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Ab initio study of electronic and magnetic properties in TM-doped 2D silicon carbide

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ABSTRACT

The magnetic properties of SiC monolayer with different TM atoms and substitutional sites are investigated using first-principles method. Magnetism is observed for all the TM dopants. The magnetic moments and binding energies are quite different between Si (TM_{Si}) and C (TM_C) sites. Dependent to the larger magnetic moments and binding energy, we also investigate the interaction between two Mn atoms in the TM_{Si} system. The results show that the ferromagnetic states are originated by the *p–d* hybridization mechanism between Mn and its neighboring C atoms. Moreover, the antiferromagnetic coupling is observed with increasing Mn-Mn distance, which can be explained by two-impurity Haldane-Anderson model using quantum Monte Carlo method.

1. Introduction

Silicon carbide (SiC) has attracted much interest due to its corrosion resistance, large band gap, high mechanical strength, low density, high hardness, high thermal conductivity and low thermal expansion coefficient [1–5]. Similar to graphene, the SiC monolayer (2D-SiC) with a honeycomb structure could be energetically stable [6,7] and SiC Monolayer exhibits a large direct band gap [8]. Several theoretical studies investigated the structure and electronic properties of SiC nano scales [9,10]. Due to its wide band gap (3.2 eV), SiC has potential applications in electronics and optics. Recently a large number of researches have given special attention to the properties of metal doped 2D materials [11–15] and high catalytic activity has been verified. However, few theoretical studies have been focused on the magnetic properties of 3d transition metal (TM) doped SiC monolayers [16,17]. In order to find its potential applications, we study the TM doped SiC monolayer by using first-principles calculations.

In this work, the magnetic properties of SiC monolayer with different TM atoms and substitutional sites are investigated using first-principles method. Magnetism is observed for all the TM dopants, but the magnetic behavior is quite different between Si and C substituted systems, shown TM_{Si} and TM_C, respectively. Among all the TM_{Si} monolayers, the Mn_{Si} system has large magnetic moments and also shows a most stable structure. Therefore, the interaction between two Mn atoms in the Mn_{Si} system is investigated. The results show the *p–d* hybridization mechanism between the Mn and its neighboring C atoms results in its ferromagnetic state. Moreover, the antiferromagnetic coupling is observed with increasing Mn-Mn distance which can be explained by two-impurity Haldane-Anderson model using quantum Monte Carlo method.

2. Method

Our calculations are performed first-principles method based on density functional theory (DFT) within the generalized gradient approximations (GGA-PBE) [18] as implemented in the VASP package [19]. The projector augmented-wave (PAW) [20] pseudo potential method is used and the cut off energy is 450 eV. The 4×4×2 k-point grids were used in both 5×5×1 and 10×5×1 supercells. The lattice parameter and bond length of SiC monolayer is 3.094 and 1.786 Å [21], respectively. The separation between two layers is 20 Å. All the calculations are self-consistent and the total energy convergence criterion is set at the value of 10^{-5} eV.

3. Result and discussions

3.1. Electronic structure and magnetism of TM doped SiC monolayer

Firstly, we calculate the equilibrium structure of pure SiC mono-

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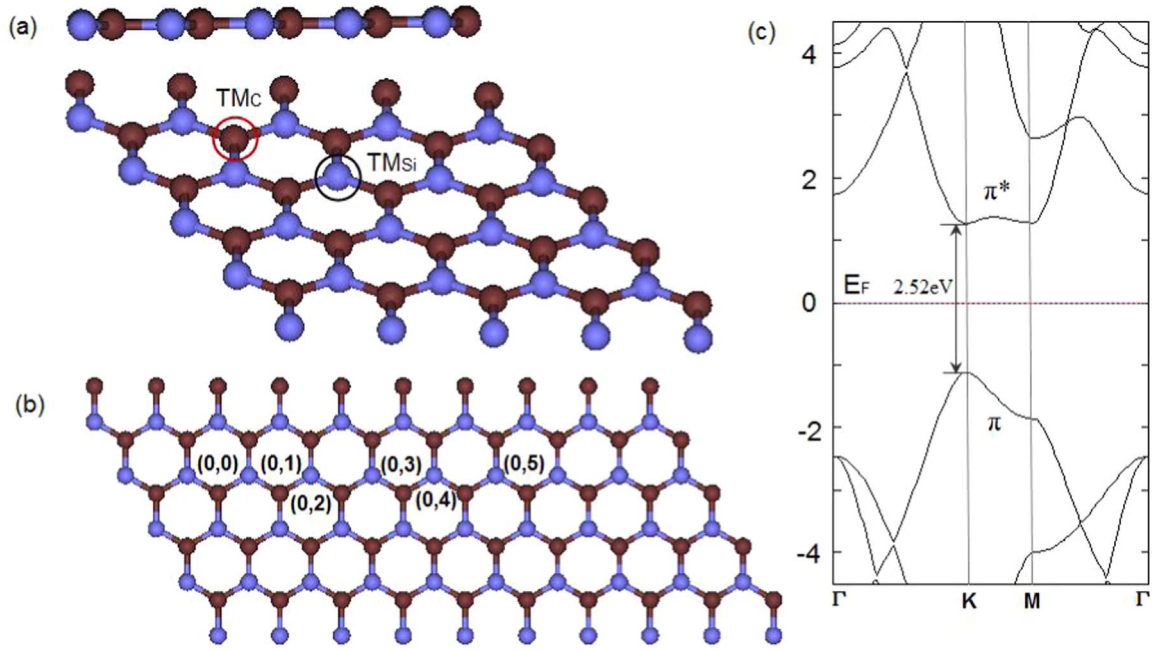

Fig. 1. Schematic structure showing (a) pristine SiC monolayer (side view) and TM-substituted SiC monolayer (top view); (b) the hexagonal structure viewed along the c axis, and the configurations in two Mn atoms-doped SiC monolayer of 10×5×1 supercell; (c) band structure of pristine SiC monolayer.

layer, which is shown in Fig. 1. Fig. 1(a) shows the schematic structure of TM-doped SiC monolayer of 5×5×1 supercell (50 atoms). The band structure of pure SiC monolayer is shown in Fig. 1(c), it has π and π* bands around K point at the Fermi level symmetrically and has a direct band gap of 2.52 eV, which agree with the previous studies [10,22]. These results verified the reliability of our methods..

Next, we study the magnetic properties of several TM (Co, Cu, Mn, Fe, and Ni) atoms substituted SiC monolayers. There are possible two TM substitutional sites in the SiC monolayer. We have shown the TM_{Si} and TM_C for the Si and C site substituted by TM atoms in Fig. 1(b), respectively. The total magnetic moments (μ_{total}), binding energy and bonding length are shown in Table 1. Here, the binding energy is estimated as $E_b=(E_{pure}+E_{TM})-E_T$, where E_{pure} and E_T is the total energy of SiC monolayer with one vacancy and with a TM dopant, respectively; E_{TM} is the energy of a TM atom. From our calculations, the values of μ_{total} are in the range of 0.299–1.571 and 1.963–2.999 μB for TM_C and TM_{Si} cases, respectively. The results indicate the stronger magnetic coupling in the TM_{Si} systems. Also, we analyze the electronic properties of TM_{Si}- and TMC-doped SiC monolayer, respectively. The total density of states (DOS) and projected density of states (PDOS) for TM-doped SiC monolayer are shown in Fig. 2. From Fig. 2(a) and (j), the spin-up and spin-down density in all the TM-doped systems are nonmagnetic and that is why the systems are nonmagnetic. For example, in the Mn-doped system, we see in Fig. 2(d) and (i), there are obvious spin spitting around the Fermi level and the symmetry of spin-up and spin-down breaks and the system exhibits magnetic behavior. We also see the hybridization between Mn and C atoms is stronger than that of Mn-Si, and then the magnetic moment of the MnSi-doped system is larger..

3.2. Magnetic coupling in Mn-substituted SiC monolayer

In Fig. 3, we have depicted the E_b variations of both TM_C and TM_{Si} cases. As it is shown the values of E_b in TM_{Si} structures are entirely higher than those of the TM_C structures, which indicate the TM_{Si} systems are more stable. Although the binding energy difference of Co_{Si}, Cu_{Si}, Fe_{Si}, Mn_{Si}, and Ni_{Si} structures is small. The Mn_{Si} system has the biggest value. Hence, we deduce that the stable structure is an essential property of Mn_{Si} system which is an advantage over other systems. Because of this, we come to investigate the interaction between two-Mn-doped system of 10×5×1 supercell, and several possible configurations of Mn dopants are discussed as shown in Fig. 1(b). We use i to mark the dopant Mn (0, i) and we position one Mn dopant atom in a fixed site [denoted 0 in Fig. 1(b)] and the other Mn dopant substitutes a Si atom at one of the marked positions i=1–5. As shown in Table 2, it is found that the ferromagnetic coupling depends on Mn-Mn distance. In addition, the stability of FM states is determined by the total energy difference for the above possible configurations. The total energy difference is estimated as$\Delta E = E_{AFM} - E_{FM}$, where E_{FM} and E_{AFM} are the total energies of two Mn atoms aligned ferromagnetically (FM) and antiferromagnetically (AFM), respectively. For the nearest Mn-Mn distance, as shown in Table 2, ΔE is 150 meV which indicates the interaction between two Mn atoms is FM. However, the situation changes with increasing Mn-Mn distance; the FM state disappears and the AFM state appears. For the cases of (0, 2) and (0, 3) in the 10×5×1 supercell, ΔE are about −41 and −12 meV, respectively. Moreover, the (0, 1) case has the lowest total energy, which indicates that the nearest two-Mn-doped SiC monolayer should be the most stable candidates for the 2D silicon carbide..

In order to understand the FM interaction between the nearest two Mn dopants, the TDOS and PDOS are shown in Fig. 4. From Fig. 4(a)–(b), the *d* state of Mn overlaps with that of *p* state of the C atom. In the minority spin channel, the *p* state of the connecting C atoms contributes significantly to the unoccupied states, which indicates a strong hybridization between Mn and its neighboring C atoms. The polarized spins in C *p* states couple with the *d* localized spins of Mn, showing a *p-d* like interaction chain, which results in an indirect FM interaction between Mn and C atoms. Because of the *p-d* interaction, the minority spin states are lifted upward together with the downward shift of the majority spin states, which lower the total energy of the system [23]. Thus, the *p-d* hybridization is responsible for FM in Mn-doped SiC monolayer..

For the nearest two Mn dopants, the calculated magnetic moment is 6.00 μ_B. It is hypothesized that the different local distortion may result in different spin distributions of the local moment. As illustrated in Fig. 5, the main spin densities are localized around two Mn dopants. The interaction between a Mn dopant and its neighboring C atoms is

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