



# The electronic, magnetic and optical properties of Cr-doped MC (M=Si, Ge and Sn): A density functional theory approach

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## ABSTRACT

The electronic, magnetic and optical properties of Cr-doped MC (M=Si, Ge and Sn) are investigated in the framework of density functional theory. The results of our calculations in mBJ-GGA approximation show that all of these compounds are half-metallic ferromagnets with a magnetic moment of  $2 \mu_B$  per supercell. We find that all of these materials have high spin-flip gaps, and they can preserve their half-metallicity up to high lattice compressions, therefore, they could be used in spintronic devices. The optical properties of pure and doped MC semiconductors such as dielectric function, absorption and reflectivity are also considered. It is found that the Cr-doped semiconductors can be used in optical devices in larger ranges of frequencies than the corresponding undoped ones.

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## 1. Introduction

Half-metallic ferromagnets have attracted much research interest because of their applications in the field of spintronic [1,2]. These kinds of materials have only one electronic spin channel at the Fermi level, and as a result, they can produce spin-polarized currents [3]. Half-Heusler and full Heusler alloys such as NiMnSb, CoVTe and Ti<sub>2</sub>VGa [4–6], some of the materials in zinc-blende (ZB), rocksalt (RS) or wurtzite (WZ) structures such as MS (M=Li, Na, K and Cs) [7–9] and MC (M=Ca, Sr and Ba) [10], and also zig-zag edged graphene nanoribbons [11] are some of the materials that were approved to be half-metallic ferromagnets. Some of the diluted magnetic semiconductors, which are nonmagnetic semiconductors doped with magnetic elements, are also

found to be half-metals [12]. For example, the compounds of III–V [12], II–VI [13] and group IV [14,15] semiconductors which are doped with magnetic elements are some of the diluted magnetic semiconductors that are found to be half-metals. These materials have also shown applicable optical properties [16–18]; for example, they could be used as optical insulators and circulators which are essential components for optical fiber networks [19].

Here, we consider the electronic, magnetic and optical properties of Cr<sub>0.25</sub>M<sub>0.75</sub>C (M=Si, Ge and Sn) compounds. To the best of our knowledge, there are not any researches on these diluted magnetic semiconductors except for Cr<sub>0.25</sub>Si<sub>0.75</sub>C that the half-metallic properties were considered with different approximation compared to our works [20]. We compare the stability of Cr-doped MC semiconductors in both RS and ZB structures because most of the appropriate semiconductors for growing these materials have fcc-based structures. The Comparison of total energies of the samples in these two structures indicates that ZB structure is more stable than RS for our samples.

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The results of our calculations show that all of these materials in ZB structure are half-metallic ferromagnets with a magnetic moment of  $2 \mu_B$  per supercell. They have also rather high spin-flip gaps which may lead to high Curie temperatures. The optical properties of the pure and doped semiconductors such as dielectric function, absorption and reflectivity are also considered. We compare the optical properties of doped and pure semiconductors, and the reasons of the changes in optical properties as a result of doping are investigated.

## 2. Computational details

The calculations were carried out on the basis of density functional theory [21] as accomplished in the WIEN2k package [22]. Full-Potential-Linearized Augmented Plane Wave (FP-LAPW) method [23] was used to solve Kohn–Sham equations self-consistently [24]. The modified Becke–Johnson (mBJ) exchange potential [25] was used to calculate the electronic, magnetic and optical properties of the compounds. The generalized gradient approximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE) [26] was employed to optimize the volume and the internal atomic coordinates. Self-consistency is achieved by choosing the amount of 0.0001 Ry as energy and 1 mRy/a.u. as force convergence criteria. For the electronic configurations of the atoms, we have used: Cr: [Ar]. $3d^5.4s^1$ , Si: [Ne]. $3s^2.3p^2$ , Ge: [Ar]. $3d^{10}.4s^2.4p^2$ , Sn: [Kr]. $4d^{10}.5s^2.5p^2$  and C: [He]. $2s^2.2p^2$ . The muffin-tin radii ( $R_{mt}$ ) were chosen such that they enclose most of the atomic charges in the sphere. The muffin-tin radii for chromium, silicon, germanium, tin and carbon in different compounds are listed in Table 1.

The wave functions in the interstitial regions were expanded in plane waves with a cut-off of  $R_{mt}K_{max}=8$ . The optimum value of 14 (a.u.)<sup>-1</sup> for  $G_{max}$  and the optimum number of 8000  $k$ -points were used in our calculations.

## 3. Results and discussion

### 3.1. Structural properties

We have used a periodic supercell which contains one Cr, three M and four C atoms to simulate  $Cr_{0.25}M_{0.75}C$  (M=Si, Ge and Sn) compounds. It is possible to obtain a dopant concentration to this amount because the empirical dopant concentration for the compounds with zinc-blende structure is from 5% to 30% [15]. Diluted magnetic semiconductors could be fabricated on the appropriate substrates by the method of molecular beam epitaxy

(MBE) [27]. For example, Mn doped GaN and GeTe were fabricated successfully by this method [28,29]. Since thin films grown on most substrates are likely to have either rocksalt (RS) or zinc-blende (ZB) structures [30], we have compared the total energies of our samples in these two structures. We find that the ZB structure is more stable than the RS for all of these samples. The total energies in the nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) phases of the compounds are also calculated to find the stable phase of our samples. We employ a  $1 \times 1 \times 2$  supercell of the compounds for the AFM phase calculations, and we find that FM is the most stable phase for these materials.

We calculate the total energy as a function of volume to obtain the equilibrium lattice constants of the supercells. We fit total energy as a function of the volume of the supercell to the Murnaghan equation of state [31]. Fig. 1 shows total energy as a function of the volume of supercell for  $Cr_{0.25}Si_{0.75}C$ ,  $Cr_{0.25}Ge_{0.75}C$  and  $Cr_{0.25}Sn_{0.75}C$  fitted to the Murnaghan equation of state. We have obtained the equilibrium lattice constants of 4.43, 4.61 and 4.97 Å for  $Cr_{0.25}Si_{0.75}C$ ,  $Cr_{0.25}Ge_{0.75}C$  and  $Cr_{0.25}Sn_{0.75}C$ , respectively. We have also calculated the lattice constants of the undoped semiconductors by the same method, and the values of 4.38, 4.62 and 5.09 Å for SiC, GeC and SnC, respectively. We can see that the lattice constant of  $Cr_{0.25}Si_{0.75}C$  is higher than SiC due to the fact that the atomic radius of Cr is higher than Si [32]. However,  $Cr_{0.25}Ge_{0.75}C$  and GeC have almost the same lattice constants that is related to almost the same atomic radii of Cr and Ge [32]. Finally, the lattice constant of  $Cr_{0.25}Sn_{0.75}C$  is lower than SnC because Cr has lower atomic radius than Sn [32].

The relaxation of atomic positions is also performed because the local structure of transition metals can affect the electronic and magnetic properties. The relaxation does not change the atomic positions of Cr and C atoms, whereas the positions of the C atoms are changed. In  $Cr_{0.25}Si_{0.75}C$ , the C atoms move away from the Cr atoms, but in  $Cr_{0.25}Ge_{0.75}C$  and  $Cr_{0.25}Sn_{0.75}C$  the C atoms approach Cr atoms. Therefore, the electronic, magnetic and optical properties of these compounds are calculated according to the relaxed atomic positions.

The formation energies of these compounds are also calculated by the following equation:

$$\Delta E_{Cr_{0.25}M_{0.75}C} = E_{Cr_{0.25}M_{0.75}C} - 0.25E_{Cr}^{bulk} - 0.75E_M^{bulk} - E_C^{bulk} \quad (1)$$

In this equation,  $E_{Cr_{0.25}M_{0.75}C}$  and  $\Delta E_{Cr_{0.25}M_{0.75}C}$  are the total and formation energies of the  $Cr_{0.25}M_{0.75}C$  sample at the most stable phase, and  $E_{Cr}^{bulk}$ ,  $E_M^{bulk}$  and  $E_C^{bulk}$  are the total energies of bulk Cr, M and C in the most stable structures, respectively. The most stable structures of Cr, Si, Ge, Sn and C are bcc, diamond cubic, fcc, centered tetragonal and simple hexagonal with a four atom basis (graphite), respectively. The formation energy values of 0.153, -0.204 and 0.106 eV are obtained for  $Cr_{0.25}Si_{0.75}C$ ,  $Cr_{0.25}Ge_{0.75}C$  and  $Cr_{0.25}Sn_{0.75}C$ , respectively. The negative value of the formation energy for  $Cr_{0.25}Ge_{0.75}C$  shows that this compound could be synthesized at normal pressure and temperature conditions. However, the positive values

**Table 1**

The muffin-tin radii for chromium, silicon, germanium, tin and carbon in different compounds.

	$Cr_{0.25}Si_{0.75}C$	$Cr_{0.25}Ge_{0.75}C$	$Cr_{0.25}Sn_{0.75}C$	SiC	GeC	SnC
Cr (a.u.)	1.9	1.8	1.8	-	-	-
Si (a.u.)	1.8	-	-	1.8	-	-
Ge (a.u.)	-	1.8	-	-	1.9	-
Sn (a.u.)	-	-	1.8	-	-	1.9
C (a.u.)	1.6	1.5	1.6	1.6	1.7	1.7

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