the partial density of states, the magnetism is formed by p-d exchange hybridization with d orbitals from transition metal and p orbitals from Te. Mn doping in GeTe remains the semiconductor with a condensed band gap. Co, Ni and Cu change the GeTe semiconductor to metal. The p-type half metal is characterized in (Ge, V)Te, (Ge, Cr)Te and (Ge, Fe)Te which become the dilute magnetic semiconductors. Finally, we believe that these computational results will serve as a basis for developing a more cloudless picture of transition metals doping in GeTe semiconductor for the spintronic applications.

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