

Predicting model for device density of states of Quantum - Confined SiC nanotube with magnetic dopant

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Abstract. Single walled (6,0) gold substituted SiC nanotube systems were studied by first principles modeling. We observed the electronic structures of SiC nanomaterials are significantly modified by the introduction of gold, and SiC:Au nanotube exhibits magnetic response. While the configurations of single walled (6,0) gold substituted SiC NTs, the energy gap decreases for the majority spin states decreases, and these systems exhibit a semimetallic behavior. From the density of states analysis, we observed that the electron orbitals arise from contributions from the C p orbitals and the 4d transition metal d orbitals. First principles results of total energy predicted the stability of the antiferromagnetic phase.

Keywords. SWSiCNT, TM-doped SiC, density of states, DMS.

1. Introduction

SiC is one of the semiconductors that has attracted considerable attention from researchers in technical applications [1-6]. Nowadays, researchers focused study of SiC in nanoscale structures according to larger flexibility coefficient and specific surface area than those of bulk configurations. The nanostructure of SiC is applied for different technological issues [7-9]. Substituted TM SWCNTs candidate for devices fabrications [1, 3, 4]. The impurities lead to charge redistribution and strengthen the ferromagnetism in SiC nanoscale structures. The ferromagnetic phase for transition metals is due to occupancy mode for d hybridization of the impurities [10, 11].

Electronic properties, magnetism for iron substituted SiCNT were simulated by the DFT using the LSDA approach [1] and the researchers found that iron substituted SiCNT has semi-metallic character, and the magnetic phase is depending on the substituting site. [12] reported that adsorption analysis of some impurity atoms substituted in SiCNT compound within DFT. It is shown that impurities can be adsorbed on the external surfaces of SWSiCNTs in the range of (1.17-3.18) eV from copper to plutonium. Heydarzadeh [13] calculated the band structure and substituted cubic SiC supercell structure and a bandgap is 2.2eV was obtained for unsubstituted SiC and a metallic character for Co-substituted compound. Electronic characteristics for (8, 0) substituted SWSiC:(Mn, Fe) NTs were simulated by ab initio and SWSiC:(Mn, Fe) systems exhibit semimetallic character, and studied compounds have potential spintronic applications [14]. [15] calculated the band structure for armchair SiCNTs by ab initio GGA approach, and obtained results indicate armchair compounds are indirect bandgap semiconductor materials, and (11,11) SiC NTs have a sufficiently large bandgap. [16] carried out ab initio DFT simulations of electronic features of single wall (6,6) silicon NT with armchair structure and results indicate this compound has indirect bandgap with 0.3 eV.

2. Calculation method

Using the Atomistic ToolKit (ATK) simulation code and using LSDA approach, we performed a DFT study of ferromagnetism in SWSiC:Au NT systems consisting of 24 atoms. The specific sample points k were generated using a $1 \times 1 \times 5$ MP grid. The value of kinetic cut-off energy taken 50 Hartree and the geometry of studied nanostructures was optimized, and for this case the strain and force toler-

ances were smaller than 0.1 GPa and 0.05 eV/Å. To predict the correct gap value and fit the experimental data, we applied the U parameters for the 4d orbitals for silicon atoms (5 eV) and 2p orbitals for carbon (4.8 eV) according to Refs. [17] and [18].

Using the Mulliken population analysis, we investigated the ferromagnetism in SiC:AuNT systems. For the analysis of the magnetic behavior for SiC nano structure compounds, the cations substituted by magnetic ions $Au^{\uparrow\downarrow}_x$ and $Au^{\uparrow\downarrow}_x$, where the signs $\downarrow\downarrow$ and $\uparrow\downarrow$ refer to the direction of the spin of gold atom.

The total magnetic moments for studied compounds are defined as the difference of occupation number between the majority and minority spin states. The projected DOS for the compounds are found within the equation (1) [19-22] and by expanding each discrete energy level

$$D_{nl\sigma}^{\alpha}(E) = \sum_i A_{nl\sigma i}^{\alpha} \frac{\delta / \pi}{(E - \varepsilon_{i\sigma})^2 + \delta^2}, \quad (1)$$

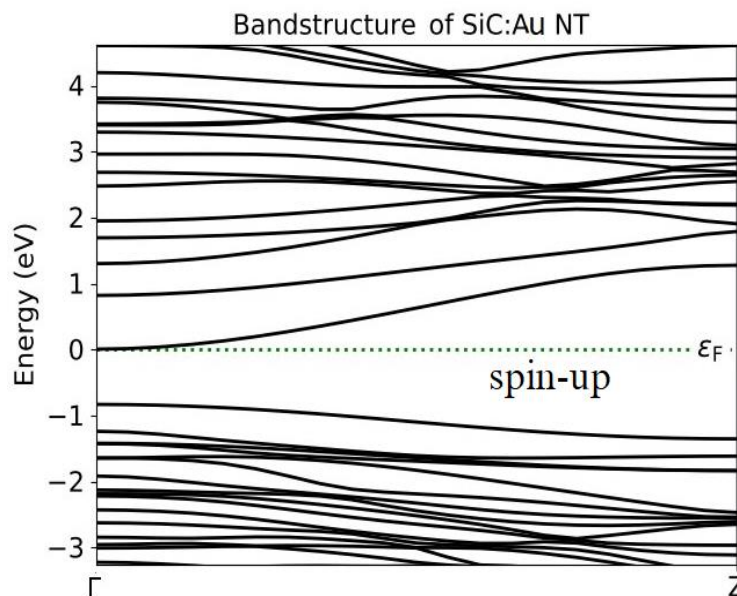
where i is the energy level index, the σ term indicates the spin, $A_{nl\sigma i}^{\alpha}$ is the orbital of atomic number α . The TDOS are defined to sum up the PDOS

$$D_{\sigma}(E) = \sum_{nl\alpha} D_{nl\sigma}^{\alpha}(E). \quad (2)$$

3. Results and discussion

3.1. Electronic characteristics in TM:SiCNT

In this paragraph, we reported the results of our calculations for the electronic structures and the electronic density of states (DOS) for SWSiC:AuNT. From the calculated minority and majority spin band structures, we have found the bandgap for gold substituted SiC NTs. The obtained results of electronic structure, DOS diagrams of SWSiC:AuNT systems shown in Fig.1, Fig.2, respectively. The ab initio results predicted that the values of bandgaps are 0.8; 0eV consist to majority, minority-spin states.



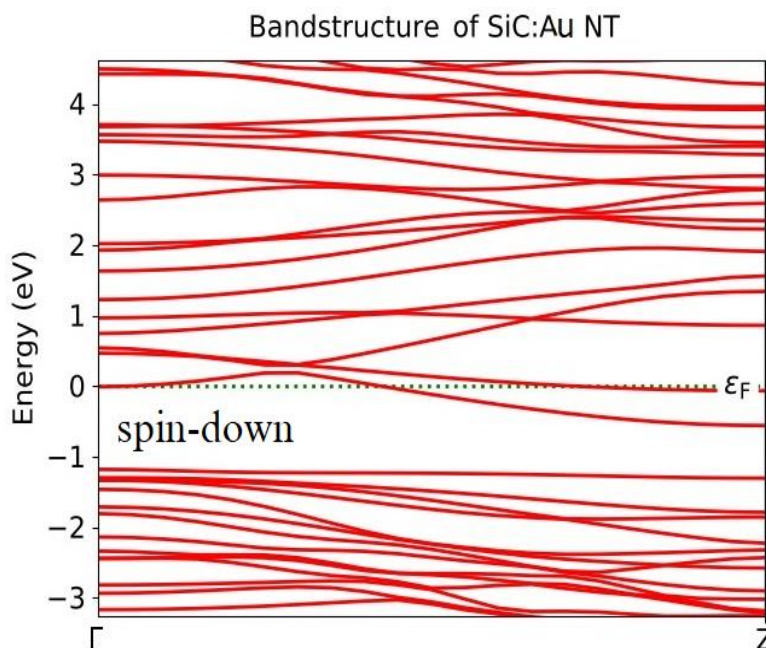
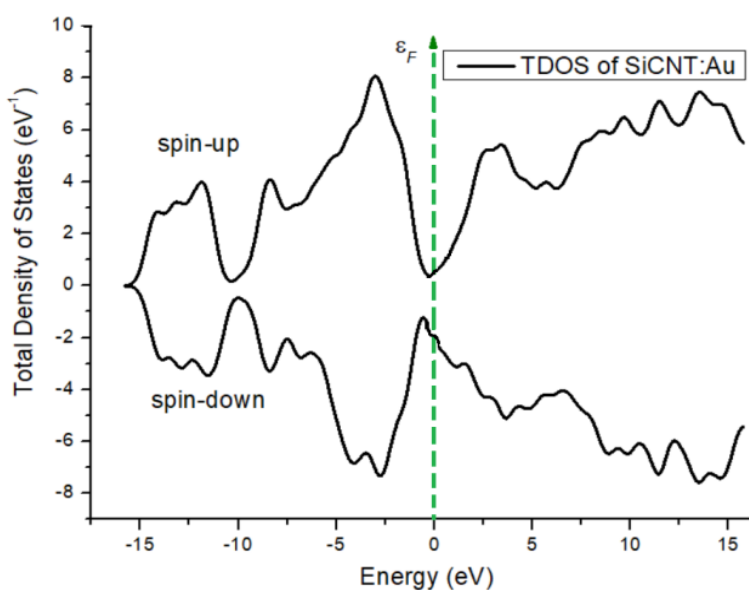


Figure 1. The calculated band structures for SWSiC:AuNTs.

From simulations, minority spin bandgap is narrowing to 0 eV after gold substituted in silicon site in the (6,0) SiC NT and studied compound with nanoscale structure exhibits metallic character. Thus, our calculations results show that the energy bands of impurity overlapping with the Fermi energy. The results for Au-substituted SiC NT predicted that the projected DOS curves mainly due to the contribution of C *p*-orbitals and *d*-orbitals of the gold. The states located at Fermi level dominated by the 4 *d* electronic orbitals of gold, indicating the presence of pd hybridization of 2 *p*-states of C and 4 *d*-states of Au.



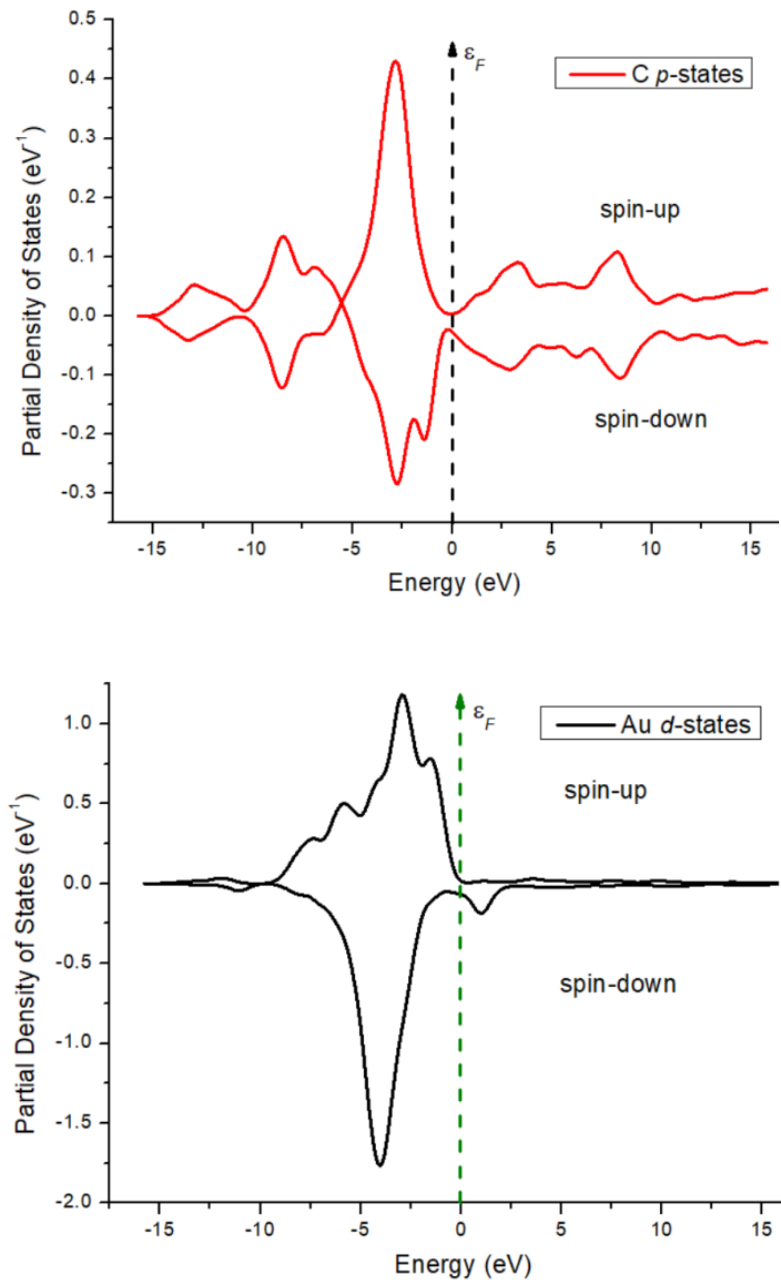


Figure 2. The calculated DOS diagrams for SWSiC:Au NTs.

3.2. Magnetic characteristics in TM:SiCNT

In this section, we simulated the magnetism in Au-substituted in SW SiC NT compounds from the analysis of Mulliken population. In the case of Au metal substituted in silicon site in the studied compound, we found the magnetic response of SiC:Au. The side view of spin-polarization for Au-substituted SiCNT structure are described in Fig.3. In Fig.3, the arrows show the directions of magnetic moments and the overall magnetization of SWSiC:AuNT is $\sim 3.2 \mu_B$. The interpretation of obtained results predicted a large contribution to magnetic response of SiC:AuNT due to three C atoms ($\sim 6 \mu_B$), chemically bonded to impurity. Fig. 4 described the DOS curves for 3C atoms. From

Fig.4, we found asymmetry for SiC:AuNT, this result indicates the magnetic response of studied compound.

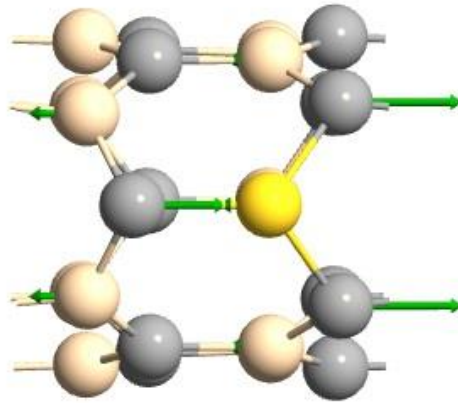


Figure 3. Spin-polarization view of SiC:Au NT: gray-carbon, beige-silicon, and yellow-gold.

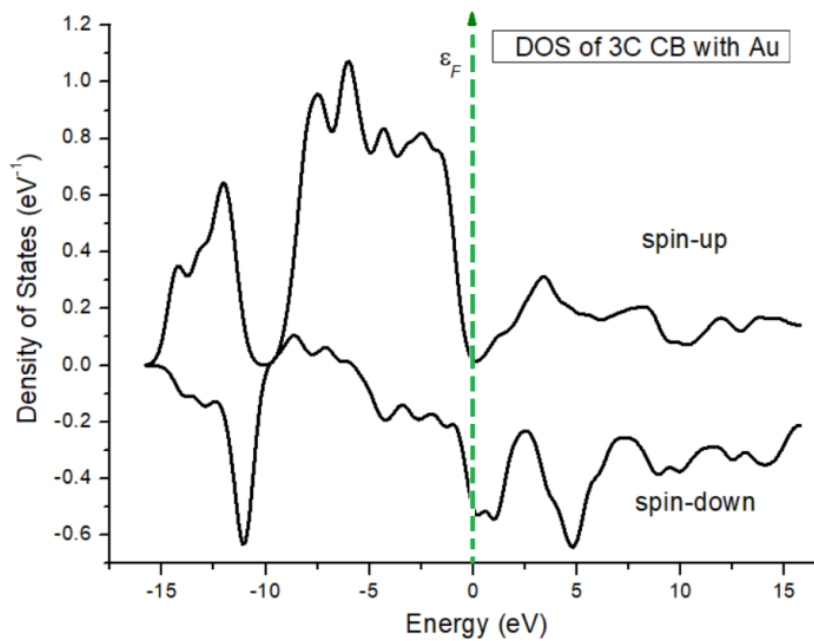


Figure 4. The calculated DOS for carbon atoms chemically bonded to Au.

The both structure atoms in SiC:AuNT contributed positive (C, $\sim 1.7 \mu_B$) and negative (Si, $\sim 4.8 \mu_B$) magnetic moments to magnetization. The values of local spin moment of impurity atom (Au) is negative ($\sim 0.8 \mu_B$; $\sim 0.3 \mu_B$ by the d electrons). Two silicon atoms weakened (see (Fig. 3) the total magnetization of SiC:AuNT within a magnetic moment of $\sim 1 \mu_B$.

It is known that, the analysis stability of FM and AFM behavior in SiC:AuNT, requires to calculate the total energies: the total energy differences between the FM and AFM phases ($E_{FM} = -6205.37207$; $E_{AFM} = -6205.48002$ eV) is positive, indicates the more stability of AFM phase than the FM for SWSiC:AuNT compounds.

4. Conclusion

Using an accurate DFT-LSDA+U approach, have been explored the spin-polarized electronic and magnetic properties of $\text{Si}_{1-x}\text{TM}_x\text{C}$ nanotube containing 24 atoms. From DFT study, we predicted the electronic and magnetic characteristics of SWSiC:AuNT compound with chirality of (6,0). The SWSiC:AuNTs exhibit semimetallic character while the Au substituted in Si site. The analysis of spin magnetization of SiC:AuNT predicted the value of magnetic moment is $\sim 3 \mu_B$ especially generated with C atoms chemically bonded to the gold. The computed total energies of SiC:AuNTs show the stability of the antiferromagnetic state.

Our study demonstrates the application possibility of SiC:AuNT compounds in optoelectronics and for spintronic devices, and also provides a reference information the analysis of magnetic feature for the Si-based compounds.

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