Technium Vol. 26, pp.1-8 (2025)
ISSN: 2668-778X
www.techniumscience.com

Prediction of ferromagnetic characteristics of gold doped SiC nanotubes for application in spintronic devices

V.N. Jafarova[1,2,3*], V.I. Eminova[3,4], M.A. Musaev[1], I. C. Scurtu[5]

[1]Azerbaijan State Oil and Industry University, 20 Azalig Ave., AZ-1010, Baku, Azerbaijan
[2]Khazar University, 41 Mehseti Str., AZ1096, Baku, Azerbaijan
[3]Ministry of Science and Education Republic of Azerbaijan, Institute of Physics, 131 H. Javid Ave., AZ-1143, Baku, Azerbaijan
[4]French-Azerbaijani University (UFAZ) under Azerbaijan State Oil and Industry University, 183 Nizami Str., AZ-1010, Baku, Azerbaijan
[5]Romanian Naval Academy, 1 Fulgerului Str., 900218, Constanta, Romania

Corresponding author: vcafarova@beu.edu.az

Abstract. Single walled (6,0) gold doped 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 these systems exhibit magnetic properties. While the configurations of single walled (6,0) gold doped SiC nanotubes, the energy gap width of the spin-up states decreases, and these systems exhibit a semi-metallic character. Partial density of states analysis shows 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: SiC:Au, nanotube, chiral, antiferromagnetic, half-metallic

1. Introduction

SiC is one of the semiconductors that has attracted considerable attention from researchers in technical applications [1–6]. Recently, researchers have focused on the study of SiC with nanoscale materials due to their larger flexibility coefficient and specific surface area than those of bulk configurations. The nanostructure of SiC is also applied for energy harvesting for biocompatibility studies, biomedical research, and sensing [7-9]. Doped TM SWCNTs have potential for technical fabrications in chemical sensors, and nanoscale devices [1, 3, 4]. The impurities lead to charge redistribution and forced magnetic behavior nearby the atoms of SiC nanostructures. The ferromagnetic (FM) behavior for TM atoms is due to the occupancy mode of d-orbital hybridization of the dopants [10, 11].

The electronic properties and magnetism for SiC:Fe NT were studied based on the DFT using the LSDA approach by Zhang et al. [1] and obtained this system of semi-metallic antiferromagnetic and ferromagnetic material depending on the doping sites. [12] reported the adsorption analysis of some

Technium Vol. 26, pp.1-8 (2025)
ISSN: 2668-778X
www.techniumscience.com

TM atoms doped on SWSiCNT using DFT methods. It is found that impurities can be chemically adsorbed on the external surface of SWSiCNT with binding energies in the range of (1.17-3.18) eV from Cu to Pt. Heydarzadeh [13] studied of electronic structure of c and doped cubic SiC supercell and a band gap of 2.2 eV was obtained for undoped SiC and a metallic nature for the Co-doped system. The electronic properties of (8, 0) doped SWSiC:(Mn, Fe) NTs were investigated by DFT method and these systems exhibit semi-metallic properties with potential spintronic applications [14]. [15] calculated the band structure for armchair SiCNTs by DFT-GGA method, and their results indicated that armchair systems are indirect-gap semiconductor materials, and SiCNTs with (11,11) chirality have a large band gap. [16] performed first-principles DFT calculations of electronic properties of SW armchair (6,6) SiNTs and obtained results indicating that this system is indirect-gap with 0.314 eV.

Studies have shown that the chirality of NT systems profoundly affects their chemical and physical properties, opening up potential for specific technical applications. The most interesting aspect of single-walled nanotubes is that their electronic structure can become either semiconducting or semi-metallic or metallic behaviors depending on the chirality. It is also interesting that the width of the energy gap also depends on the chirality.

2. Computational details

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 1×1×5 Monkhorst-Pack grid. The cutoff energy was taken at 50 Ha and the geometry of studied nanostructures was optimized, and for this case the strain and force tolerances 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 states of Si atoms (5 eV) and 2p states for C atoms (4.8 eV) according to Refs. [17] and [18].

Using the Mulliken population analysis, we investigated the ferromagnetism in SiC:AuNT systems. To investigate the FM and AFM behavior for diluted SiC nanotubes, the cations were randomly substituted by magnetic ions $Au^{\uparrow\uparrow}{}_x$ and $Au^{\uparrow\downarrow}{}_x$, where the signs ↓↓ and ↑↓ refer to the direction of the spin of gold atom.

3. Results

3.1. Electronic properties of SiC:Au nanotube

We calculated the majority and minority spin band structures and the density of states (DOS) for SWSiC:AuNT. From the calculated first-principles band structures, we estimated band gap of these systems. The results of the first-principles band structure and DOS diagrams for SWSiC:AuNT systems are shown in Figs. 1 and 2. From the calculated band structures, we found the width of band gap and obtained the majority (0.8 eV) and minority spin states (0 eV).

Technium Vol. 26, pp.1-8 (2025)
ISSN: 2668-778X
www.techniumscience.com

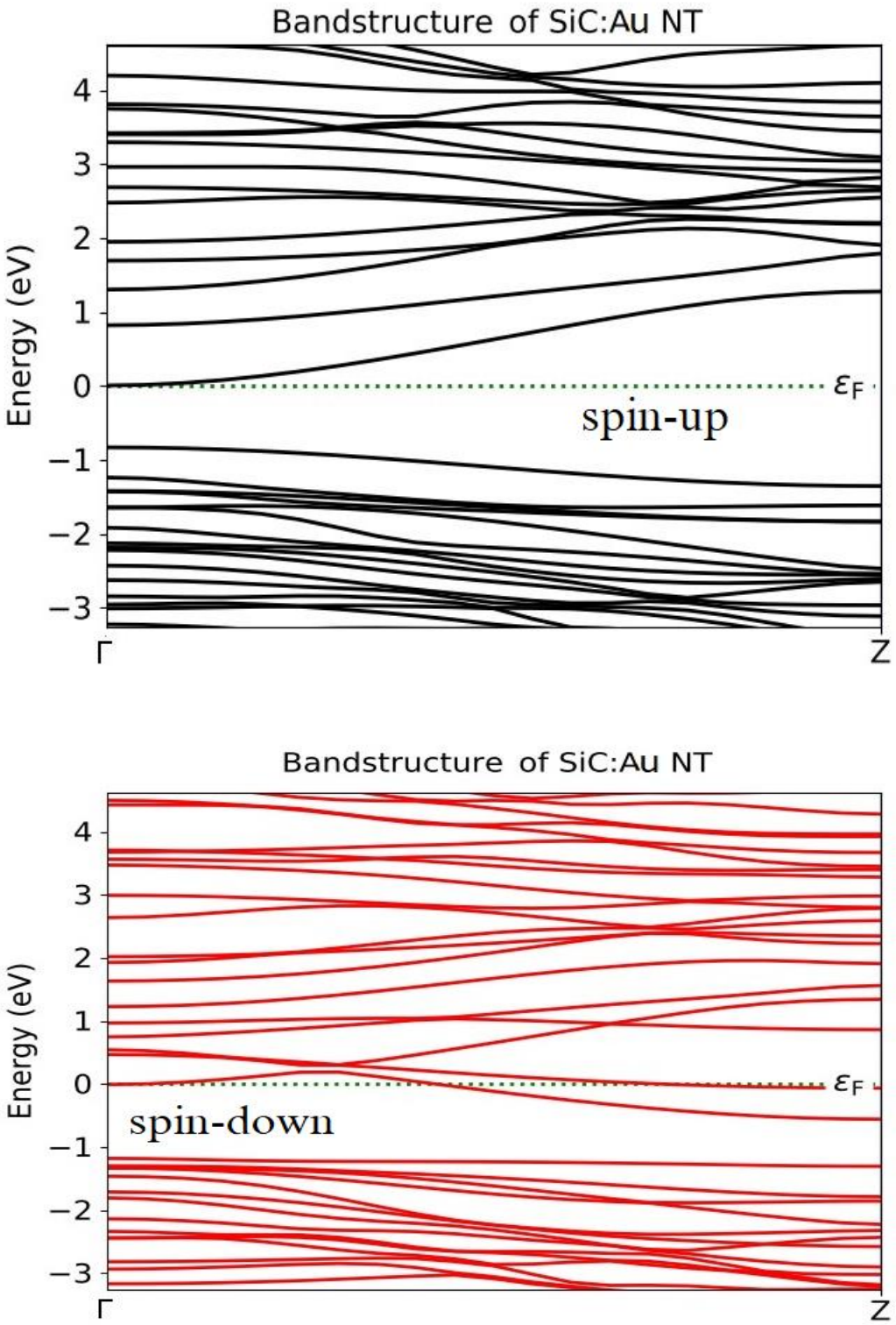
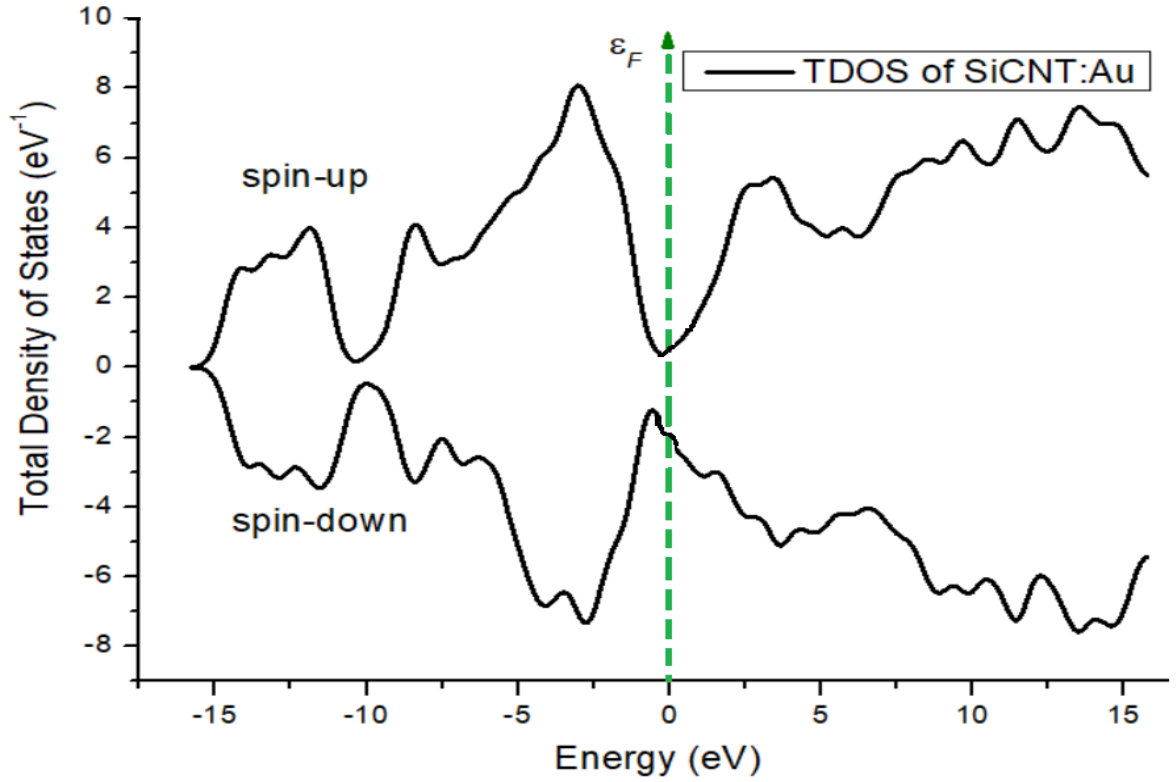
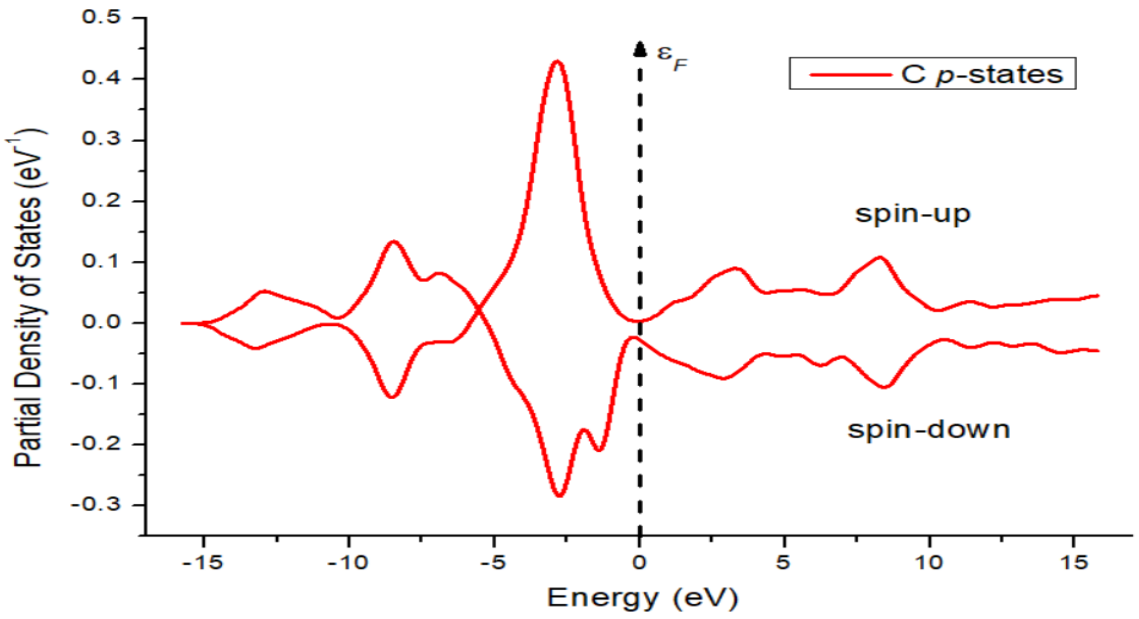


Figure 1. The calculated band structures for SWSiC:AuNTs.


Total Density of States (eV-1)
Energy (eV)
εF
TDOS of SiCNT:Au
spin-up
spin-down


Partial Density of States (eV-1)
Energy (eV)
εF
C p-states
spin-up
spin-down

Technium Vol. 26, pp.1-8 (2025)
ISSN: 2668-778X
www.techniumscience.com

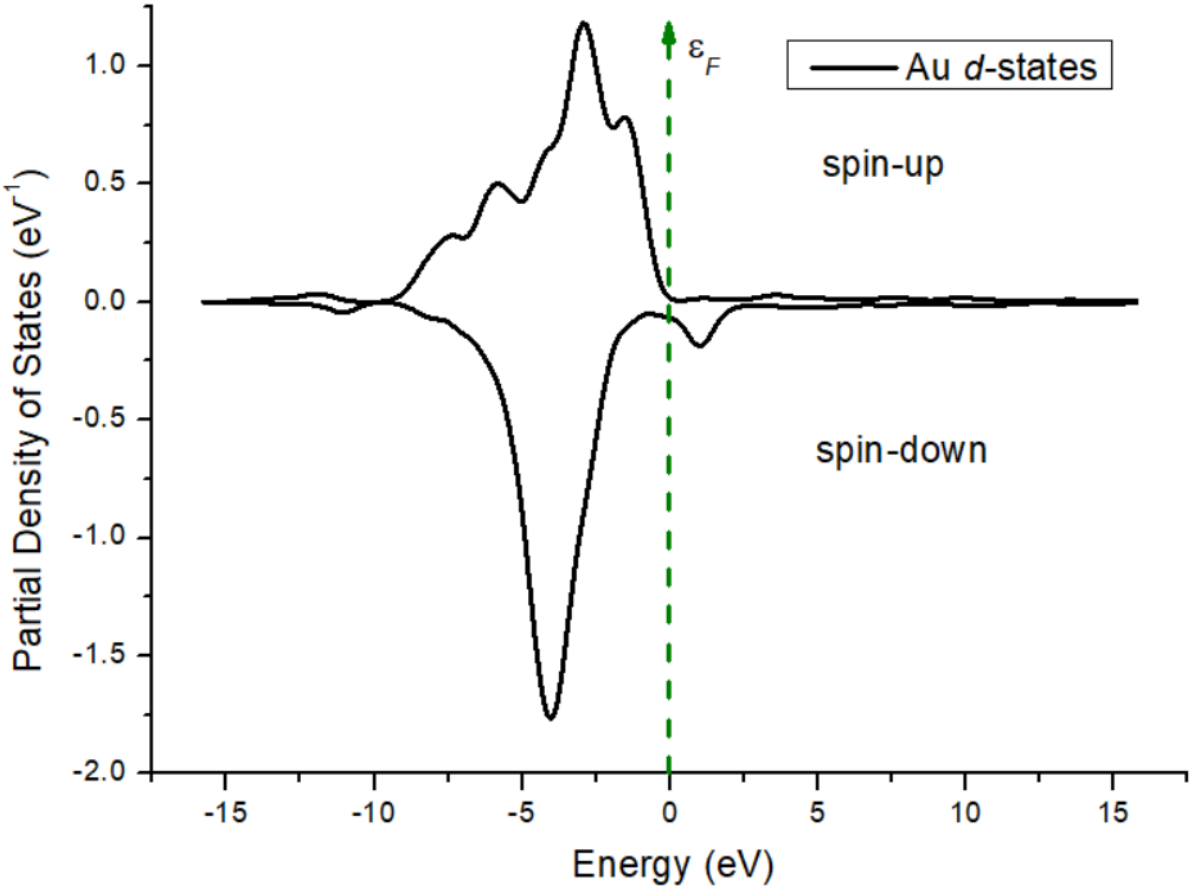


Figure 2. The calculated DOS diagrams for SWSiC:Au NTs.

From first-principles simulations, the minority spin band gap of the Au-doped (6,0) SWSiCNT is reduced to 0 eV, and this nanosystem becomes metalized. The bands that are located nearby the Fermi energy overlap with the another conduction band and cross the Fermi level. An investigation of the projected DOS curves for the Au-doped (6,0) SWSiCNT system shows these states mainly due to the contribution of the *p* orbitals of the host carbon and *d* electrons of the gold atom. From first-principles calculations, we obtained the states located at the Fermi level are dominated by the 4*d*-states of gold, demonstrating the presence of hybridization between 2p-states of C and 4d-states of Au.

3.2. Magnetism in SiC:AuNT

In this paper, we also studied the magnetism in gold-doped SWSiCNT systems from Mulliken population analysis using ATK code. The introduction of an Au into the structure of a SiC NT leads to magnetization of the studied systems. The spin-polarization view of Au-doped SiC NT are given in Fig. 3 and in this figure, the green arrows show the spin moments and the overall magnetization of the SWSiC:AuNT is 3.174 μ_B. The analysis of the results shows that a large contribution to the magnetization of Au-doped SiCNT systems comes from 3 carbon (~ 6.3 μ_B), which are chemically bonded to the dopant. The density of states for three carbon atoms chemically bonded with dopant is plotted in Fig. 4 and we observed strong asymmetry in this figure that indicate magnetization of the Au-doped SiCNT system.

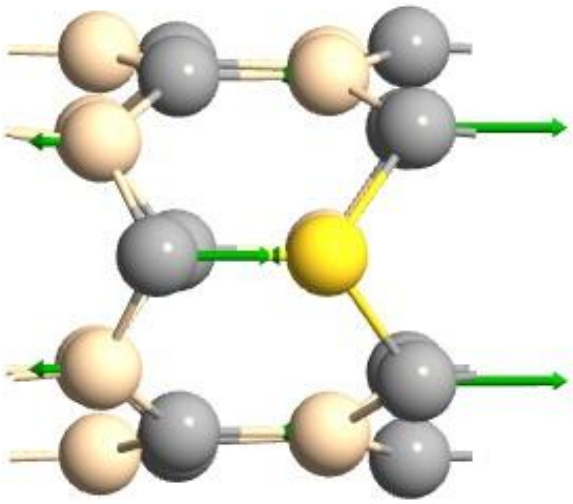


Figure 3. Spin-polarization view of SiC:Au NT: gray-carbon, beige-silicon, and yellow-gold.

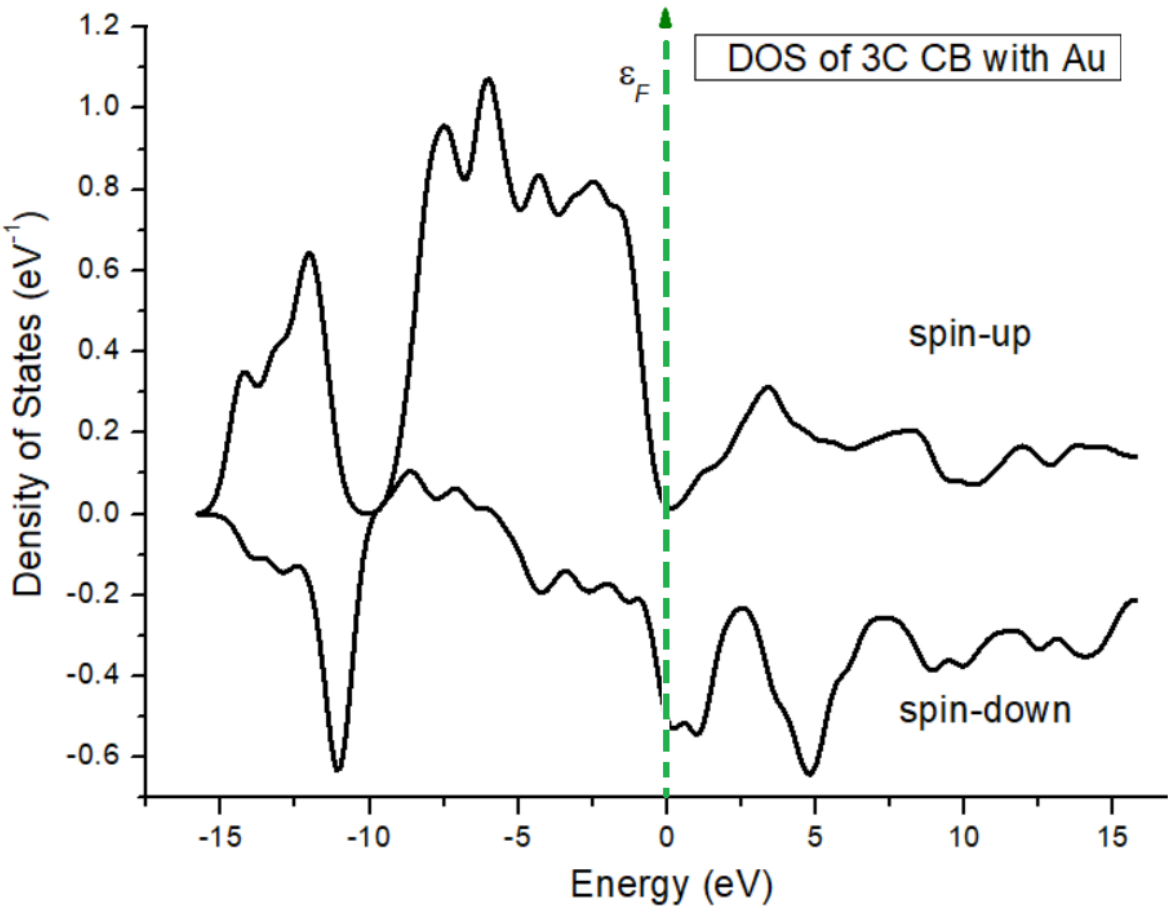


Figure 4. Spin-polarization DOS diagrams for 3C atoms chemically bonded with Au.

The other host carbon and silicon atoms of SiC NT structure give positive (~1.7 μ_B) and negative (~4.8 μ_B) contributions to the magnetization of systems. The local spin moment of Au is equal to -0.8 μ_B (~0.3 μ_B from d electrons). As can be seen from Fig. 3, two Si atoms weaken the magnetization of the SiC:AuNT with a magnetic moment of ~1 μ_B.

To analyze the FM and AFM behavior of Au-doped SiC nanotubes, we also calculated the total energies for these states. We found that the total energy difference between the FM (- 6205.37207 eV) and AFM (-6205.48002 eV) states is positive and this result indicates that for the SWSiC:Au NT, the AFM state is more stable than the FM state.

4. Conclusion

In this work, we report the study of the electronic and magnetic properties of and Au-doped (6,0) SWSiCNTs using DFT simulations. We found that these physical properties of investigated systems are changed significantly by transition metal functionalization. The (6,0) SWSiCNTs exhibit half-metallic characteristics for gold-doped on Si sites. The spin-polarized electron density results for Au-doped SiCNT indicate that the overall magnetic moments (~3.2 μ_B) of the systems are mainly generated by three carbon atoms (~6 μ_B) that are chemically bonded to the gold atom. The total energy results of SiC:AuNTs show the stability of the antiferromagnetic state.

Our study demonstrates the application of Au-doped (6,0) SWSiCNTs in optoelectronics and spintronics, and provides a reference information for the analysis of magnetism in graphene-like semiconductor compounds. All first-principles results of our studies show that the TM doped SWSiCNT could be a potential material to produce important magnetic materials for application in optoelectronic and spintronic devices.

References

[1] W. Zhang, F. Zhang, Z. Zhang, S. Lu, Y. Yang, “Electronic structure and magnetism of Fe-doped SiC nanotubes,” *Science China Physics, Mechanics & Astronomy*, vol. 53, no. 9, pp. 1582-1589, 2010, doi: 10.1007/s11433-010-4089-8.

[2] R. Madar, “Silicon carbide in contention,” *Nature*, vol. 430, pp. 974-975, 2004, doi: 10.1038/430974a.

[3] A. Gali, “Ab initio study of nitrogen and boron substitutional impurities in single-wall SiC nanotubes,” *Phys. Rev. B*, vol. 73, pp. 245415-1-9, 2006, doi: 10.1103/PhysRevB.73.245415.

[4] K.M. Alam, A.K. Ray, “Hybrid density functional study of armchair SiC nanotubes,” *Phys. Rev. B*, vol. 77, no. 3, pp. 035436-1-10, 2008, doi: 10.1103/PhysRevB.77.035436.

[5] B. Baumeier, P. Krüger, J. Pollmann, “Structural, elastic, and electronic properties of SiC, BN, and BeO nanotubes,” *Phys. Rev. B*, vol. 76, no. 8, pp. 085407-1-10, 2007, doi: 10.1103/PhysRevB.76.085407.

[6] S. Mukherjee, A.K. Ray, “Ab initio study of molecular hydrogen interaction with SiC nanotube-a precursor to hydrogen storage,” *J. Comput. Theor. Nanosci.*, vol .5, no. 7, pp. 1210-1219, 2008, doi: 10.1166/jctn.2008.2556.

[7] J.S. Ponraj, S.C. Dhanabalan, G. Attolini, G. Salviati, “SiC nanostructures towardbiomedical applications and its future challenges,” *Crit. Rev. Solid State Mater. Sci.*, vol. 41, no. 5, pp. 430-446, 2016, doi: 10.1080/10408436.2016.1150806.

[8] R. Yakimova, Jr.R. M. Petoral, G.R. Yazdi, C. Vahlberg, A.L. Spetz, K. Uvdal, “Surface functionalization and biomedical applications based on SiC,” *J. Phys. D: Appl. Phys.*, vol. 40, pp. 6435-6442, 2007, doi: 10.1088/0022-3727/40/20/S20.

[9] A.M. Manal, S.H. Kenawy, M.A.H. Esmat, T.E.-B. Gehan, I.K. El Zawawi, “Influence of silicon carbide on structural, optical and magnetic properties of Wollastonite/Fe_2O_3 nanocomposites,” *Ceram. Int.*, vol. 47, no. 9, pp. 12047-12055, 2021, doi: 10.1016/j.ceramint.2021.01.048.

[10] M.L. Sun, Q.Q. Ren, Y.M. Zhao, J.P. Chou, J. Yu, W.C. Tang, "Electronic and magnetic properties of 4D series transition metal substituted graphene: A first-principles study," *Carbon*, vol. 120, pp. 265–273, 2017, doi: 10.1016/j.carbon.2017.04.060.
[11] E. Santos, A. Ayuela, D. Sanchez-Portal, "First-principles study of substitutional metal impurities in gr aphene: Structural, electronic and magnetic properties," *New J. Phys.*, vol. 12, no. 5, pp. 053012-1-32, 2010, doi: 10.1088/1367-2630/12/5/053012.
[12] J.X. Zhao, Y.H. Ding, "Silicon carbide nanotubes functionalized by transition metal atoms: A density-functional study," *J. Phys. Chem. C*, vol. 112, no. 7, pp. 2558-2564, 2008, doi: 10.1021/jp073722m.
[13] H. Heidarzadeh, "Transition metal-doped 3C-SiC as a promising material for intermediate band solar cells," *Opt. Quantum Electron.*, vol. 51, no. 1, pp. 32-1-11, 2019, doi: 10.1007/s11082-019-1742-y.
[14] A.T. Mulatu, K.N. Nigussa, L.D. Deja, "Electronic and optical properties of TM-doped (8,0) SiC SWNT and the prospect of hydrogen storage," *Opt. Mater. A*, vol. 134, pp. 113094-1-12, 2022, doi: 10.1016/j.optmat.2022.113094.
[15] Ch. Vatankhah, Badehian H.A., "Electronic and optical properties of armchair silicon carbide nanotubes from first principles," *Optik*, vol. 237, pp. 166740-1-7, 2021, doi: 10.1016/j.ijleo.2021.166740.
[16] W. Wang, J. Xu, Y. Zhang, G. Li, "First-Principles Study of Electronic Structure and Optical Properties of Silicon/Carbon Nanotube," *Comp. Chem.*, vol. 5, no. 4, pp. 159-171, 2017, doi: 10.4236/cc.2017.54013.
[17] S.L. Dudarev, G.A. Botton, S.Y. Savrasov, C.J. Humphreys, A.P. Sutton, "Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+U study," *Phys. Rev. B*, vol. 57, no. 3, pp. 1505-1509, 1998, doi: 10.1103/PhysRevB.57.1505.
[18] A.I. Liechtenstein, V.I. Anisimov, J. Zaanen, "Density-functional theory and strong interactions: Orbital ordering in Mott-Hubbard insulators," *Phys.Rev.*, vol. 52, no. 8, pp. R5467-R5471, 1995, doi: 10.1103/physrevb.52.r5467.