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Impact of isotropic strain on electronic and magnetic properties of O-adsorbed SiC monolayer

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ABSTRACT

Electronic and magnetic properties of two-dimensional (2D) silicon carbide (SiC) with the O adatom have been studied by the first-principles calculations. Different adsorption sites have been investigated. Magnetism is observed, while the O adatom binds to Si or situates in the middle of hexagons. We further study the effects of strain on the magnetism in the O-adsorbed 2D-SiC, we apply an isotropic tensile and compressive strain on the system. On the basis of our calculations, tunable magnetism shows as the strain increases. The analysis of the PDOS shows that the p-p hybridization between O and C/Si atoms results in such magnetic behavior. Moreover, under the compressive strain, the O-adsorbed SiC monolayer could transfer from semimetal to metal states. The adsorption of the O atom might show potential applications in SiC-based nanoscale devices.

1. Introduction

Graphene, as a typical monolayer honeycomb structure, has extraordinary properties and has been applied in various kinds of applications [1–3]. Discovery of graphene has led to the emergence of other two-dimensional (2D) materials, which will have potential applications for future nanoscale devices [4,5]. However, the 2D materials still face important challenges, such as growth of large areas, the integration in current Si-based nanotechnologies, which seriously restricts its practical application. In this aspect, searching substitutable 2D materials, which have supereminent chemical and physical properties, is under significant research interests [6–9].

In recent years, graphene-like 2D silicon carbide (SiC) has been investigated by many researchers because of their interesting properties [10–12]. Different from graphene, the 2D-SiC has a zero band gap, which is attributed to their strong π-bonding between two nearest-neighbor P_z orbitals. Therefore, potential applications in electronic and optoelectronic devices have been well investigated [13,14]. To realize the wide applications, the doping characteristics of transition-metal (TM) in SiC have got much interest [15–18]. Different from the magnetism induced by the d electrons of TM atoms, the magnetic moment induced by the sp states of nonmetal atoms has much stronger exchange interactions [19,20]. Very recently, theoretical studies predicted that nonmetal elements, such as B, C, F, N, and O atoms, could induce magnetic moments in MoS_2 [21], arsenene [22], and phosphorene [23]. In addition, theoretical investigations have revealed that strain is effective and promising tools to control electronic properties of 2D materials. The band gap of graphene could be open by strain engineering [24]; By applying the biaxial stress, the silicon transfers from semimetal to metal states [25]. It is also demonstrated that the electronic structures of multi-layers MoS_2 are tuned continuously by the tensile strain [26]. All these studies reveal that the application of strain could be a powerful and important way to change the properties of 2D materials. Motivated by the above studies, the effects of strain on the magnetic and electronic properties of O-adsorbed SiC are interesting from the perspective of fundamental understanding and spintronic applications.

In this paper, based on first-principles calculations, the magnetic and electronic properties of O-adsorbed 2D-SiC are systematically studied. The magnetism depends on the adsorption sites. The O atom binding to the C atom is always nonmagnetic. While the O atom binds to Si or situates in the middle of hexagons, magnetic moments of 1.98 and 1.86 μB are induced. On the basis of the analysis of spin-density and PDOS, the magnetism originated from p-p hybridization between the O adatom and C/Si atom. Then, we studied the magnetic properties of O-adsorbed 2D-SiC under an isotropic strain. Based on our results, the O-adsorbed in the middle of the Si-C hexagon changed from magnetic to nonmagnetic states. The magnetic moment disappeared under the tensile strain and gradually decreased as the compressive strain increased. It might be explained by different p-p hybridizations between the O adatom and C/Si. Moreover, under the compressive strain, the O-

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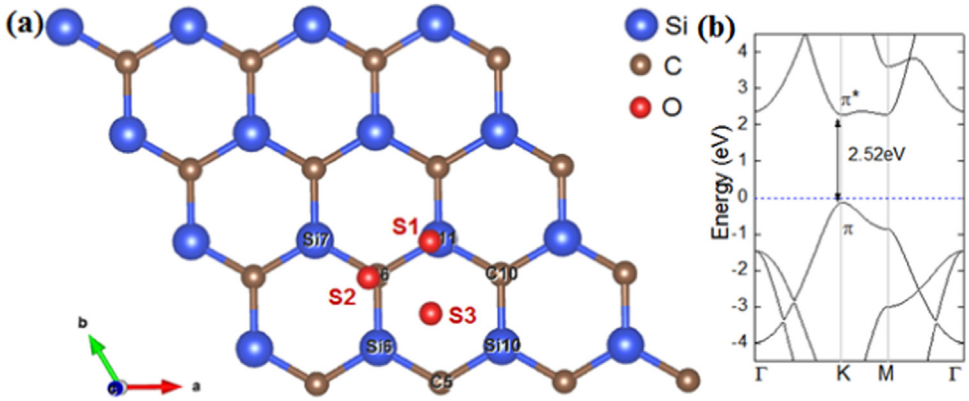

Fig. 1. (a) Three different adsorption sites of the O atom on the 4 × 4 × 1 SiC monolayer marked S1, S2 and S3. (b) The band structure of pure 2D-SiC.

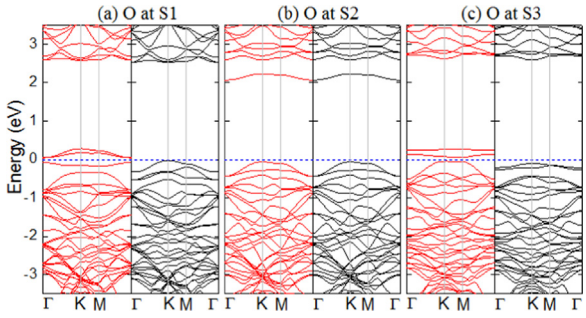

Fig. 2. Band structures of SiC monolayer with one O adatom at different adsorption sites (a) S1, (b) S2, and (c) S3. The Fermi level is indicated by the dotted line.

adsorbed SiC monolayer could transfer from semimetal to metal states. Our findings provide promising candidates for the O-adsorbed SiC monolayer in future spintronic devices.

2. Method

The electronic and magnetic properties in this paper are performed by the density functional theory (DFT) implemented in the VASP code [27]. The Perdew-Burke-Ernzerhof (PBE) of exchange-correlation calculations with the generalized gradient approximation (GGA) are used [28]. The projector-augmented wave (PAW) potentials [29] are used with a 450 eV cut-off energy. A set of 5 × 5 × 1 k-points is used. The lattice parameter and bond length of SiC monolayer is 3.094 and 1.786 Å [12]. To ensure negligible interactions between SiC layers images, a vacuum of 15 Å along the z-direction is added. In the following the magnitude of the biaxial tensile strain is expressed as

$$\varepsilon = \frac{a - a_0}{a_0} \times 100\%,$$

where a and a_0 are the lattice parameters of strained and unstrained SiC monolayer, respectively [30]. Here, the negative (positive) values of ε correspond to the compressive (tensile) strains. All the structures are fully relaxed until the force is less than 10^{-2} eV/Å and the self-consistent of energy is set at 10^{-5} eV.

3. Results and discussions

3.1. Magnetism of 2D-SiC with different adsorption sites

Firstly, we study the magnetic properties of 2D-SiC with one O adatom. Three possible adsorption sites are considered, as shown in Fig. 1a. The O atom might bind to Si or C atoms, or situate in the middle of hexagons, marked as S1, S2, and S3. For pure 2D-SiC, as shown in Fig. 1b, the system is nonmagnetic semimetal with π and π* bands crossing K point at the Fermi level (E_F), which agrees with previous studies [15,31]. Magnetic moments of 1.98 and 1.86 μB are observed while the O atom is adsorbed at S1 and S3. No magnetism is observed at S2 on the 2D-SiC surface. The calculated band structures of O-adsorbed

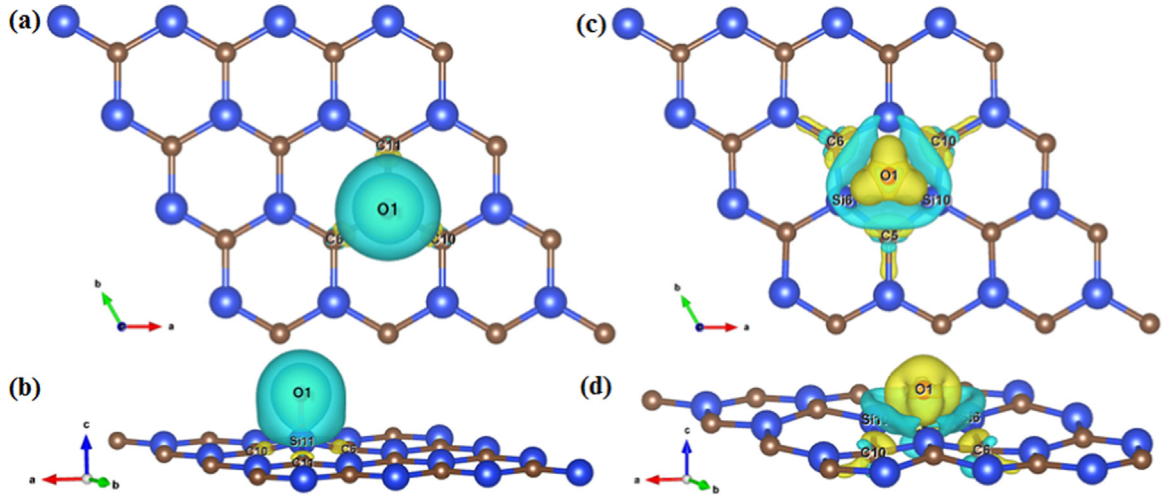

Fig. 3. (a) Top and (b) side views of calculated spin density distribution of 4 × 4 × 1 SiC monolayer with one O atom adsorbed at S1; (c) top and (d) side views of calculated spin density distribution of one O atom at S3. Yellow and cyan isosurfaces represent positive and negative spin densities (0.008 e/Å^3). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.).