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Curvature induced magnetic nanonodes in (6, 0) SiC/C nanotube heterojunction superlattice

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HIGHLIGHTS

- The electronic and magnetic properties of the zigzag (n, 0) ($n=6$–10) SiC/C nanotube superlattices are investigated by using the first-principles calculations.
- The (6, 0) SiC/C nanotube superlattice shows magnetic property with $2.0\mu_B$ magnetic moments due to the curvature effect.
- The spin densities distribute periodically along the axial direction and mainly locate at the CNT segment, thus forming the magnetic nanonodes.

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ABSTRACT

The zigzag (n, 0) ($n=6$–10) SiC/C nanotube superlattices are investigated by using the first-principles calculations. Our calculations indicate that the (n, 0) ($n=7$–10) SiC/C nanotube superlattices are semiconducting and non-magnetic. However, the (6, 0) SiC/C nanotube superlattice shows magnetic property with $2.0\mu_B$ magnetic moments due to the curvature effect. The spin densities distribute periodically along the axial direction and mainly locate at the CNT segment, thus forming the magnetic nanonodes. The proposed magnetic nanonodes offer a method to obtain the periodic magnetic structure and thus have potential applications in future nanoscale devices.

1. Introduction

One dimensional (1D) axial heterostructures between different 1D nanomaterials have recently been of particular interest owing to their potential application in future high-performance nano-optoelectronic and nanoelectronic devices [1–3]. Compared with single-component 1D structures, 1D nanoscale heterojunctions provide the possibility to take advantages of distinct functional and properties of the individual nanosized components. The formation of 1D heterojunctions can also lead to materials with unique properties and multiple functionalities not realized in single-component structures that are useful for a wide range of applications [4–7].

Inspired by the interesting properties and potential applications of axial heterostructures, great interest has rapidly grown in nanotube–nanotube heterojunction in recent years. Theoretically, Thesing et al. [8] and Farahani et al. [9] studied the AlN/BN nanotube junction. The electric dipole was found inside the AlN/BN nanotube hollow region and the distinct electronic distribution of the valence and conduction bands suggest a spatial selective character of the hybrid nanotube [8]. There are significant changes in the nuclear magnetic response (NMR) values for the N atoms as compared to such values for the Al and B atoms within AlN/BN nanotubes [9]. The electronic and field emission properties of BN/C heteronanotubes have been investigated using the density functional theory (DFT) [10–12]. In addition, Chen et al. performed the *ab initio* elongation method calculations on the nonlinear optical properties of the BN/C single-walled nanotube heterostructure [13]. Experimentally, the BCN/C nanotube junctions have been synthesized [14], and their rectification behaviors have been evaluated. The electronic transport characteristic of an individual CN_x/C nanotube Schottky junction have been investigated [15]. Based on the individual CN_x/C heterojunction, high performance field-effect transistors were fabricated by focus ion-beam technology [16].

Since bulk silicon carbide materials possess unique physical properties, such as high hardness, high thermal conductivity, and superior radiation resistance, scientists were interested in understanding the properties of silicon carbide related materials, i.e. silicon carbide nanotubes (SiCNTs). Sun et al. have successfully synthesized the SiCNTs [17]. As the SiCNTs are formed via reaction of silicon with CNTs in the experiments, the heterojunction composed of SiCNT and CNT is worth studying. The system

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containing a large number of heterojunctions can be achieved by making the superlattices of the two constituent nanotube (SiCNT and CNT), which may be called as SiC/C nanotube superlattices (NSLs). In this work, we studied the zigzag SiC/C NSLs. It is found that the (6, 0) SiC/C NSL is spin-polarized due to the curvature effect, while the $(n, 0)$ $(n=7–10)$ SiC/C NSLs are nonspin-polarized. The obtained net magnetic moments for the unit cell in the (6, 0) SiC/C NSL is $2.0\mu_B$. The spin mainly locates at the CNT segments, thus forming the magnetic nanonodes.

2. Method and model

All calculations were performed using the Vienna *ab initio* simulation package (VASP) code adopting the projector augmented wave (PAW) potentials [18] and Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) exchange correlation functional [19]. The kinetic energy cutoff of 400 eV for the plane wave expansion is employed. The Monkhorst–Pack special *k*-point method [20] is used with a grid of $1 \times 1 \times 9$. The achieved total energy convergence is less than 2 meV. The entire systems were relaxed by conjugate gradient method until the force on each atom is less than 0.02 eV/Å. Both nonspin-polarized and spin-polarized calculations are considered.

Periodic boundary condition was applied to the nanotube superlattice along tube axis, and 15 Å lateral separation between tubes to exclude the mirror interactions. To mimic the $(n, 0)$ $(n=6–10)$ SiC/C nanotube heterostructures, two primitive unit cells for both SiCNT and CNT are employed in our calculations. The relaxation of lattice constant along the axial direction is also considered.

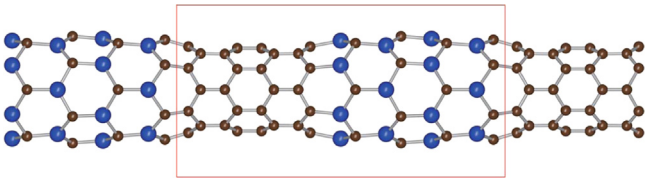

Fig. 1. Schematic view of geometric structure for the (6, 0) SiC/C nanotube superlattice. Large and blue balls denote the Si atoms, and small and brown balls denote the C atoms. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

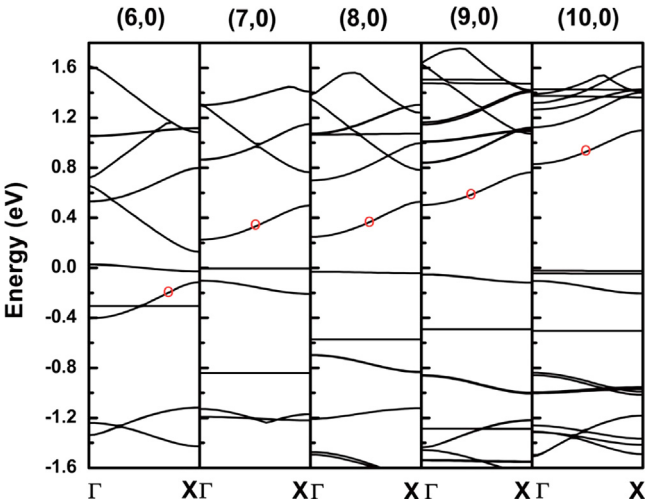

Fig. 2. Energy band structures without spin-polarization of the $(n, 0)$ $(n=6–10)$ SiC/C nanotube superlattices. The Fermi levels are all set to 0 eV.

3. Results and discussions

The optimized structure of the (6, 0) SiC/C NSL with the interface perpendicular to the tube axis is plotted in Fig. 1. Due to the lattice mismatch between CNT and SiCNT with identical structural indexes, the distortion occurs near the interface. The nearest distances between C and C atoms (d_{C-C}) and between C and Si atoms (d_{C-Si}) at the interfaces are 1.42 Å and 1.80 Å, respectively, which are slightly larger than those bonds along the axis in the middle of individual segments, i.e. 1.41 Å for d_{C-C} and 1.78 Å for d_{C-Si}. Along radial direction, C and Si atoms in SiCNT segments at the interfaces move inward, while C atoms in CNT segments at the interfaces move outward. Neither bonding mismatch nor defect is found at the interfaces. Similar results can be observed for $(n, 0)$ $(n=7–10)$ SiC/C NSLs.

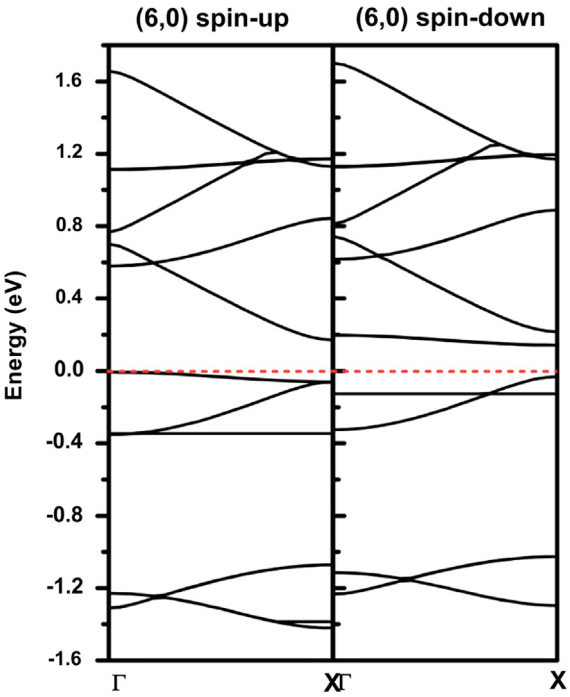

Fig. 4. Energy band structures with spin-polarization of the (6, 0) SiC/C nanotube superlattice. The Fermi levels are both set to 0 eV.

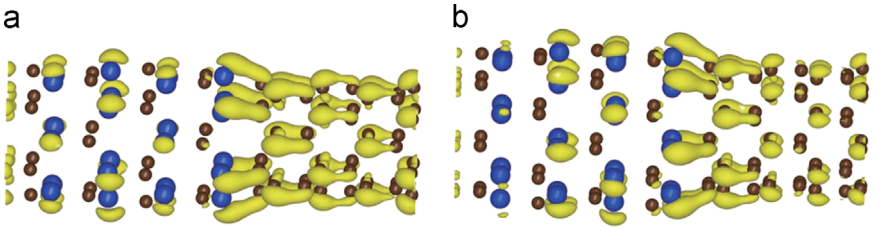

Fig. 3. Partial charge densities of the labeled band in Fig. 2 at the Γ point for (a) the (6, 0) SiC/C nanotube superlattice, and (b) the (7, 0) SiC/C nanotube superlattice.