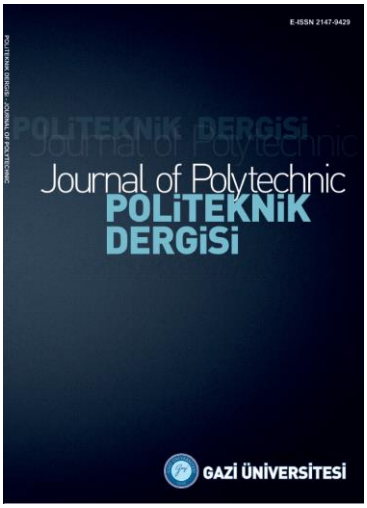

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Electronic and magnet properties of cobalt doped SiCNT:A first-principles study

Kobalt katkılı SiCNT'nin elektronik ve mıknatıs özellikleri: İlk prensip çalışması

Yazar(lar) (Author(s)): *Sevda Rzayeva[1], Vusala Nabi Jafarova[2]*

ORCID[1]: 0009-0006-9747-3972

ORCID[2]: 0000-0002-0643-1464

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Highlights

- Using the DFT+LSDA+U method successfully improved the energy gap/DFT+LSDA+U yönteminin kullanılması enerji boşluğunu başarıyla iyileştirdi
- Introduction of 3d transition metal ion in SiC NT show the magnetic response/SiC NT'de 3 boyutlu geçiş metal iyonunun tanıtımı manyetik tepkiyi gösteriyor
- Calculations of the total energies predicted the stability of the antiferromagnetic phase/Toplam enerjilerin hesaplanması antiferromanyetik fazın kararlılığını tahmin etti
- Results of the current find predict that SiC:Co NT will be a promising candidate for spintronic devices/ Mevcut bulgunun sonuçları SiC:Co NT'nin spintronik cihazlar için umut vadeden bir aday olacağını tahmin ediyor

Graphical Abstract

In this study, the defect effect on the electronic and magnetic properties of single-walled SiC:Co nanotubes with chirality (6,0) were studied based on density functional theory. We obtained that the electronic properties of the single-walled SiC nano systems are significantly changed by metal introduction and these systems show magnetic properties. / Bu çalışmada, kiralite (6,0) ile tek duvarlı SiC:Co nanotüplerin elektronik ve manyetik özellikleri üzerindeki kusur etkisi yoğunluk fonksiyonel teorisine dayalı olarak incelenmiştir. Tek duvarlı SiC nano sistemlerinin elektronik özelliklerinin metal girişiyle önemli ölçüde değiştiğini ve bu sistemlerin manyetik özellikler gösterdiğini elde ettik.

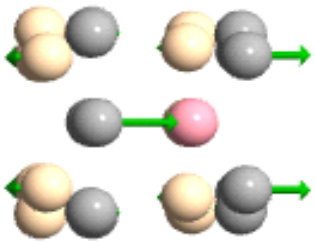

Figure. Spin-polarization view of SiC:Co nanotube / **Şekil.** SiC:Co nanotüpünün spin-polarizasyon görünümü

Aim

The aim of this work to obtain magnetic materials and to define new application opportunity. / Bu çalışmanın amacı manyetik malzemeler elde etmek ve yeni uygulama fırsatları tanımlamaktır.

Design & Methodology

We simulated physical properties of SiC:Co nanomaterials using density functional theory and implementing Atomistic Tool Kit code. / Yoğunluk fonksiyonel teorisini kullanarak ve Atomistic Tool Kit kodunu uygulayarak SiC:Co nanomalzemelerinin fiziksel özelliklerini simüle ettik.

Findings

The simulations predicted that SiC:Co is a magnetic material with ~1.9 μ_B magnetic moment. */ Simülasyonlar, SiC:Co'nun ~1,9 μB manyetik momente sahip manyetik bir malzeme olduğunu öngörmüştür.*

Conclusion

Results of the current find predict that SiC:CoNT will be a promising candidate for spintronic devices. / Mevcut bulgunun sonuçları SiC:CoNT'nin spintronik cihazlar için umut vadeden bir aday olacağını tahmin ediyor.

Declaration of Ethical Standards

The authors of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission. / Bu makalenin yazarları, bu çalışmada kullanılan materyal ve yöntemlerin etik kurul izni ve/veya yasal-özel izin gerektirmediğini beyan eder.

Electronic and Magnet Properties of Cobalt Doped SiCNT:A First-Principles Study

Research Article

Sevda Rzayeva[1,2], Vusala Nabi Jafarova[2,3,4*]

[1]Azerbaijan State University & Economics, 6 Istiglaliyyat Str., AZ-1123, Baku, Azerbaijan
[2]Ministry of Science and Education Republic of Azerbaijan, Institute of Physics, 131 H. Javid Ave., AZ-1143, Baku, Azerbaijan
[3]Department of Physics, Azerbaijan State Oil and Industry University, 20 Azalig Ave., AZ-1010, Baku, Azerbaijan
[4]Khazar University, 41 Mehseti Str., AZ 1096, Baku, Azerbaijan

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ABSTRACT

The defect effect on the physical properties of single-walled SiC:Co nanotubes with chirality (6,0) were studied based on density functional theory. We obtained that the electronic properties of the single-walled SiC nano systems are significantly changed by metal introduction and these systems show magnetic properties. Due to the mutability of data at the atomic and molecular scale, correct prediction of the density of states applying the ab-initio and density functional theory formalisms is complicated. The computed energy band gaps of 3.3 and 0.98 eV were obtained for the SiC bulk structure and nanotube within local density and local spin density approaches using the Hubbard U method. Our analysis indicates that, the magnetic moment of the SiC:Co system is equal to ~1.9 μ_B and the undoped SiC is a nonmagnetic system. According to the results SiC:Co nanotubes induce magnetism. The calculations of the total energies predicted the stability of the antiferromagnetic phase. Thus, the tunable electronic and magnetic properties of metal-doped SiC systems provide a flexible design method for more suitable SiC-based spintronics and field-electron emission devices.

Keywords: SiC nanotube, Quantum-confined, ferromagnetism, cobalt doped SiC, metallic.

Kobalt Katkılı SiCNT'nin Elektronik ve Mıknatıs Özellikleri: İlk Prensip Çalışması

ÖZ

Kiralite (6,0) ile tek duvarlı SiC:Co nanotüplerin fiziksel özellikleri üzerindeki kusur etkisi yoğunluk fonksiyonel teorisine dayalı olarak incelenmiştir. Tek duvarlı SiC nano sistemlerinin elektronik özelliklerinin metal girişiyle önemli ölçüde değiştiğini ve bu sistemlerin manyetik özellikler gösterdiğini elde ettik. Atomik ve moleküler ölçekte verilerin değişebilirliği nedeniyle, ab-initio ve yoğunluk fonksiyonel teorisi formalizmlerini uygulayarak durum yoğunluğunun doğru tahmini karmaşıktır. Hubbard U yöntemi kullanılarak yerel yoğunluk ve yerel spin yoğunluğu yaklaşımları içinde SiC yığın yapısı ve nanotüp için 3,3 ve 0,98 eV'lik hesaplanan enerji bant aralıkları elde edilmiştir. Analizimiz, SiC:Co sisteminin manyetik momentinin ~1,9 µB'ye eşit olduğunu ve katkısız SiC'nin manyetik olmayan bir sistem olduğunu göstermektedir. Sonuçlara göre SiC:Co nanotüpler manyetizma indükler. Toplam enerjilerin hesaplanması antiferromanyetik fazın kararlılığını öngörmüştür. Böylece, metal katkılı SiC sistemlerinin ayarlanabilir elektronik ve manyetik özellikleri, daha uygun SiC tabanlı spintronik ve alan elektron emisyon cihazları için esnek bir tasarım yöntemi sunmaktadır.

Anahtar Kelimeler: SiC nanotüp, Kuantum-sınırlı, ferromanyetizma, kobalt katkılı SiC, metalik.

1. INTRODUCTION

In recent years, SiC with nanostructures have attracted great interest in spintronic devices due to their unique chemical and physical characteristics. Carbon nanotubes have high sensitivity, quick response, low size and low operating temperature [1-4]. Wide band gap semiconductor materials doped with 3d transition metal (TM) (V, Cr, Co, Fe, Mn, and Ni) elements are attracting great attention for the application for dilute magnetic semiconductor (DMS) devices. The studied material, silicon carbide (SiC), is the main candidate for replacing Si in the production of electronics operating in hostile environments [5]. Due to its unique physical and electronic properties, (high mechanical strength, low density, corrosion resistance, high hardness and thermal conductivity, a wide band gap, chemical inertness, etc.) SiC may be of interest to researchers [2-9].

In a number of theoretical works, electronic, magnetic and structural features of silicon carbide nanosheets, nanoribbons and nanotubes have been studied [10-13]. However, in this work [14], the authors reported that on the basis of partial charge analysis, the TM-doped single-walled CTM NTs have localized net charge distributions, whereas the spin densities in SWC:(Sc,Co,Cu) NTs are delocalized over the entire NTs.

The SWC:TM NTs are mostly metallic materials with narrow-gap semiconducting behavior. The electronic and magnetic properties of these TM-doped SWCNTs were

*Corresponding Author:
vusala.cafarova@asoiu.edu.azr

calculated within density functional theory (DFT). The TM-doping silicon carbide systems have a significant redshift and better absorption capacity of visible light and TM co-doped 3C-SiC system combines electrical properties with magnetic characteristics and has higher magnetic moments [15].

Depending on the types of defects (vacancy or impurity), the physical properties of SiC compounds change differently and these properties make them useful materials in the field of optoelectronic and spintronic devices [16]. Experimentally studied from X-ray fluorescence spectrometers the magnetic properties of nanocrystalline β-SiC and obtained the saturation magnetization arising from magnetic impurities like Fe, Ni, and Co [17].

The two-dimensional structure induces electronic properties which are essential in spintronic devices [18, 19], and energy conversion [20, 21]. Success in wet etching of 2D SiC prompts further investigation of SiC-based systems [22].

The magnetic SiC nanomaterial could be more effective than carbon nanotube for different application nanotechnology (for example nanocomposites, nanoelectronics etc.) and biotechnology (for example ceramic, alloys etc.) and suggests exciting possibilities in spintronic devices. Lately, the features of transition metal-doped 2H-SiC (hexagonal polytype) and single-walled silicon carbide nanotube (SWSiCNT) between its polytypes are of high scientific interest. The present study is a useful investigation for the construction of spintronic devices based on DMS materials with Curie temperatures. In this paper we report the study of the physical properties, such as electronic structure and magnetic properties of single-walled cobalt-doped SiC nanotubes with chirality (6,0).

2. COMPUTATİONAL METHOD

In this paper, using the DFT approach SiC bulk and (6,0) SWSiC nano structures are analytically modeled. Thus, the electronic characteristics of SiC nanotubes, as well as the change in their features when doped with magnetic materials, are studied. The calculations of electronic and magnetic feature of SiCNT and SiC wurtzite structure were carried out by DFT method within Local Spin Density Approximation (LSDA) and Local Density Approximation (LDA) implemented Atomistic ToolKit (ATK) code (http://quantumwise.com/). This is a software for atomic-scale modeling and simulation of nanosystems. ATK combines DFT with non-equilibrium Green's functions for first-principles electronic structure and

transport calculations of molecules, periodic systems etc. DFT is infamous for foretelling very small band gaps. It is well known that LDA functional generally underestimate band gaps and that hybrid DFT or self-interaction corrected calculations correct these issues more universally in most systems. The last progress of LDA functional and using Hubbard U semiempirical corrections have given us an opportunity to determine correct band gaps of materials.

The interactions among the ions and electrons, and exchange correlation were described by the Fritz-Haber-Institute (FHI) Perdew Zunger (PZ) functional and ion pseudopotentials, respectively. The Kohn-Sham wave functions were expanded by a linear combination of atomic orbitals with a kinetic energy cutoff of 50 and 75 Ha (1 Ry=2 Ha) for the bulk and nanostructure, respectively. When calculate electronic structural feature for pure compound, the primitive cell of SiC wurtzite containing 2 silicon and 2 carbon atoms and the atomic positions are optimized until the stress and v on each atom converges to less than 0.001 eV/Å3 and 0.001 eV/Å respectively. The containing dopant atom and pure SiC nanotube systems were optimized with stress and force tolerances of 0.01 eV/Å3 and 0.01 eV/Å, respectively. The reciprocal space integration was performed using Monkhorst-Pack k-point sampling of 1×1×5 nano systems and 7×7×7 bulk systems and a standard electron temperature of 300 K.

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. The Hubbard U corrections taken 5 eV for Si and 4d and 4.8 eV for C 2p-states. Note that, for all calculations Brillouin zone integration k-point sampling of SiC and the convergence of the plane-wave basis set cutoff energy are tested. In Table the simulation parameters for the DFT based analytical model are shown. Table 1 lists the simulation parameters for the DFT-based analytical model.

In this study, the configurations of metal Cobalt doped SiC systems were investigated. The doping atoms include not only eight 3d-series TM atoms but also one semi-metal atom and one other metal atom. The electronic and magnetic performances were investigated at the most stable structures systematically.

The high stability in Ti-SiC was explained by the complete bonding states between the Ti atom and the neighboring carbon atoms because of the same valence electron number with the substituted Si atom. The magnetism evolution in transition metal-doped SiC was attributed to the occupation mode of hybridization orbitals nearby the Fermi level.

3. RESULTS AND DISCUSSION

3.1. Electronic Properties of Pure SiC Wurtzite

The studied wurtzite compound SiC has a wide indirect band gap of about 3.3 eV, and this property was useful for applications in electronics and optics. Because this material has high thermal conductivity and temperature resistance, it can be applied as high temperature heating material due to high melting temperature and thermo-physical properties [23]. Some theoretical studies investigate the electronic properties of the SiC nanostructure [24-27] and the wurtzite structure [28, 29]. However, less theoretical studies devoted to the study of the magnetic properties of Co- doped SiC nanotubes.

Table 1. Simulation parameters for DFT based SiC nanotubes

Parameters	Value	Details
Configuration	(A, B, C)	The SiC NT structure along (X, Y, Z) axes.
Electrodes' Fermi level	0eV	The left and right electrodes' Fermi level lies at 0eV
Force tolerance	0.01eV/Å	When minimum then sustainability increase
Poisson Equation Solver	Multi-grid	Algorithm used
Maximum interaction range between electron orbitals	1 nm	Numerical accuracy parameters
No. of steps for iteration	100	Increasing steps increasing accuracy
Step size	0.25 nm	Step size increasing the time of simulation
Electron temperature	300K	Room temperature operation

In Ref [28] the authors were informed about the results for the electron bands and density of states (DOS) using DFT and generalized gradient approximation methods with the GW scheme.

Z. Huang et al. [13] and A.V. Sinelnik et al. [28] studied electronic band structure for SiC-2H structure using GGA and obtained a result for a band gap of 2.3 eV, which this result underestimated is about 1.0 eV from the experimental result.

In the present work, for U=5 eV for Si 4d states and U=4.8 eV for C 2p states, we obtained first-principles direct and indirect band gap values of 5.2 and 3.3 eV for SiC with wurtzite structure and this is compared with other theoretical and experimental results and list in Table 2. This result highlights that the compound is an indirect semiconductor and is very close to the experimental results obtained by the experimental result as 3.33 eV [30].

Table 2. Energy band gaps (eV) of the DFT-LDA+U approximation for SiC. Theoretical and experimental results of other authors are included for comparison

Method	E_g (direct)	E_g (indirect)	Refs.
LDA+ U	5.2	3.3	This work
GGA	4.06	2.33	[14]
GW	5.18	3.17	[14]
GGA		2.3	[13]
GW		3.68	[17]
GGA		3.01	[18]
GW		3.15	[19]
GW		3.12	[20]
QPscGW		3.75	[20]
Experiment		3.330	[31]

Using DFT-LDA+U, the electron energy band structure in the energy range from -20 to 10 eV along the high symmetry directions in the first Brillouin zone (BZ) was obtained, and the TDOS diagrams for wurtzite SiC are shown in Figs.1 and 2, respectively.

In all figures, the Fermi energy level is set to 0 eV, and in our calculations the conductivity minimum for SiC wurtzite is located at the K symmetry point of the BZ. Figure 1 describes the LDA+U calculated band structure for SiC wurtzite.

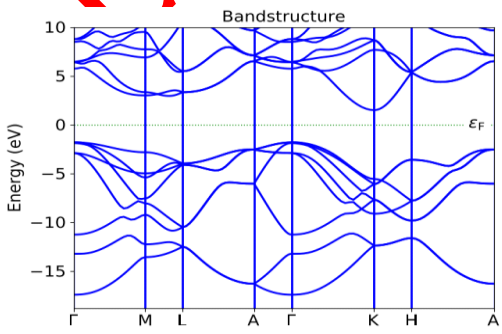

Figure 1. DFT-LDA+U calculated band structure for SiC wurtzite (E_g=3.3 eV)

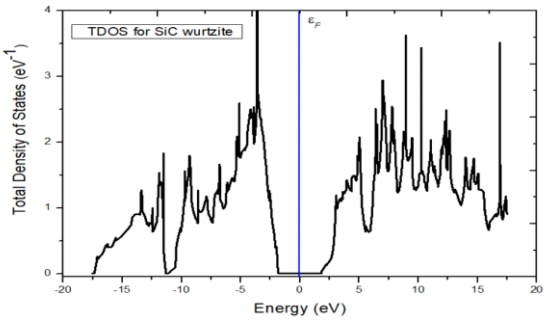

Figure 2. DOS diagrams for pure SiC with wurtzite structure

From the total density of states (TDOS) and the computed energy band structure we can divided two parts the valence bands: the low valence bands are ranging from -17.4 eV to -13.2 eV and upper valence bands are ranging from -11.2 eV to -1.87 eV and this valence bands are formed from p-states of C atom. Our results show that the conduction band is mainly composed of Si p and d-states, but Si and C d-states make almost no contribution to the valence band.

3.2. Electronic Properties for Pure SWSiCNT

Spin-polarized band structure, total and partial DOSs diagrams for undoped (6,0) single wall SiC NT are shown in Figs. 3 and 4. From DFT-LSDA+U calculations we obtained that the chiral SiCNT has a direct band gap (Γ- Γ) and wide of the band gap is 0.98 eV for undoping SWSiC nonmagnetic NT and this result smaller than that of the pristine SiCNT and this fact is closer to the result in [28-35].

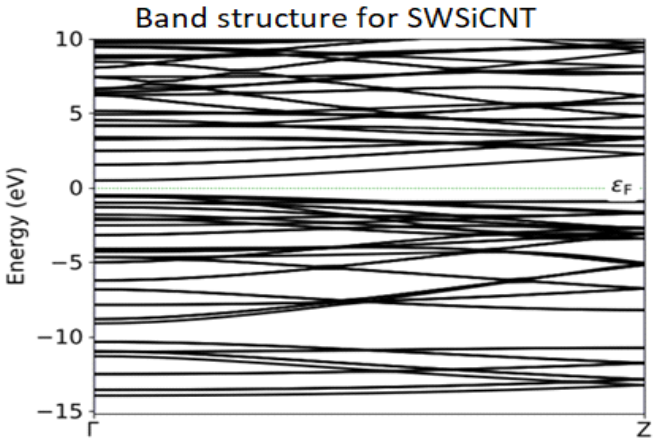

Figure 3. Electronic band strcucture for undoped SWSiC (6,0) nanotube (E_g=0.98 eV)

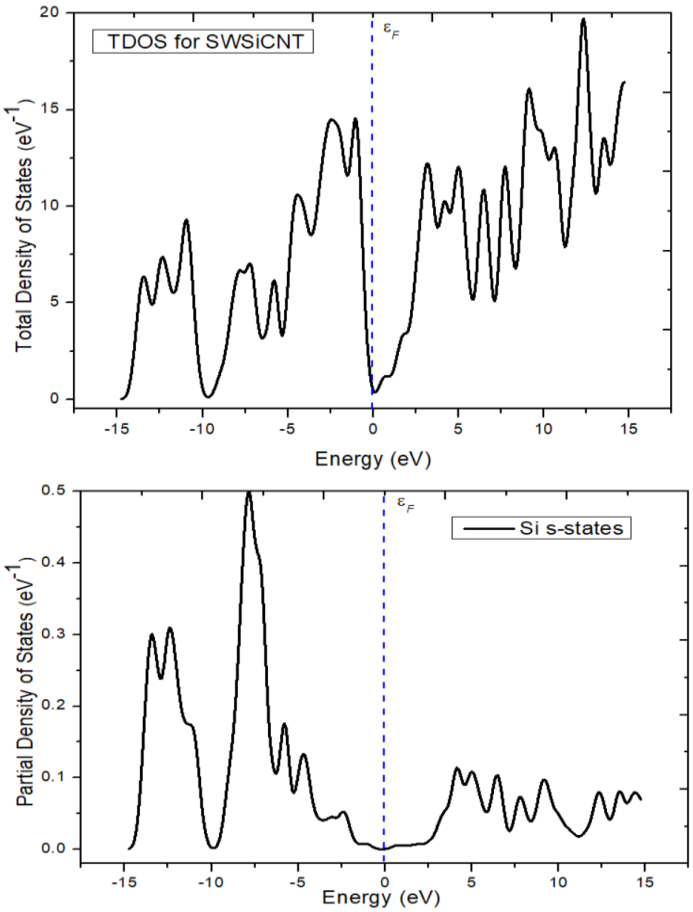

Figure 4. Spin-polarized DOSs diagrams for undoped (6,0) SWSiC NT

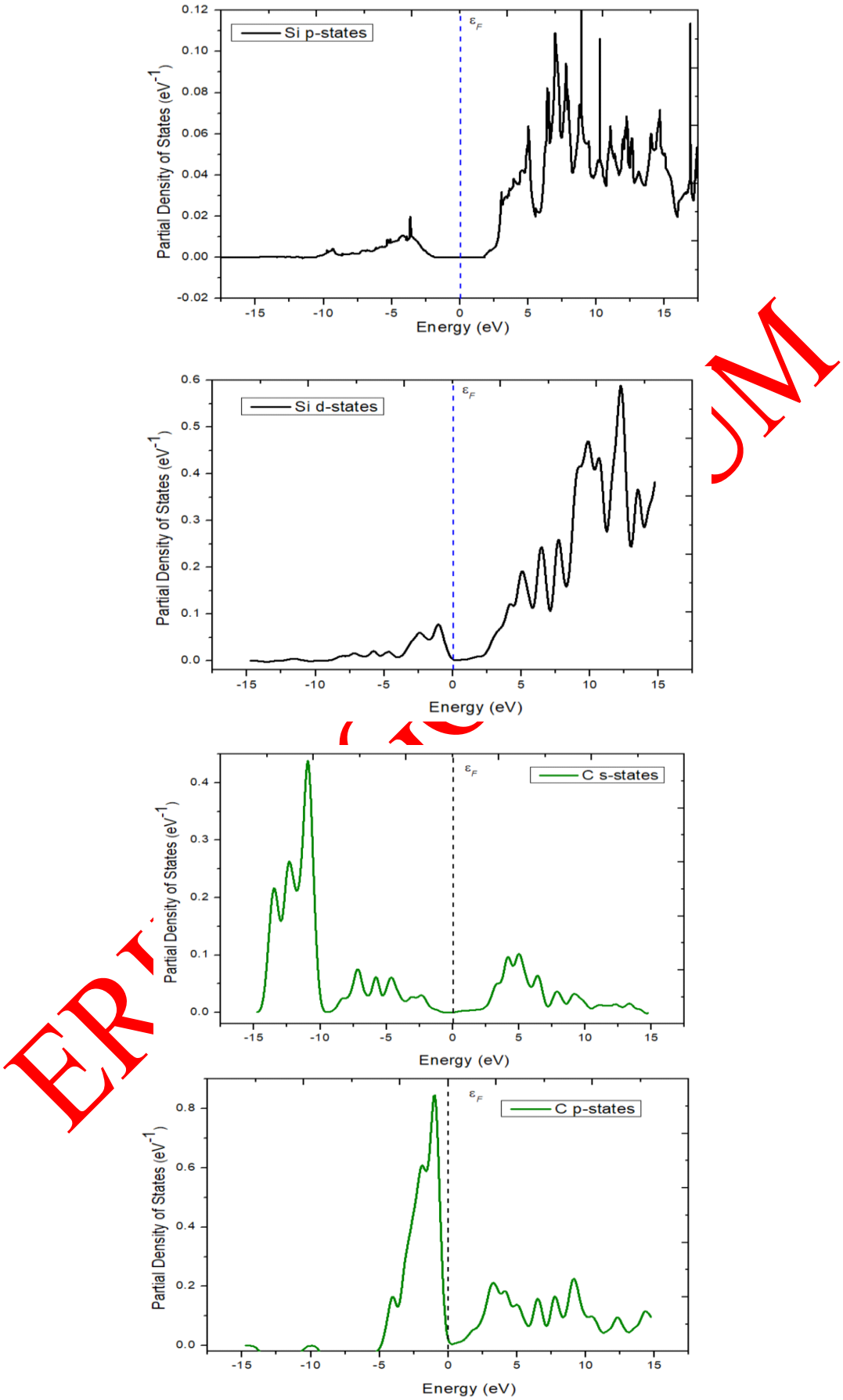

Figure 4. (cont.) Spin-polarized DOSs diagrams for undoped (6,0) SWSiC NT

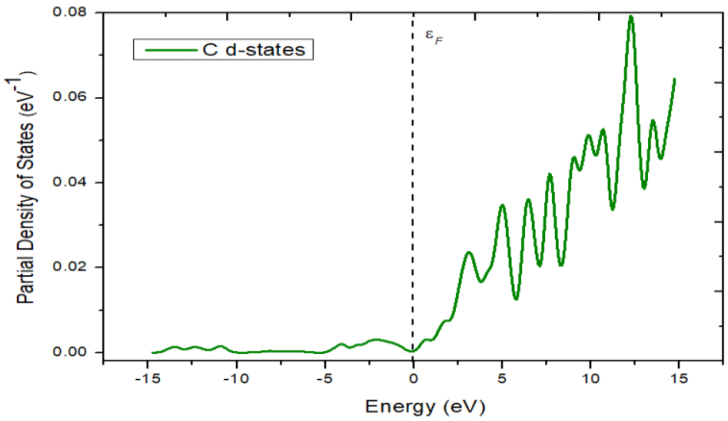

Figure 4. (cont.) Spin-polarized DOSs diagrams for undoped (6,0) SWSiC NT

In the future, we will also investigate the electronic and magnetic properties of TM-doped SiC NT materials. It is known that many physical characteristics of compounds depend on their defect configurations [36, 37].

3.3. Electronic properties of Co-doped SWSiCNTs

The defect engineering of the SiC nanosystems has remained an important motivation in materials science research as the fundamental physical and chemical properties of silicon carbide must depend on their defect structures. It is because of the complex nature of the defects that SiC is being discovered and rediscovered repeatedly.

This section is devoted to simulate electronic properties of undoped and Co-doped single wall SiC nanotubes (SWSiCNTs) with chirality of (6,0). This analytical model of nonmagnetic SiC chiral nanotubes is designed using DFT based formalisms. SWSiCNT is semiconductor material with the band gap energy ranging from 0.9 to 1.83 eV [10]. This nanotube is then doped with magnetic material like Cobalt in Silicon site. From first-principles simulations the Co-doped single wall SiC nanotube (SWSiC:CoNT) exhibits the metallic behavior. Figure 5 describes the structure of SWSiC:Co (6,0) NT.

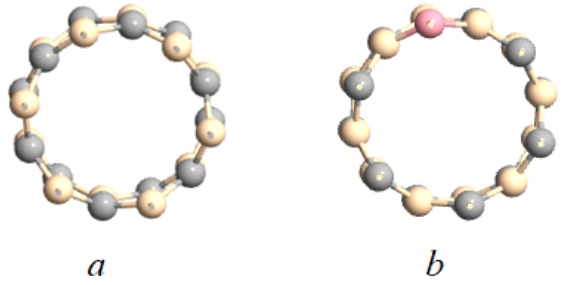

Figure 5. Structure of Co-doped SWSiC (6,0) NT (silicon-beige, carbon-gray, cobalt-pink)

A.T. Mulatu et. al [11] reported the results for undoped (8,0) SiCNT using the DFT-GGA method and found that the band gap is 1.05 for this system. E.V.Larina et. al [12] investigated different NTs and show that the pure (5,0) SWSiCNT has metallic conductivity. In [38] J.W. Sun et al. was studied the influence of the structure for the magnetic doping SiC film and obtained that Co-doped film exhibit intrinsic ferromagnetism at 300 K. From partial DOS calculations (see Figure 4), we obtained that the Si and C d-states give insignificant contribution to valence band. But the conduction bands treated mainly from Si d-orbitals and small contributions come from d-states of C atoms. From first principles simulations result of spin-polarized band structures for spin-up and spin-down states for SWSiC:CoNT system shows metallic character.

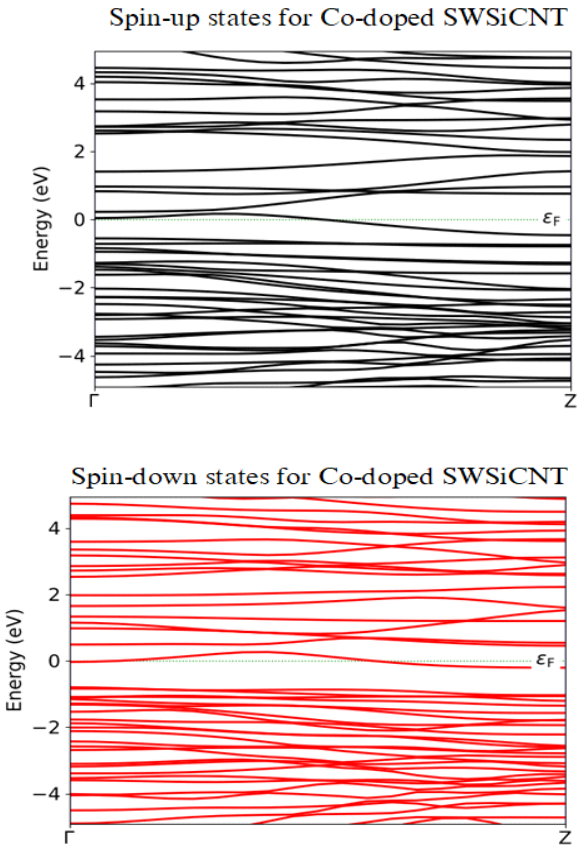

Figure 6. Spin-polarized band structures for Co-doped (6,0) single wall SiCNT

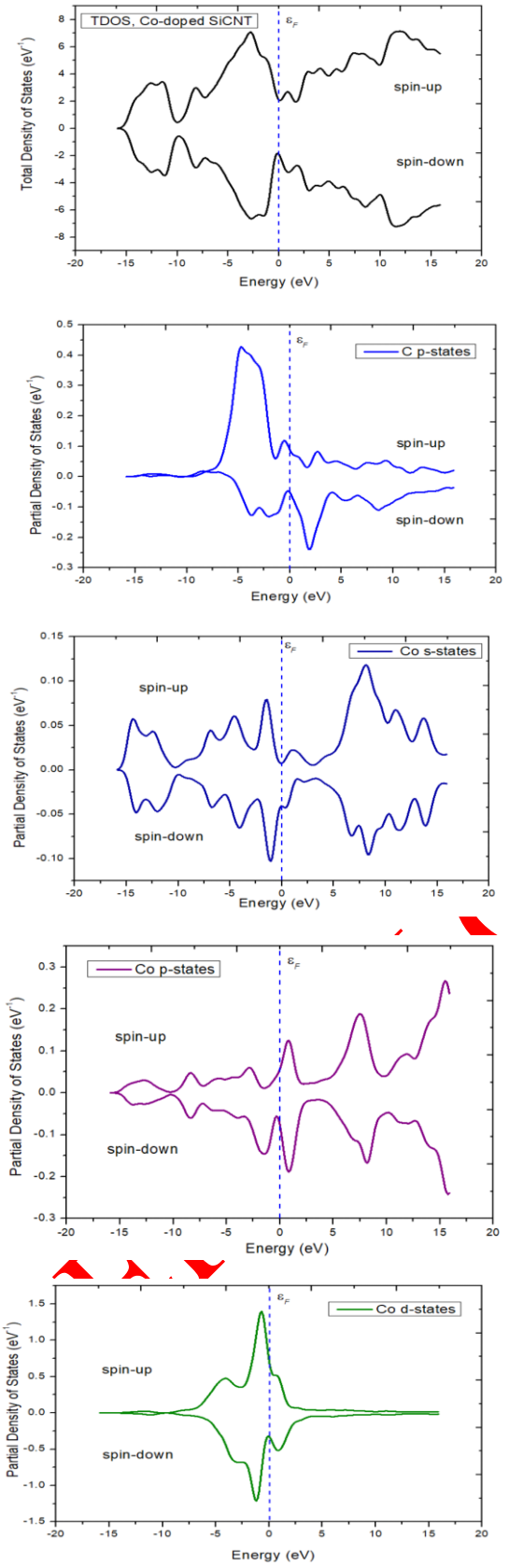

Figure 7. Spin-polarized DOS diagrams for Co-doped (6,0) single wall SiC NT

Figures 6 and 7 show the spin-polarized band structures (black curves describe spin-up states and red curves show spin-down states) and DOS diagrams for SiC:Co NTs. From Fig. 6, there are some asymmetry behaviours in the Co s, p-states and significant imbalances in the C p- and Co d- states: indicates that the system is magnetic.

4. MAGNETISM IN SWSIC:CONTS

In this work, the features of ferromagnetic (FM) and antiferromagnetic (AF) coupling, overall and local magnetic moments are modeled on the basis of Mulliken's population analysis. We also received overall energies for both phases for SWCNTs (6,0) to find out. From first principles calculations of spin-polarized band structures for majority and minority spin bands, we found that single-walled SiCTN doped with cobalt has a metallic nature. Figure 8 shows the spin polarization pattern of Co-doped SiCNT. According to our first-principles simulations, the total magnetic moment of the double- and single-Co^{+2}-doped SiCNT systems is 5.2 and ~1.8 μ_B, respectively. Our results are closer to the experimentally observed value of ~1.7 μ_B, arising from magnetic impurities [17].

This fact is due to double exchange between C 2p and Co 3d-states as a result of pd orbital hybridization and the carbon p-orbitals play significant roles in the stability of FM phase. The main contribution to nanotube magnetization comes from 3 C atoms (~3.26 μ_B) chemically bonded to the Co impurity atom and a slight negative contribution to the magnetization from the impurity atom is ~0.16 μ_B, respectively.

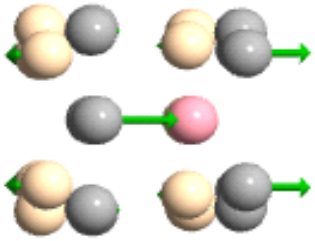

Figure 8. Spin polarization side view for SiC:CoNT: Si-beige, C-grey, Co-pink. Magnetic moments are indicated by green arrows

From the total energy calculations for AFM (EFM=-5479.61682 eV) and FM (EFM=-5479.56293 eV) phases the result of energy difference ($\Delta E = E(AFM) - E(FM)$) indicating that the AFM state more stable than FM state for SiC:CoNT.

5. CONCLUSION

DFT-LDA+U modeling were used to study the influence of native defects on the electronic and magnetic properties. We found that bulk SiC has an indirect band gap (3.3 eV), but chiral SWSiCNTs are direct band gap semiconductors (0.98 eV) at Γ point. The introduction of the dopant atom leads to the magnetization of the

systems, resulting from the double exchange between the p-d hybridization among the C 2p- and Co 3d- states. The d-states of the Co play an important role in inducing magnetism in SWSiC:CoNTs. From first principles simulations the Co-doped SWSiCN is a magnetic material with metallic character and total magnetic moments for the single and double Co-doped SiCNT are ~1.9 and ~5 μ_B, respectively. The results of the current find predict that single-walled SiCNT will be a promising candidate for use in Si-based diluted magnetic nanomaterial for spintronic devices in the future.

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 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.

DECLARATION OF ETHICAL STANDARDS

The authors of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

AUTHORS' CONTRIBUTIONS

Sevda RZAYEVA: Wrote the manuscript.

Vusala Nabi JAFAROVA: Perofrmed the simulations and analyse the results.

CONFLICT OF INTEREST

There is no conflict of interest in this study.

REFERENCES

[1] Li K., "Wang W., Cao D., "Metal (Pd, Pt)-decorated carbon nanotubes for CO and NO sensing", ***Sensors and Actuactors B: Chemical***, 158 (1):171-177, (2011).

[2] Eleni C.V., Romanos G.E., Karanikolos G.N., Kanellopoulos N.K., "Catalytic NOx removal by single-wall carbon nanotube-supported Rh nanoparticles", Journal of Hazardous Materials, 194:144-155, (2011).

[3] Wang R., Zhang D., Liu C., "The germanium-doped boron nitride nanotube serving as a potential resource for the detection of carbon monoxide and nitric oxide", ***Computational Materials Science,*** 82:361-366, (2014).

[4] Liu L., Jin J., Hou F., Li S., C. Lee H., "Catalytic Effects of calcium and potassium on a curved char surface in fuel reburning: a first-principles study on the adsorption of nitric oxide on single-wall carbon nanotubes with metal decoration", ***Energy,*** 125:459-469, (2017).

[5] Matsunami H., "Technological Breakthroughs in Growth Control of Silicon Carbide for High Power Electronic Devices", ***Japanese Journal of Applied Physics***, 43:6835, (2004).

[6] Ivanov P.A., Chelnokov V.E., "Recent developments in SiC single-crystal electronics, Semicond" ***Science and Technology***, 7: 863, (1992).

[7] Narushima T., Goto T., Hirai T., Iguchi Y., "High temperature oxidation of Silicon Carbide and Silicon Nitride", ***Matererials Transactions JIM***, 38: 821-835, (1997).

[8] Wang S.Z., Xu L.Y., Shu B.Y., Xiao B., Zhuang J.Y., Shi E.W., "Physical properties, bulk growth, and applications of SiC single crystal", ***Journal of Inorganic Materials***, 14:527-534, (1999).

[9] Watari K., "High thermal conductivity non-oxide ceramics", ***Journal of the Ceramic Society of Japan***, 109: 1265, (2001).

[10] Zhao M., Xia Y., Li F., Zhang R.Q., Lee S.T., "Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculation", ***Phyical Review B***, 71:085312, (2005).

[11] Mulatu A.T., Nigussa K.N., Daja L.D., "Structural and electronic properties of zigzag single wall (8, 0), (9, 0), and (10, 0) silicon carbide nanotubes", ***Materialia***, 20:101257, (2021).

[12] Larina E.V., Chmyrev V.I., Skorikov V.M., D'yachkov P.N., Makaev D.V., "Band Structure of Silicon Carbide Nanotubes", ***Inorganic Materials***, 44(8):823–834, (2008).

[13] Huang Z., Lü T.Y., Wang H.Q., Zheng J.Ch., "Thermoelectric properties of the 3C, 2H, 4H, and 6H polytypes of the wide-band-gap semiconductors SiC, GaN, and ZnO", ***AIP Advances,*** 5,:097204, (2015).

[14] Chen Y.K., Liu L.V., Tian W.Q., Wang Y.A., "Theoretical Studies of Transition-Metal-Doped Single-Walled Carbon Nanotubes", ***Journal of Physical Chemistry C***, 115:9306-9311, (2011).

[15] Wang J., Yan W., Gao T., Gao Y., Liu Y., "Analysis of the magnetic and optical properties of (Fe, V)-co-doped 3C–SiC using first-principles calculations", ***Journal of Physics and Chemistry of Solids,***181(21):111527, (2023).

[16] Zhang Y., Jiang S., Li Y., Chen C., Chen Z., Wang X., "The influence of point defects on the electronic structures and optical properties of 3C-SiC", ***AIP Advances,*** 14:055009, (2024).

[17] Mishra G., Mohapatra S., Prusty S., Sharma M. K., Chatterjee R., Singh S. K., Mishra D. K., "Magnetic Properties of Nanocrystalline β-SiC,"***Journal of Nanoscience and Nanotechnology***, 11(6):5049-5053, (2011).

[18] Cui Z., Bai K., Ding Y., Wang X., Li E., Zheng J., Wang S., "Electronic and Optical Properties of Janus MoSSe and ZnO vdWs Heterostructures", ***Superlattices and Microstructures***, 140:106445, (2020).

[19] Cui Z., Luo Y., Yu J., Xu Y., "Tuning the Electronic Properties of $MoSi_2N_4$ by Molecular Doping: A First Principles Investigation", ***Physica E: Low-dimensional Systems and Nanostructures,*** 134, 114873, (2021).

[20] Sun M., Ren Q., Zhao Y., Chou J.P., Yu J., Tang W., "Electronic and Magnetic Properties of 4d Series Transition Metal Substituted Graphene: a First-Principles Study", ***Carbon***, 120: 265–273, (2017).

[21] Sun M., Yan Y., Schwingenschlögl U., "Beryllene: A Promising Anode Material for Na- and K-Ion Batteries with Ultrafast Charge/Discharge and High Specific Capacity", ***The Journal of Physical Chemistry Letters***, 11:9051–9056, (2020).

[22] Chabi, S., Kadel, K., "Two-dimensional Silicon Carbide: Emerging Direct Band Gap Semiconductor", ***Nanomaterials***, 10: 2226, (2020).

[23] Gürcan K., Derin B., Ayas E., "Effect of SiC particle size on the microstructural, mechanical and oxidation properties of In-situ synthesized HfB2-SiC composites", ***Journal of Polytechnic***, 24(2):503-510, (2021).
[24] Sun L., Li Y., Li Z., Li Q., Zhou Z., Chen Z., Yang J., Hou J.G., "Electronic structures of SiC nanoribbons", ***The Journal of Chemical Physics,*** 129(17):174114, (2008).
[25] Alfieri G., Kimoto T., "Engineering the band gap of SiC nanotubes with a transverse electric field", ***Applied Physics Letters***, 97: 043108, (2010).
[26] Lou P., Lee J.Y., Electrical control of magnetization in narrow zigzag silicon carbon nanoribbons, ***The Journal of Physical Chemistry C***, 113(50): 21213-21217, (2009).
[27] Bekaroglu E., Topsakal M., Cahangirov S., Ciraci S., "First-principles study of defects and adatoms in silicon carbide honeycomb structures", ***Physical Review B***, 81(7): 075433, (2010).
[28] [28] Sinelnik A.V., Semenov A.V., "Theoretical study of the band structure of 2H-SiC and 4H-SiC of silicon carbide polytypes", ***Condensed Matter Physics***, 24:23706,(2021).
[29] Park C.H., Cheong B.H., Lee K.H., Chang K.J., "Structural and electronic properties of cubic, 2H, 4H, and 6H SiC", ***Physical Review B***, 49:4485, (1994).
[30] Harris G. L. (Ed.), "Properties of Silicon Carbide, INSPEC, Institution of Electrical Engineers", ***London***, (1995).
[31] Wenzien B., Kackell P., Bechstedt F., "Quasiparticle band structure of silicon carbide polytypes", ***Physical Review B***, 52:10897, (1995).
[32] Jafarova V.N., Rzayeva S.S., Scurtu I.C., Stanca C., Acomi N., Raicu G., Prediction of ferromagnetism in GaN:Ag and SiC:Ag nanotubes, ***Advances in Natural Sciences Nanoscience and Nanotechnology,*** 15(3), 035012 , (2024).
[33] Ummels R.T., Bobbert P.A., Haeringen W .Van, "Ab initio quasiparticle energies in 2 H, 4 H, and 6 H SiC", ***Physical Review B***, 58:6795, (1998).
[34] Gao S.P. Zhu T., "Quasiparticle band structure calculation for SiC using self-consistent GW method", ***About Acta Physica Sinica***, 61:137103, (2012).
[35] Methfessel M., Paxton A., "High-precision sampling for Brillouin-zone integration in metals", ***Physical Review B***, 40, 3616, (1989).
[36] Gözükizil M.F., Birelli A., "Al, Cu doped-undoped TiO_2 thin film deposition and the effect of doping on film properties", ***Journal of Polytechnic***, 27(3):1081-1087, (2024).
[37] Zan R., Altuntepe A., Erkan S., Seyhan A., "Nitrogen doped graphene film synthesis and characterization", ***Journal of Polytechnic***, 25(2):667-673, (2022).
[38] Sun X.K., Liu J.W., Liu K.L., Wang S.H., Zhao L.L., Qin, W., Wang G.L., Meng M., Li J.T., Dong X., "Effect of temperature on the structure and magnetic properties of Co doped SiC films", ***Superlattices and Microstructures***, 107:144–149, (2017).