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Electronic and magnetic characteristics of Vanadium doped single-walled silicon carbide nanotubes: DFT study

Sevda Rzayeva[a,b,c], Vusala Nabi Jafarova[b,d,e,1],

[a]Azerbaijan State University & Economics, 6 Istiglaliyyat Str., AZ-1123, Baku, Azerbaijan
[b]Ministry of Science and Education Republic of Azerbaijan, Institute of Physics, 131 H. Javid Ave., AZ-1143, Baku, Azerbaijan
[c]Azerbaijan State Oil and Industry University, 20 Azadlig Ave., AZ-1010, Baku, Azerbaijan
[d]Department of Physics, Azerbaijan State Oil and Industry University, 20 Azalig Ave., AZ-1010, Baku, Azerbaijan
[e]Khazar University, 41 Mehseti Str., AZ 1096, Baku, Azerbaijan

Abstract: In this study, the physical properties of vanadium-doped single-walled silicon carbide (SWSiC:V) nanotubes are theoretically investigated using local spin density estimation and density functional theory methods with Hubbard U-corrections. These properties were modeled for the cases where one or two silicon atoms were replaced by vanadium atoms in the structure of silicon carbide nanotubes. The SiC nanotube with V doping of ~1.0 μ_B induces magnetization, and this magnetic material has a net magnetic moment even though the undoped SiC system is non-magnetic. The population density calculations showed that the magnetization of the single-walled SiC:V nanotube is mainly due to the 3d and 2p- orbitals of the V dopant and the orbital carbon atoms. According to the results of total energy calculations, the ferromagnetic phase is more stable than the antiferromagnetic phase.

Keywords: DFT, band structure, magnetism, vanadium doped SiC, density of states.

1. Introduction

Recently, diluted magnetic semiconductors (DMSs) materials have attracted much attention from researchers for the use in spintronic, optoelectronic and magnetoelectronic equipment [1-4]. The study of ferromagnetism has opened up new technical possibilities in carbon and carbon-based compounds for 3d transition metals (TMs) doped systems [5-7]. SWSiCN has uniform physical characteristics because it can behave as metals or semiconductors depending on the tube curvature, chirality, length and diameter silicon carbide is the most complex material with a wide energy gap, high thermal conductivity, and radiation resistance and is suitable for use in electronic equipment. SiC binary composite is also used in ceramics, metals and alloys, and for biotechnology purposes, silicon carbide nanosystems are suitable for the application of nanosensors and nanodevices, which can be used under high power, high temperature and high frequency [8-9].

A number of theoretical works have studied the electronic, magnetic and structural features of silicon carbide nanosheets, nanoribbons and nanotubes [10-13]. However, the magnetic features of 3d TM-doped silicon carbide nanotubes have been investigated less by theoretical researchers. Various explore groups have synthesized SiC nanotubes [14-20]. Theoretical [21-24] and experimental [25] studies focusing on the interaction of transition metal atoms with SWSiCNTs have reported significant changes in the electronic, magnetic and structural features of these systems.

[1] Corresponding Authors
e-mail: vusale.cafarova@asoiu.edu.az

In this paper, we report the electronic and magnetic features derived from our DFT results for the junctions of V-doped single-walled (6,0) SiC nanotubes. Nowadays, in the polymer industry, the trade-off between the performances of rubber material plays a crucial role [26], and the molecular modeling of the dynamic physical characteristics of the vulcanized rubber material can be evaluated using DFT.

2. Computational Method

The electronic and magnetic properties of the undoped SiC and doped SiC:V nanosystems were modeled using Density Functional Theory (DFT). The exchange-correlation effects are taken into account in the local density approximation (LDA) and local spin density approximation (LSDA) frameworks, respectively, and Hubbard U semi-empirical corrections for the Atomistix ToolKit (http://quantumwise.com/) code. DFT is infamous for foretelling very small band gaps. It is well known that local density approximation (LDA) functional generally underestimate band gaps and that hybrid DFT or self-interaction corrected calculations correct these issues more universally in most systems. Nevertheless, the last progress of LDA functionals and using Hubbard U semiempirical corrections have given us an opportunity to determine correct band gaps of materials. By successfully correcting the electronic band structure of the investigated compounds using Hubbard U semiempirical correction, can future extend the study of magnetic properties of doped systems. First-principles computations were performed using linear combinations of atomic orbitals (LCAO) and the pseudopotential method. The Perdew Zunger (PZ) functional and Fritz-Haber-Institute (FHI) ionic pseudopotentials within the Double Zeta Polarized (DZP) basis set were described the exchange correlations and interactions between electrons and ions, respectively. The kinetic energy cut-off of 75 Ha, which has Kohn-Sham wave functions, was extended in a linear combination with atomic orbitals. Single-walled SiC:V nanotubes with a chirally (6.0) equilibrium configuration were prepared by holding the atomic coordinates until the strain resistance and maximum atomic force were below 0.001 eV/Å3 and 0.001 eV/Å, respectively. Cross-spatial integration was performed using a standard electron temperature of 300 K and a 1×1×5 Monkhorst-Pack *k*-point sampling method. Note that for all simulations, the plane-wave fundamental set cut-off energy approach and the SiC *k*-point sampling Brillouin grid zone integration are tested, thus yielding Hubbard U corrections of 5 eV for Si 4d- and 4.8 eV for C 2p-states. The Hubbard U correction is applied using the simplified approach according to Dudarev et al. [27], which corresponds to the case J=0 in the more elaborate expression by Lichtenstein et al. [28].

Using Mulliken population analysis we computed the values of magnetic moments of 3d metal-doped SWSiC:V NTs. The Mulliken population analysis has been performed to obtain the occupation number of each atom orbital. Thus the magnetic moments are defined as the difference of occupation number between the spin-up and spin-down states. The partial density of states of the spin is obtained by expanding each discrete energy level according to the Lorentzian formula (1) [29]

$$D^{\alpha}_{nl\sigma}(E)=\sum_{i}A^{\alpha}_{nl\sigma i}\frac{\delta/\pi}{\left(E-\varepsilon_{i\sigma}\right)^{2}+\delta^{2}} \quad ..(1)$$

where i and σ are the indexes of energy level and spin, respectively, $A^{\alpha}_{nl\sigma i}$ is the Mulliken population of atomic orbital of atom α. The total density of states of the spin is defined as the sum of the partial density of states

$$D_{\sigma}(E)=\sum_{nl\alpha}D^{\alpha}_{nl\sigma}(E) \qquad (2)$$

In modeling the antiferromagnetic position of dilute magnetic nanotubes, cations (Si) were randomly replaced by magnetic ions V↓x/2 and V↑x/2 through the signs ↓↑, associated with the direction of local moments of impurities. Silicon, vanadium and carbon atoms with valence electrons were defined as [Ne] $3s^2$, $3p^2$, [He] $2s^2$, $2p^2$, and [Ar] $3d^3$, $4s^2$, respectively.

3. Results and discussion

3.1 Electronic properties of pure SiC NTs

The studied wurtzite compound SiC has a wide indirect band gap of about 3.3 eV and this property has been useful for applications in electronics and optics. Some theoretical studies have investigated the electronic properties of SiC nanostructure [27-

30] and wurtzite structure [31, 32]. However, less theoretical studies have been devoted to the magnetic properties of SiC:Co nanotubes. The authors were informed about the results for the electronic bands and density of states (DOS) using DFT and generalized gradient approximation (GGA) with GW scheme [31].

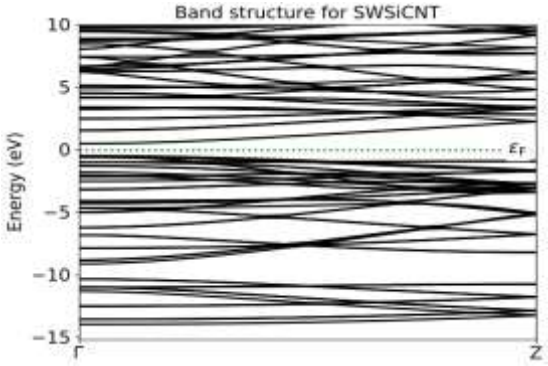
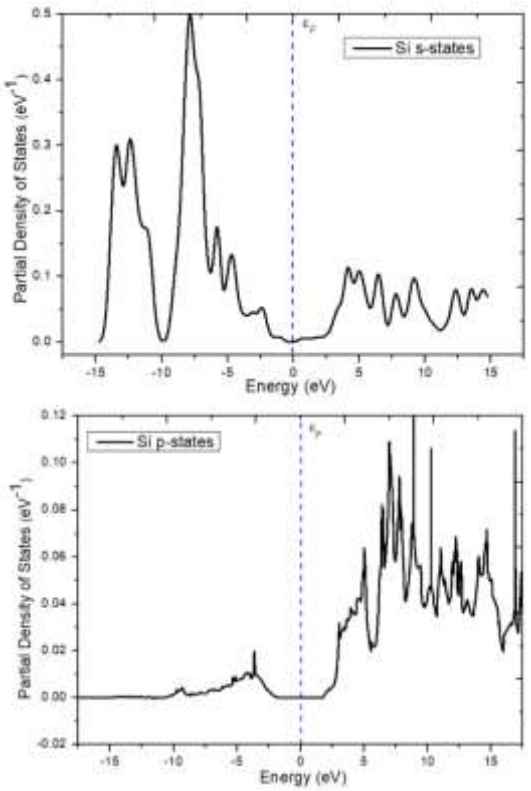


Figure 1. Electronic band structure for undoped SWSiC (6,0) nanotube (E_g=0.98 eV) within LDA.



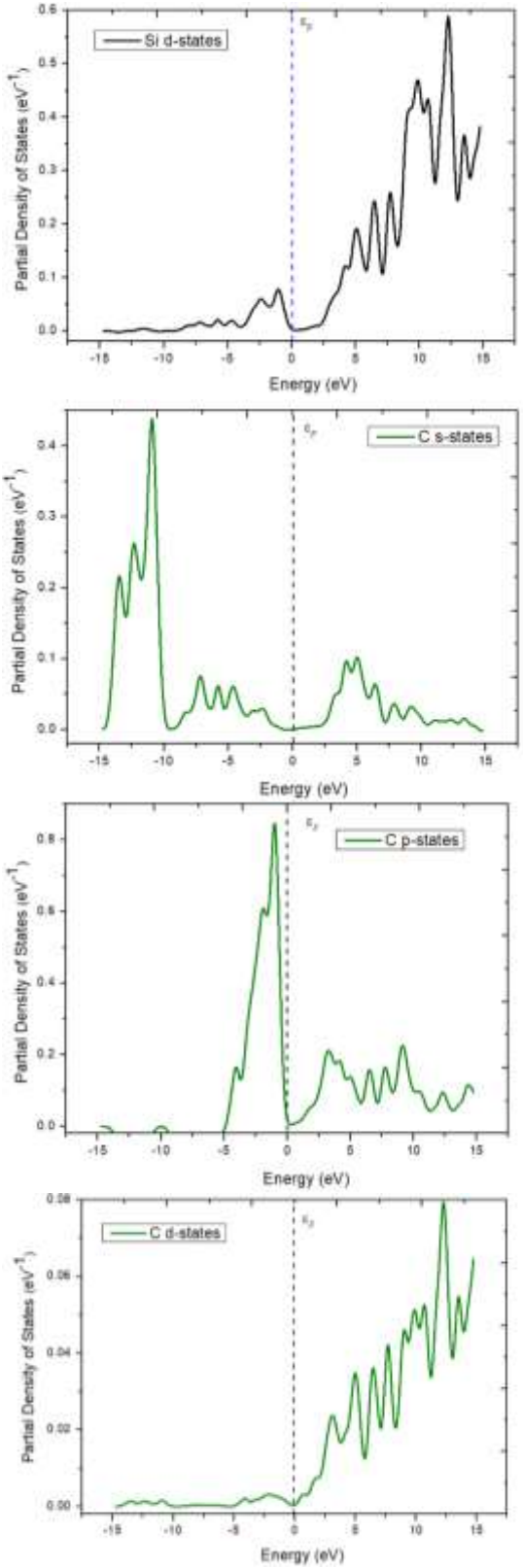


Figure 2. Spin-polarized DOS diagrams for undoped (6,0) SWSiC NT within LDA.

In this work, the calculated energy gap is about 3.17 eV for the hexagonal structure of SiC. The

electronic band structure for the SiC-2H structure was studied using GGA and the result for the band gap of 2.3 eV was obtained, which was about 1.0 eV lower than the experimental result [31]. In this work, for U=5 eV for Si 4d states and U=4.8 eV for C 2p states, we obtained the first-principles values of direct and indirect band gap of 5.2 and 3.3 eV. The spin-polarized band structure, total and partial density of states (PDOS and TDOS) diagrams for undoped (6,0) single-walled SiC NT are shown in Figs. 1 and 2.From DFT-based calculations, we obtained that chiral SiC NT has a direct band gap (Γ- Γ), and the band gap is 0.98 eV for undoped non-magnetic SWSiC NT, and this result is smaller than that of pure SiC NT. This fact is closer to the result in [31, 32].

3.2 Electronic properties of SiC:V NT

In this work, one (Figure 3) and two silicon atoms were removed from the SiC nanotube structure and replaced by vanadium atoms. In order to obtain the energy gap for this system more accurately, we apply the semi-empirical Hubbard corrections U and LSDA: for the d-states of silicon U =5 eV and for the p-states of carbon U=4.8 eV. In this situation, at the end of our first-principles simulations, we found that our results were closer to the experimental result (E_g = 3.330 eV), and the obtained values of the direct and indirect band gaps are 5.2 and 3.3 eV for the wurtzite structure of bulk SiC [34-36]. When we obtain the energy gap for this bulk structure, we will continue our studies for SWSiC NT systems. From DFT-LSDA+U simulations we find that the energy gap is 0.98 eV for the undoped non-magnetic system and the chiral SWSiCNT (6.0) has a direct energy gap with Γ-Γ transition, this truth is closer to the conclusion in [29, 35].

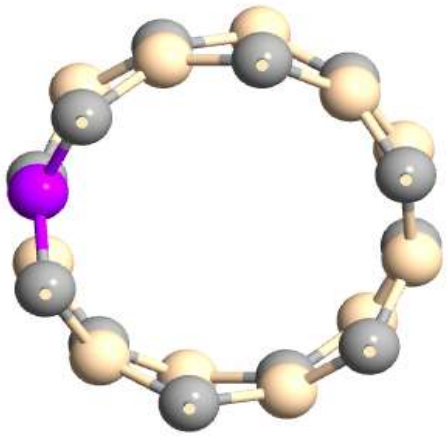


Figure 3. Top view of single-walled (6,0) SiC:V NTs. Gray balls are carbon, beige balls are silicon and purple balls are vanadium.

The first-principles DFT-based calculations of the electronic properties of the SiC:V supercell performed in the ADF-BAND code were presented in [28]. The electronic and magnetic properties of vanadium doped 2D SiC were studied using the VASP code and the first-principles energy gap was shown to be 2.574 eV [30]. However, the authors have not found enough references in the literature on V doping of chiral SiC nanotubes yet. The effect of single atom doping on the electronic and magnetic properties of the hexagonal 4H-SiC supercell was investigated based on first-principles modeling and reported that the energy gap for the SiC:V system is ~0.45 eV [37].

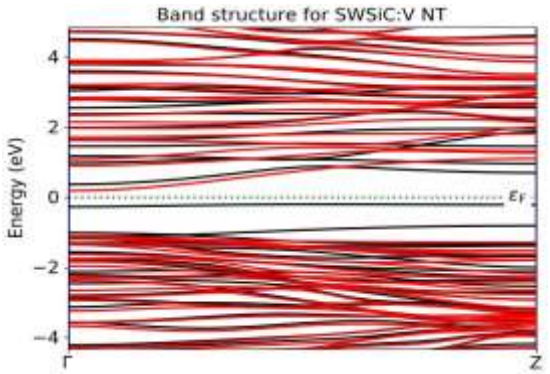


Figure 4. Spin-polarized energy structures for single-wall SiC:V NT: black and red curves correspond to the majority and minority spin states.

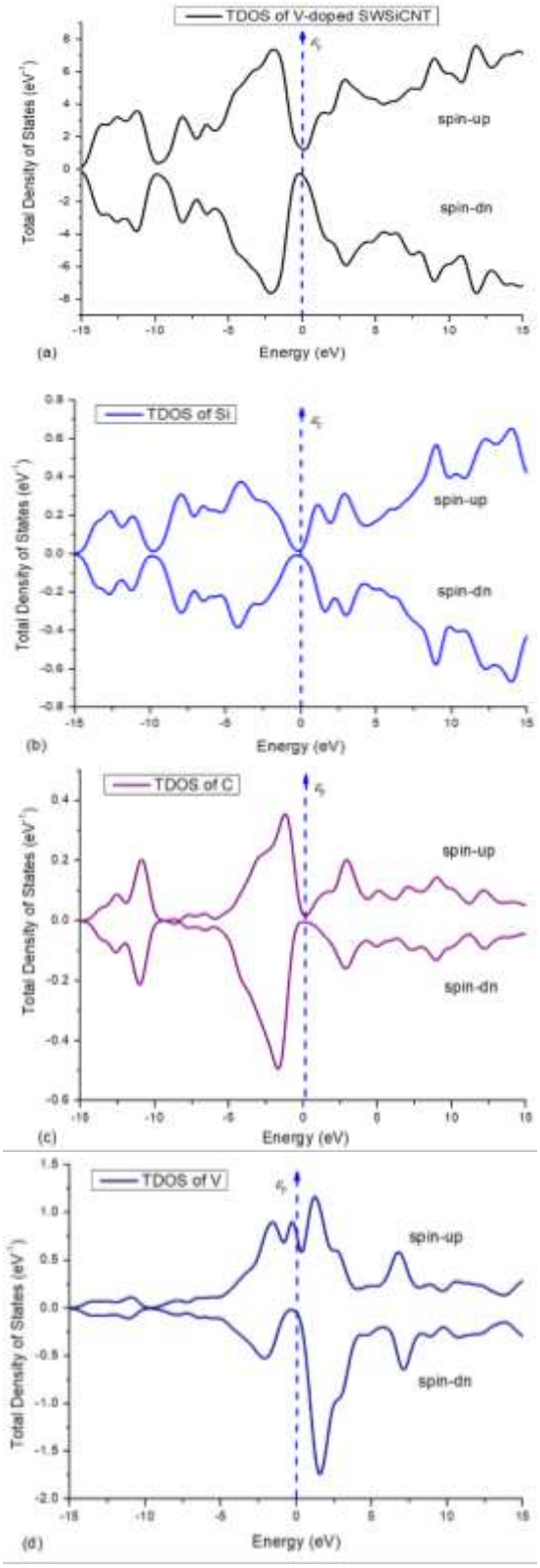


Figure 5. TDOS diagrams for SiC:V NTs.

We obtained first-principles simulations for the spin-polarized band structures using DFT-LSDA+U method, respectively for the majority and minority spin states, we obtained a single-walled (6,0) SiC:V NT structure as shown in Figure 4, which is not a semi-metallic material. The Fermi level for all figures is shown as a dotted line (set to 0 eV).

As shown in Figure 5, the PDOS and TDOS states of the SiC:V NT system were calculated. The negative and positive energy values in the DOS figures correspond to the majority and minority spin energy states. In Figure 5, we found that the TDOS of SiC:V NT system and some V 3d-states and PDOS after doping, the atoms in the C 2p states become asymmetric. The SiC:V NT system is not ~~a~~ half-metallic as can be seen in Fig. 3, i.e., the majority and minority spin states are not accessible at the Fermi level. Vanadium-doped SWSiCNT systems can be ferromagnetic due to a specific behavior based on the p-d hybridization between the C and V electronic states of 2p and 3d, respectively.

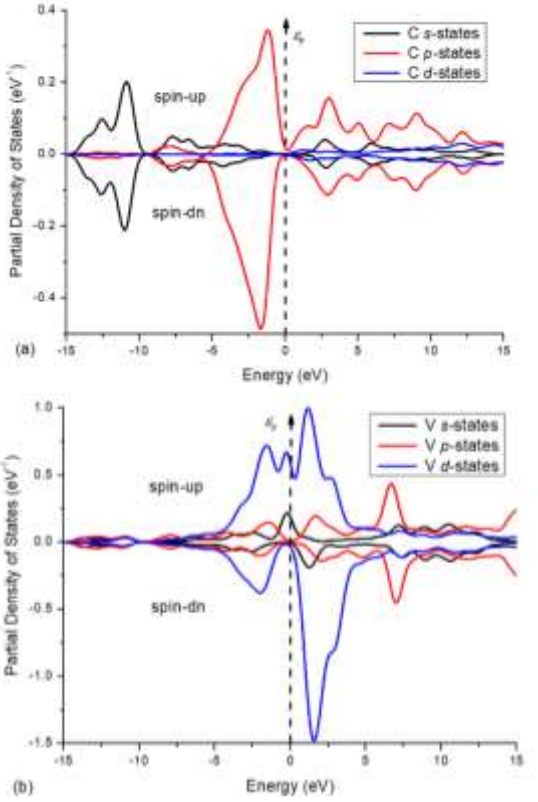


Figure 6. PDOS for C s-, p-, and d-states (a); PDOS for s-, p- and d-states of V (b).

3.3 Magnetism in Vanadium doped Silicon Carbide

In this work, the ferromagnetic (FM) and antiferromagnetic (AFM) coupling features, spin

moments are modeled based on Mulliken population analysis. We also obtained the total energies for both phases for SWCNT (6,0) to elucidate this.

When doped with V-shaped SiC, the resulting magnetic moments are 1.24 μ_B and this sistem displays the stability of AFM configuration [29]. The authors obtained a total magnetic moment of 1 μ_B for the 2D SiC:V system using DFT-Based study [37]. They calculated a magnetic moment of 2.12 μ_B for the SiC:V supercell structure and showed that this structure is metallic in nature [37]. The first-principles studies of the effect of vanadium dopants on the magnetic properties of the SiC-4H polytype were published in [38]. According to the GGA+Hubbard U results, the magnetic moment of the SiC:V system is about 2.03 μ_B, and it was reported that the 6H structure of vanadium-doped SiC is a FM phase at room temperature [39]. SiC:V nanowires were both theoretically and experimentally investigated and shown that the cubic structure of SiC:V can demonstrate half-metallic and FM states [40]. The authors informed that silicon carbide nanowires with low vanadium impurity concentrations possess ferromagnetic, paramagnetic or diamagnetic phases and have a spin moment of 1 μ_B [40]. For the vanadium doped Si cluster, the local magnetic moment was found 0.67 μ_B [41-46]. The illustration of spin polarization is displayed in Fig. 5. The vanadium impurity atom (~1.6 μ_B) makes the major contribution to the magnetization of the NT structure. Significant negative contributions come from 3 carbon atoms (~1.3 μ_B) chemically bonded to vanadium. Based on the first principles results, due to the presence of V impurity at the Si site, the magnetic moment of SiC:V NT is 1.0 μ_B, and the impurities play an important role in generating the magnetization of the single-walled (6.0) SiC:V NT. The host atoms of the 12 C and 11 Si provide negative ~1.2 μ_B and positive ~0.6 μ_B contribution to the magnetization of the single-wall SiC:V nanotube with a chillarity of (6.0).

This result indicates that E(AFM)= -4374.17385 eV and E(FM)= -4374.18175 eV, and the difference between these energies is negative, and which means that the FM phase for SWSiC:V NT system is more stable than the AFM phase.

4. Conclusions

In this study, a more accurate research method such as application was realized. In addition, this method can calculate the band structure with high accuracy, which is closest to the known experimental result. The introduction of vanadium atoms, which leads to magnetization of the systems, is caused by the double exchange of p-d hybridization between 2p-carbon and 3d-electron states of vanadium. The impurity atoms in the d-states play a crucial role in shaping the magnetization of V^{2+}-doped single-walled (6,0) SiC NTs. SWSiC:V NT is a non-semi-metallic magnetic material, and the total energy calculation results indicate a stable FM phase for this system. The 12 C and 11 Si structures atoms give negative ~1.2 μ_B and positive ~0.6 μ_B contributions to the magnetization of single-walled SiC:V nanotubes with a chillarity of (6.0), and the total spin moment is ~1.0 μ_B.

The research method applied in this work can be used in the future to study many physical properties of Si-based materials. It is our future scientific research plan to investigate the electronic, optical, magnetic, etc. properties of SiC nanotubes and nanosheets doped with 3d transition elements and to investigate the new technical application of defect-structured Si-based nanosystems as a result of the scientific researches performed.

The results of this work predict that single-walled SiC:V nanotube systems may be promising candidates for spintronic devices producing dilute carbon-based magnetic nanomaterials applications in the coming days. At the same time, this study proved that vanadium doped silicon carbide exhibits good magnetic properties and can be used as a ferromagnetic material in the field of spintronics.

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