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Ferromagnetism induced by intrinsic defects and carbon substitution in ZnO nanowires

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HIGHLIGHTS

- The possible ferromagnetism (FM) in ZnO nanowire is investigated.
- Cation vacancy could induce FM in ZnO nanowire.
- Carbon substitution could induce FM in ZnO nanowire.

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ABSTRACT

The possibilities of magnetism induced by intrinsic defects and carbon substitution in ZnO nanowires are investigated by *ab initio* calculations. The calculated results indicate that an ideal ZnO nanowire is nonmagnetic. The zinc (Zn) vacancy can induce the magnetic moments rather than oxygen vacancy, which is originated from the polarization of O 2p electrons. A couple of zinc vacancies can lead to the ferromagnetic coupling. A carbon substitution for oxygen also produces magnetic moments. When substituting two carbon atoms, the characteristics of exchange coupling depend upon the distance of two carbon atoms. The longer distance of two carbon atoms prefers the ferromagnetic coupling, whereas the shorter distance leads to the antiferromagnetic coupling.

1. Introduction

Room temperature ferromagnetism (FM) in pure semiconductors or insulators without any ferromagnetism element has attracted much attention in recent years. The experimental results indicated that observed FM originated from the oxygen vacancies for oxides HfO_2, CeO_2, Al_2O_3, ZnO, In_2O_3, SnO_2 and TiO_2 [1–5], but from neutral cation vacancies for MgO [6–9]. Most of *ab initio* calculations demonstrated that neutral cation vacancies were responsible for the magnetic moments in oxides such as TiO_2, ZnO, SnO_2, ZrO_2 and MgO [10–19]. Ferromagnetism could also be produced by doping non-magnetic sp elements such as C, N, Mg and Al in oxides, nitrides and sulfides [20–40]. Recently, focus has been shifted to low-dimensional nano-structures since the future spintronics requires dilute magnetic semiconductor (DMS) in reduced dimensionality and size, such as one-dimensional (1D) nanowires, nanotubes and nanobelts, owing to their high thermal stability, chemical resistivity and excellent mechanical properties. Nowadays, high-quality ZnO nanowires (NWs) have been successfully synthesized, and their formation mechanism and relative stability have been studied [41–46]. The synthesis of perfect single-crystal ZnO NWs opens up new possibilities of fabricating ZnO-based new functional spintronics devices taking advantage of their spin degree of freedom, due to its lower mass density, high porosity, and very large surface to weight ratio. Extensive calculations based on density functional theory demonstrated that Zn vacancy could introduce magnetic moments in ZnO [11]. However, up to now, theoretical mechanism of vacancy (or substitution) induced ferromagnetism in ZnO NWs is still lacking. In the present work, we perform *ab initio* calculations on the magnetism of ZnO NWs by the GGA method. Calculation results demonstrate that Zn vacancy could induce large magnetic moment in ZnO nanowire, which is located mainly on the neighboring O atoms around Zn vacancy. A couple of neutral Zn vacancies could lead to a ferromagnetic state of the system. A single carbon substitution for oxygen could also produce large local magnetic moments. When substituting two carbon atoms, the characteristics of exchange coupling depend upon the distance of two nitrogen atoms. The longer distance of two carbon atoms prefers the ferromagnetic coupling, whereas the shorter distance leads to the antiferromagnetic coupling.

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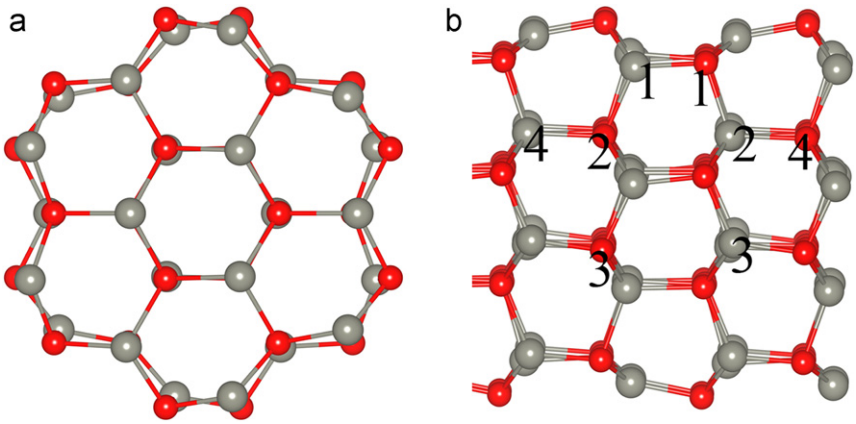

Fig. 1. (a) Top view and (b) side view model of an ideal ZnO nanowire.

2. Computational details

The present calculations were performed using the plane-wave pseudopotential method in the Vienna *ab initio* simulation package (VASP) [47,48]. The projector augmented wave (PAW) [49] potentials were employed, and the generalized gradient approximation (GGA) was used to describe the exchange correlation energy. A ZnO nanowire containing 96 atoms was relaxed to investigate the magnetic properties with the presence of vacancies and carbon substitution. Fig. 1(a) and (b) shows us the top view and side view model of the ideal ZnO nanowire relaxed by VASP. By removing one neutral zinc atom or two zinc atoms, we obtained the concentrations of 2.08% or 4.17% V^0_{Zn} vacancies in the ZnO nanowire model. The cases of 2.08% and 4.17% carbon substitutions for oxygen were also taken into account. Each case had been relaxed before calculating the magnetic moments and density of states (DOS). A plane wave cut off of 400 eV was used for the basis set. $1\times1\times7$k-points were used for the sampling of one-dimensional Brillouin zone. We also calculated the formation energies of the V^0_{Zn} vacancies. In general, the formation energy of a neutral point defect can be defined as [50]

$$E_f=(E^v_{tot}-E^0_{tot}+n_i\mu_i)/n_i,$$

where E^v_{tot} and E^0_{tot} are the total energies of supercells with and without defects, respectively, n_i is the number of atoms removed, and μ_i is the chemical potential of the corresponding atom. For the ZnO system, the formation energy of a single V^0_{Zn} vacancy can be calculated using the following equation:

$$E_f(V_{Zn})=(E^v_{tot}(V_{Zn})-E^0_{tot}(ZnO)+n_i\mu_{Sn})/n_i.$$

In thermodynamic equilibrium, the chemical potentials of Zn and O should satisfy the stability condition defined as

$$\mu_{Zn}+\mu_O=\Delta H(ZnO),$$

where ΔH is the formation enthalpy of ZnO. Under extreme O-rich condition, the oxygen potential μ_O is subjected to an upper bound given by the energy of O in an O_2 molecule, namely, $\mu^{max}_O=1/2\mu_{O_2}$. Therefore, μ_{Zn} can be obtained from

$$\mu^{min}_{Zn}=\Delta H(ZnO)-\tfrac{1}{2}\mu_{O_2}.$$

Similarly, under extreme Zn-rich condition, the lower limit of oxygen chemical potential is

$$\mu^{min}_O=\Delta H(ZnO)-\mu_{Zn},$$

where μ_{Zn} is the energy of Zn in bulk zinc. In the present work, we just consider the formation energies of V^0_{Zn} vacancies under extreme O-rich condition.

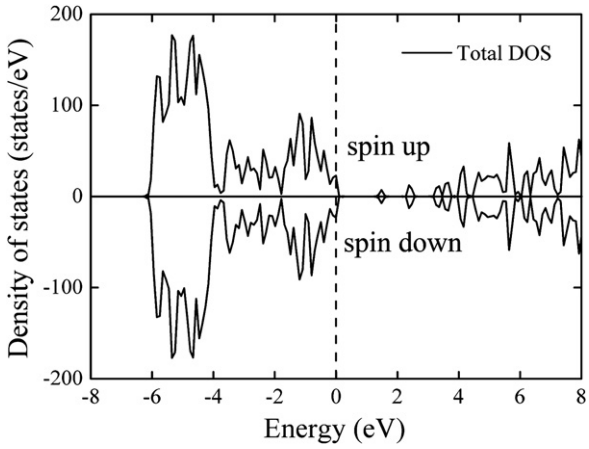

Fig. 2. Total DOS of an ideal ZnO nanowire.

3. Results and discussion

In the ideal ZnO nanowire, the Zn is in a +4 state due to the donation of its four valence electrons to the O_2 complex, which is in a −4 state. This results in ideal ZnO nanowire as a nonmagnetic and wide band-gap material where all bands are occupied. According to our calculations, the formation energies for Zn_1, Zn_2, O_1 and O_2 vacancies are 8.88, 9.34, 6.45 and 6.85 eV, respectively, which show that the O_1 vacancy is more stable than the others. Fig. 2 displays the spin-resolved total DOS of the ideal ZnO nanowire. No spin-polarization emerges around the Fermi energy level which is just crossing the valence band. Therefore, it can be concluded that the ideal ZnO nanowire is non-magnetic. The total energies of the supercell for spin-polarized and nonspin-polarized on various vacancies are considered. Results show that the magnetic states are more stable for O and Zn vacancies in the ideal ZnO nanowire. Fig. 3(a) and (b) separately presents the total DOS's of the ZnO nanowire with 2.08% $V^0_{O_1}$ and $V^0_{O_2}$ vacancies (neutral oxygen O_1 or O_2 atom is removed from ZnO nanowire, as shown in Fig. 1). Obviously, the introduction of the oxygen vacancy could not bring about magnetic moments. Fig. 3(c) and (d) shows the total DOS and partial DOS projected onto p orbital of O atoms and p, d orbitals of Zn atoms when the concentration of V^0_{Zn} vacancy is 2.08% (removing Zn_1 and Zn_2 in Fig. 1). From these figures, the total DOS exhibits an obvious spin–split around the Fermi level, indicating the existence of local magnetic moments. The partial DOS indicates that the spin-polarization of 2p electrons of oxygen atoms is responsible for the induced magnetic moments. Although the p, d orbitals of the Zn atoms

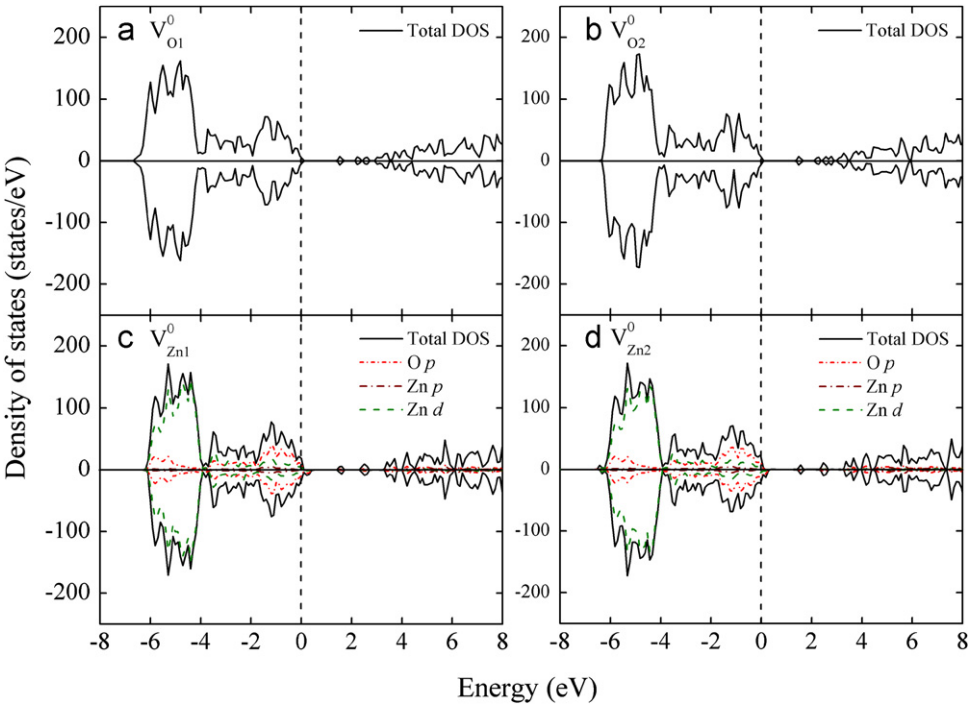

Fig. 3. Total DOS of (a) ZnO nanowire with 2.08% $V^0_{O_1}$ vacancy and (b) ZnO nanowire with 2.08% $V^0_{O_2}$ vacancy. Total DOS and partial DOS of (c) ZnO nanowire with 2.08% $V^0_{Zn_1}$ vacancy and (d) ZnO nanowire with 2.08% $V^0_{Zn_2}$ vacancy. The vertical dotted line indicates the Fermi level.

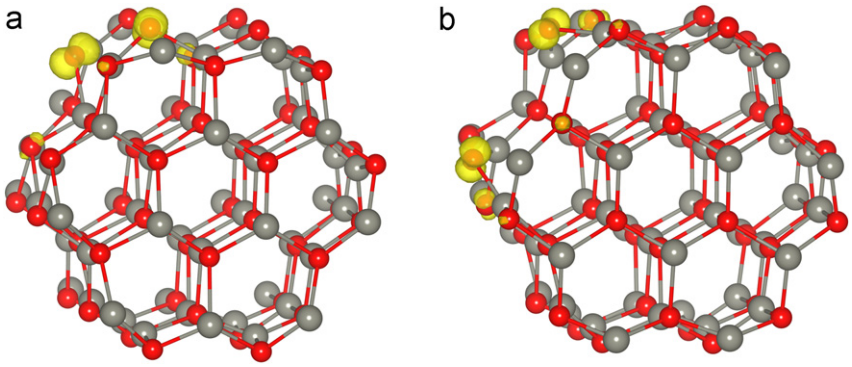

Fig. 4. Three-dimensional iso-surfaces (the iso-value is 0.02 e/Å^3) of magnetization density (spin up minus spin down) of (a) ZnO nanowire with 2.08% $V^0_{Zn_1}$ vacancy and (b) ZnO nanowire with 2.08% $V^0_{Zn_2}$ vacancy. The small red balls and large gray balls represent the O and Zn atoms, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

also exhibit spin-polarization, their contribution to the spin-polarization of the whole system is subtle. As the presence of V^0_{Zn} vacancy leads to a loss of donor charge, leading to introduce non-zero magnetic moments. As shown in Fig. 4(a) and (b), we present three-dimensional magnetization density (spin up minus spin down) for the ZnO nanowire with 2.08% V^0_{Zn} vacancy. The small red balls and large gray balls represent the O and Zn atoms, respectively. Clearly, the magnetization density is mainly localized at the O atoms near the V^0_{Zn} vacancy. According to our calculations, the system presents a net magnetic moment of $2.08\mu_B$ with a concentration of 2.08% $V^0_{Zn_1}$ vacancy. In addition, the magnetic moments of the O atoms take percentages of 85.8% in the total net moments. For the ZnO nanowire with 2.08% $V^0_{Zn_2}$ vacancy, the magnetic moment is $2.07\mu_B$, and the magnetic moments of the O atoms take percentages of 85.8% in the total net moments. For the ZnO nanowire with 4.17% Zn vacancies, we investigate three distributions of two isolated neutral Zn vacancies at the nanowire. The three cases are removing of Zn_1 and Zn_2, Zn_1 and Zn_3, and Zn_2 and Zn_4 from the ZnO nanowire (see Fig. 1). The calculated results show that the total DOS of each case could exhibit obvious spin-polarization, which originates mainly from the spin-polarization of O 2p electrons, and indicates the existence of large local magnetic moments. Table 1 lists the relative stabilities (ΔE), relative formation energies (ΔE_f), relative energies of the states between FM and AFM (ΔE_{AFM-FM}) and the total net magnetic moments (M_{tot}), calculated for the ZnO nanowire with 4.17% Zn vacancies. We can see that the magnetic moments for the above three cases are $3.64\mu_B$, $3.56\mu_B$, and $3.85\mu_B$. In order to investigate the magnetic coupling between the two isolated vacancies, we studied the relative energies of the states between ferro- and antiferromagnetic coupling ($\Delta E_m = E_{AFM} - E_{FM}$) by GGA calculations. For the above three cases, the total energies of the states with ferromagnetic coupling are lower than the energies of the states with antiferromagnetic coupling. That is to say, ferromagnetic coupling is energetically favorable for each case. Recently, Zunger et al. pointed out that the ferromagnetic

interaction in bulk ZnO with Zn vacancies is actually negligible due to the localization of hole states, which is overestimated in the LDA and GGA [51]. However, the correction with cancellation of nonlinearity (CONL) cannot carry out in current VASP package, and the properties of ZnO can be different in various forms, such as bulk, surface, nanowire, nanotube, and nanorod. Therefore, we still calculated the magnetic properties of ZnO NWs with the GGA method. A comparison of the total energies provides us with the information that when Zn_1 and Zn_2 are removed, the system has a total energy of −403.2 eV, which is 0.11 and 0.09 eV lower than the energies of the other three cases, respectively. The relative formation energies indicate that removing Zn_1 and Zn_2 is the most favorable. As the distance between Zn_1 and Zn_2 (3.2 Å) is the first-neighboring among the considered three structures of the ZnO nanowire with two isolated V_{Zn}^0 vacancies, it is possible that the vacancies could prefer to gather in the nanowire.

The ferromagnetism without any transition metal impurities (so-called d^0 ferromagnetism) is one of the hottest topic in DMS research. There are many theoretical investigations of d^0 magnetism [10–40]. As a consequence, the ferromagnetism of C substitution in ZnO NWs is considered. Replacement of a single O atom by one C atom (O_1 or O_2 substituted by C, see Fig. 1) in the ZnO nanowire corresponds to a 2.08% carbon concentration. The energy of spin-polarized state for O substituted by C is lower than that of nonspin-polarized state. For O_1 substituted by C, Fig. 5(a) presents the corresponding total DOS as well as partial DOS projected onto the 2p orbitals of O and C, and p, d orbitals of Zn atoms. A comparison between the total DOS of ideal ZnO nanowire and that of the ZnO nanowire with one C substitution shows that the introduction of C substitution produces obviously spin-polarized impurity states around the Fermi level. The partial DOS indicates that the spin–split of the total DOS is mainly contributed by the spin-polarization of the 2p electrons of C and O atoms. For O_2 substituted by C atom, the total DOS and partial DOS also show an obviously spin–split impurity states around the Fermi level, which mainly originated from the O and C 2p electrons (see Fig. 5(b)). Fig. 5(c) is the three-dimensional iso-surface magnetization density (spin up minus spin down) for the ZnO nanowire with 2.08% C substitution for O_1. The magnetization density mainly concentrates on the C atom. According to our calculations, the magnetic moment of the C atom is $1.122\mu_B$, and the total magnetic moment of the O atoms is $0.676\mu_B$. The two parts together take a percentage of nearly 91.7% in the total magnetic moments ($1.96\mu_B$) of the whole system. In Fig. 5(d), the three-dimensional iso-surface density for the ZnO nanowire with 2.08% C substitution for O_2 shows that the spin density is mainly distributed on the C atom. The magnetic moment of the C atom is $1.207\mu_B$, and the total magnetic moment of O atoms is $0.714\mu_B$. Both of them take a percentage of nearly 95.1% in the total magnetic moments ($2.02\mu_B$).

To examine long-range magnetic coupling of magnetic moments in C-doped ZnO nanowire, we consider three different configurations of a couple of C atoms doped ZnO nanowire, corresponding to a dopant concentration of 4.17%. The three structures are obtained by two C atoms substituting two O atoms at O_1 and O_2, O_1 and O_3, and O_2 and O_4 with different C–C

Table 1
Values of the relative stabilities ($\Delta E = E(\mathrm{ZnO}) - E(\mathrm{ZnO})_{lowest}$), relative formation energies ($\Delta E_f = E_f(\mathrm{ZnO}) - E_f(\mathrm{ZnO})_{lowest}$), relative energies of the states between FM and AFM ($\Delta E_m = E_{AFM} - E_{FM}$) and total net magnetic moments (M_{tot}), calculated for the ZnO nanowire with 4.17% V_{Zn}^0 vacancies.

Atoms removed	ΔE (eV)	ΔE_f (eV)	ΔE_m (meV)	M_{tot} (μ_B)	Distance (Å)
Zn_1 and Zn_2	0	0	44	3.64	3.2
Zn_1 and Zn_3	0.11	0.16	32	3.56	5.6
Zn_2 and Zn_4	0.09	0.14	52	3.85	5.2

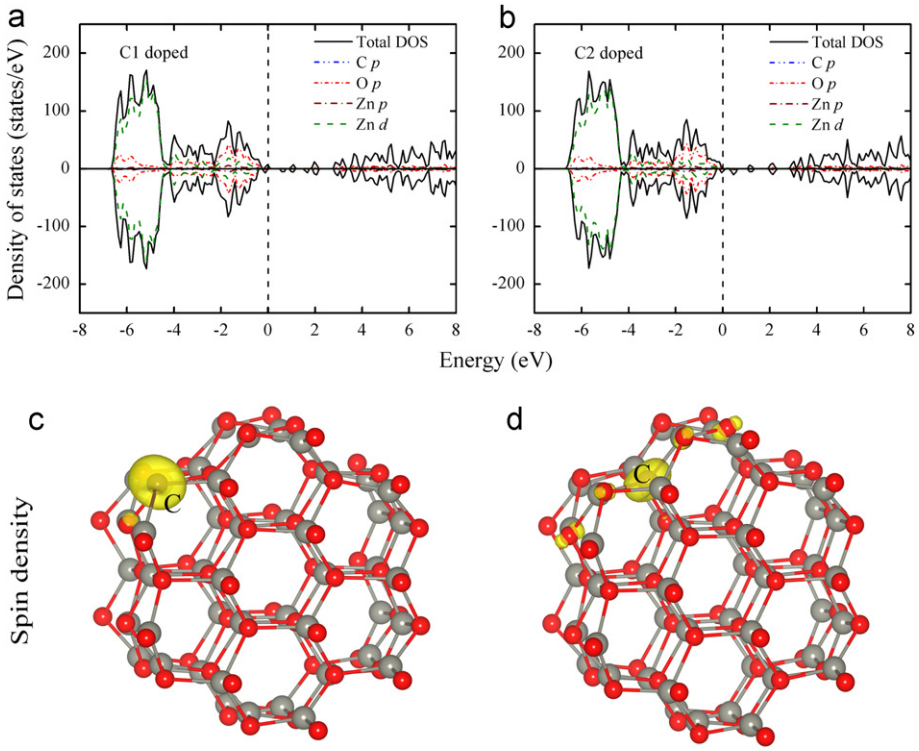

Fig. 5. Total DOS's and partial DOS's of the ZnO nanowire with 2.08% C substitution for (a) O_1 and (b) O_2. The vertical dotted line indicates the Fermi level. Three-dimensional iso-surfaces (the iso-value is 0.02 e/Å^3) of magnetization density (spin up minus spin down) of the ZnO nanowire with 2.08% C substitution for (a) O_1 and (b) O_2. The small red balls and large gray balls represent the O and Zn atoms, respectively. The C atom is labeled. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

distances(see Fig. 1). Table 2 shows the relative stabilities (ΔE), the relative formation energies (ΔE_f), the relative energies of the states between FM and AFM ($\Delta E_m = E_{AFM} - E_{FM}$) and the total net magnetic moments (M_{tot}), calculated for the ZnO nanowire with two O atoms substituted by C atoms. The obtained relative stabilities (ΔE) indicate that the relatively stable state is substituting two C atoms for O_1 and O_2. When O_1 and O_2 atoms are substituted by C atoms, the antiferromagnetic coupling is more favorable and the ferromagnetic moment is zero. The corresponding total DOS and the partial DOS are shown in Fig. 6(a)–(c). Clearly, there is no spin-polarization that emerges around the Fermi energy in total DOS (Fig. 6(a)). Interestingly, the partial DOS of two C atoms given in Fig. 6(b) and (c) , are spin polarized. However, their magnetic moments are in opposite directions, resulting in a total magnetic moment of zero. When O_1 and O_3 as well as O_2 and O_4 are substituted by C atoms, the systems could exhibit spin-polarization (see Fig. 6(d)–(i)), and for these cases, the magnetic moments are $4.05\mu_B$ and $3.91\mu_B$ according to the present calculations, respectively. Further investigation indicates that for these structures, the ferromagnetic coupling is lower than the antiferromagnetic coupling. That is to say that, the ferromagnetic coupling is energetically favorable.

Table 2
Values of the relative stabilities ($\Delta E = E(\text{C:ZnO}) - E(\text{C:ZnO})_{lowest}$), relative formation energies ($\Delta E_f = E_f(\text{C:ZnO}) - E_f(\text{C:ZnO})_{lowest}$), relative energies of the states between FM and AFM ($\Delta E_m = E_{AFM} - E_{FM}$) and total net magnetic moments (M_{tot}), calculated for the ZnO nanowire with 4.17% carbon substitution for oxygen.

Atoms substituted	ΔE (eV)	ΔE_f (eV)	ΔE_m (meV)	M_{tot} (μ_B)	Distance (Å)
O_1 and O_2	0	0	−64	–	3.2
O_1 and O_3	1.85	0.61	37	4.05	5.6
O_2 and O_4	1.79	0.54	48	3.91	5.2

4. Conclusion

In summary, we performed *ab initio* calculations on the magnetism of the ZnO nanowire with various vacancies and C substitutions

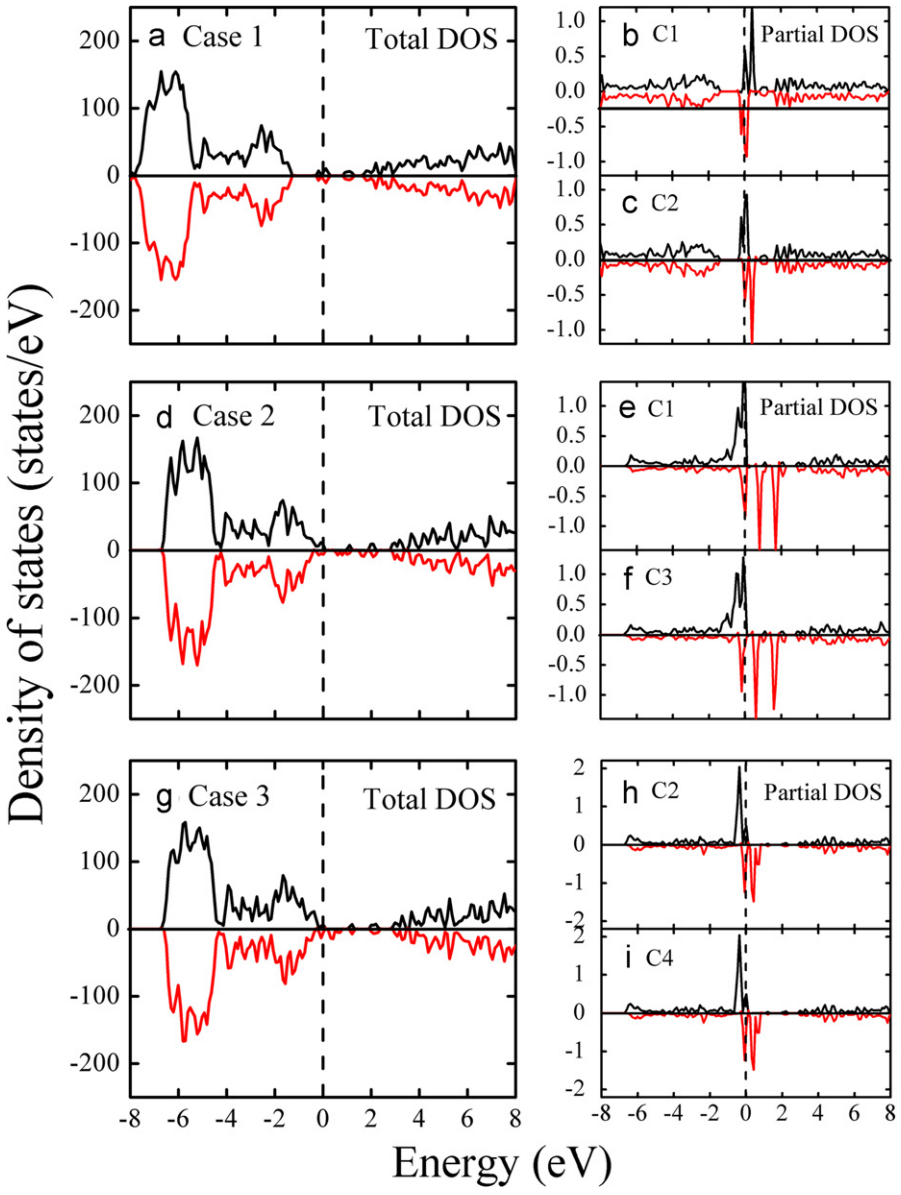

Fig. 6. Total and partial DOS plots of the ZnO nanowire with two C substitutions. The (a)–(c) represent two C atoms substitution for O_1 and O_2 atoms. The (d)–(f) represent two C atoms substitution for O_1 and O_3 atoms. The (g)–(i) represent two C atoms substitution for O_2 and O_4 atoms. The vertical dotted line indicates the Fermi level.

for O atoms. The results show that the ideal ZnO nanowire is non-magnetic, and V_O^0 vacancies introduce zero magnetism. V_{Zn}^0 vacancies could bring about large local magnetic moments in the ZnO nanowire, localized mainly on the neighboring O atoms around Zn vacancy. A couple of neutral V_{Zn}^0 vacancies could lead to a stable state with ferromagnetic coupling. A single C substitution for oxygen also produces large local magnetic moments. When substituting two C atoms, the characteristics of exchange coupling depend upon the distance of two nitrogen atoms. The longer distance of two C atoms prefers the ferromagnetic coupling, whereas the shorter distance leads to the antiferromagnetic coupling.

Acknowledgments

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