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# Functionalization of short clusters of carbon nanotubes (6.0) by copper and nickel atoms: a theoretical investigation

© N.P. Boroznina,[1] D.F. Sergeev,[1,2] S.V. Boroznin,[1] I.V. Zaporotskova[1]

[1]Volgograd State University,
400062 Volgograd, Russia
[2]All-Russian Research, Design and Technological Institute of Oil Refining and Petrochemical Equipment,
400078 Volgograd, Russia
e-mail: boroznina.natalya@volsu.ru

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The results of a theoretical study of the effect of surface functionalization of pure (6,0) carbon nanotubes with copper and nickel atoms on their conductive properties are presented. The analysis was performed using density functional theory within the B3LYP functional with the 6-31G basis set. The calculations allowed us to determine the optimal positions of copper and nickel atoms on the carbon nanotube surface. These positions were found to be located above the center of the nanotube hexagon. Computer simulations of the regular adsorption of selected metal atoms on the nanotube surface were conducted. Analysis of the electron-energy state of the resulting nanosystems allowed us to determine the energy band gap. With this type of regular adsorption, a decrease in the band gap is observed, indicating improved conductive properties of the resulting systems compared to „pure“ carbon nanotubes.

**Keywords:** nanotechnology, nanomaterials, metallization, surface adsorption.

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## Introduction

Recently, the use of metal composites has increased markedly in various industry sectors [1,2], which is explained by the fact that such materials often exhibit improved characteristics relative to their individual components [1–3]. The composite materials are generally composed of the two or more underlying components such as matrix and carcass having various properties [2,3]. The matrix is a connecting material, and the carcass is an embedded component to obtain the necessary characteristics [3]. It should be stressed that distribution of the carcass material is critical in obtaining the performance properties required from a composite [4]. The progress in strong benefits of composites with an underlying metal matrix has led to engineering of the aluminum metal-matrix composites. Such composites have a good ratio of mechanical characteristics to the total mass of the material, electrical and thermal characteristics, as well as a reasonable cost [2,5–8].

However, the new industrial sector challenges dictate the need for the materials and devices miniaturization in parallel with their properties improvement [9]. Given the above, it is worth paying special attention to the carbon nanotubes (CNT), as they are quite a valuable material for use in various fields, including developments in electronics, energy storage, sensors, composites and coatings [10–14]. Because CNT are featuring a pool of highly valued properties for the specific areas, they are very prosperous for use in different sectors. Such properties include high mechanical characteristics, high conductivity and adsorption capacity, and chemical stability [10,14–22].

At that, special mention should be made of the option of changing or improvement of CNT properties, since the manipulations related to the structural modifications or functionalization of the CNT surface allow getting even more pronounced properties [12,15,19–25]. It should be emphasized that the improved CNT demonstrate higher rate of their use in experiments, fabrication and use of nanomaterials, as well as in the systems made on their basis [26].

The studies [20,27–29] may serve as an example with sensor properties of CNT studied in them after the CNT modification or functionalization using various metals. The research data often indicate that critical properties of the harmful substance detectors have been improved, e.g., they have better selectivity and sensitivity.

In other studies [30–33], after similar manipulations, it was possible to achieve increased electrical conductivity, rapid electron transfer, high specific capacity, electrical stability and mechanical strength. All the above-mentioned is of great value for the contemporary electronic devices used both in household appliances and in the industry sector.

This paper outlines a theoretical study of the mechanism of CNT (6.0) interaction with the atoms of copper (Cu) and nickel (Ni), modifying the CNT surface.

## 1. Methodology

Density functional theory (DFT) is a well-recognized and proven method both for conducting model experiments and for quantum chemical analysis. This method is also characterized by the ease of use when calculating the CNT-based systems. According to DFT, the properties of a multi-electronic system, including its energy, can be determined

from the electron density in the absence of information about wave functions [34].

B3LYP — is a hybrid approximation method, a three-parameter functional (the exact Hartree-Fock exchange operator, Becke functional and Slater functional), with its correlation part being a combination of LYP and VWN functionals. It is a unique method because the three exchange components are taken with weight coefficients. This method has semi-emprirical nature, thus, allowing to get higher calculations accuracy [34].

Basis 6-31G is a more advanced version of a set of mathematical functions, since it is a valence-split basis in which the valence orbitals of atoms are described by several basic functions in a molecule [34].

## 2. Discussion of research results

### 2.1. Interaction of CNT (6,0) with Cu and Ni atoms —single adsorption

To determine the perspective and mechanism of the functionalization of the CNT (6.0) surface with Cu and Ni atoms, a study of their interaction was conducted. To more accurately identify the position of Cu and Ni atoms relative to CNT surface, as well as to identify their effect on the conductive properties of the functionalized CNT, three models were created for each of the analyzed atoms, namely, when they are located above the carbon atom, above the carbon atom bond center, and above the hexagon center (Fig. 1). The CNT length was about 17 Å or 8 hexagons, the uncompensated valences at the cluster boundaries are closed with hydrogen atoms to avoid the margin effects. Figure 1 shows a complete cluster of CNT to visually demonstrate the removal of the adsorption center from the CNT boundaries, and then (Figure 2) — to demonstrate the regular arrangement of metal atoms.

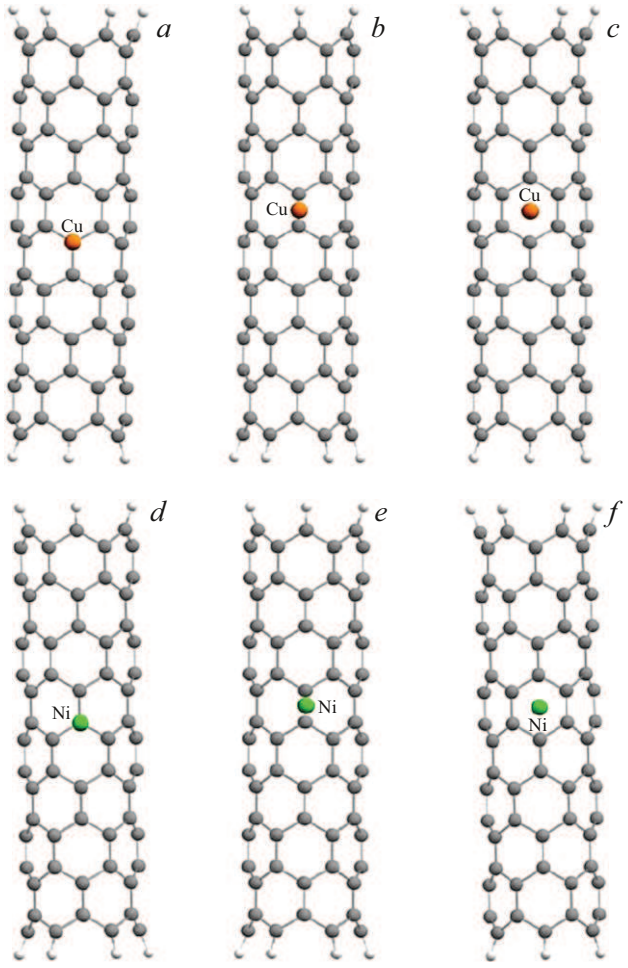


**Figure 1.** CNT with attached copper and nickel atoms, single adsorption: $a, d$ — above the carbon atom; $b, e$ — above the carbon bond center; $c, f$ — above the center of CNT hexagon.

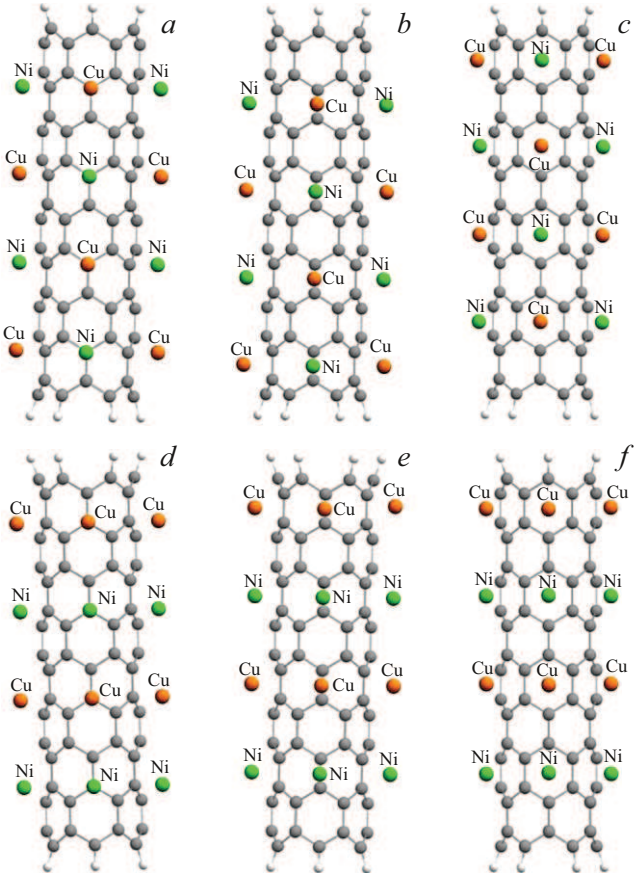


**Figure 2.** CNT with attached copper and nickel atoms, regular adsorption: $a, d$ — Cu and Ni above the carbon atom; $b, e$ — Cu and Ni above the center of the carbon bond; $c$, $f$ — Cu and Ni above the center of CNT hexagon.

To obtain the required amount of data, the simulation of CNT (6.0) interaction with Cu and Ni atoms took place in increments of 0.01 nm to each of the adsorption centers (Fig. 1, $a$–$f$). These atoms were approached perpendicular to the longitudinal axis of CNT, where at each step the estimated energy of the resulting system was calculated. The calculated data were used to plot the graphs reflecting the

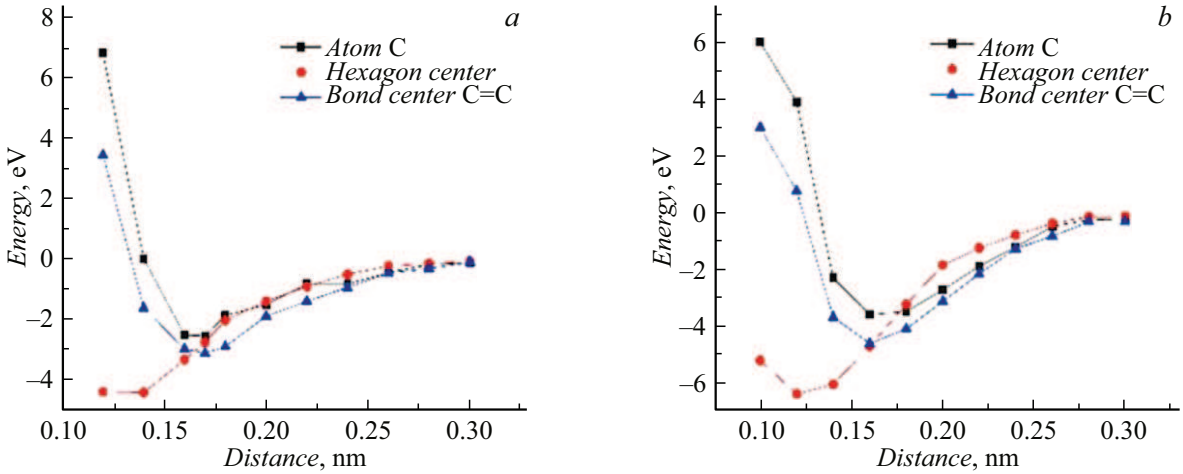


**Figure 3.** Profiles of the potential energy surface of the atom attachment process: *a* — Cu to CNT surface for three atomic arrangement options; *b* — Ni to CNT surface for three atomic arrangement options.

**Table 1.** Comparative table of the electron-energy characteristics of the studied systems with a single adsorption

| Structure type | Distance of interaction, nm | energy interaction, eV | band gap width, eV |
|---|---|---|---|
| CNT (6.0) before functionalization | | | 0.69 |
| CNT−Cu above C atom | 0.17 | −2.50 | 0.26 |
| CNT−Cu above the bond center C−C | 0.17 | −3.07 | 0.20 |
| CNT−Cu above the center of hexagon | 0.12 | −4.38 | 0.51 |
| CNT−Ni above the atom C | 0.16 | −3.59 | 0.53 |
| CNT−Ni above the center of C−C bond | 0.16 | −4.61 | 0.64 |
| CNT−Ni above the center of hexagon. | 0.12 | −6.39 | 0.57 |

surface profiles of the potential energy of CNT interaction with the studied atoms (Fig. 3). Based on the energy minima, we determined the best interaction distances of Cu and Ni with the CNT surface, as well as their energy values. After analyzing the electron-energy states of the obtained systems, their band gap values were calculated. The results are provided in Table 1.

The study allowed identifying the most probable locations of Cu and Ni atoms on the surface of CNT (6.0) during its functionalization from the energy standpoint. It is the location of the atoms of these metals above the hexagon center of CNT surface (Fig. 1, *c*,*f*): it was identified based on the best interaction energy of all the analyzed systems.

The theoretical calculations made it possible to plot the graphs reflecting the densities of the states of the analyzed systems (Fig. 4). The band gap widths for all possible locations of the metal atoms above the CNT (6.0) surface are given in Table 1.

By studying the electron-energy structure of the created CNT,+,Cu and Ni complexes, it was found that the molecular orbitals were grouped into a conduction band and a valence band separated by the band gap. The densities of states are a family of graphs where, in addition to the total density of states, densities of alpha and beta electron states are indicated, which differ from each other in the direction of spin. The newly occurred additional densities of states were associated with impurity levels that appeared in the structure after addition of a metal atom. The values of the valence band top and conduction band bottom were determined by the total density of the system states, also shown in these figures.

The band gap is the energy difference between the upper occupied and lower vacant orbitals. Using the band gap, it is possible to find the materials conductive properties, including properties of various nanostructures. To find the band gap the following formula is used:

$$\Delta E_g = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}. \qquad (1)$$

The band gap of CNT (6.0) before functionalization made 0.69 eV. When Cu atom is attached to this type of CNT in any of its arrangements the band gap values decline (Fig. 4, *b*–*d*) if it is located above the hexagon center —

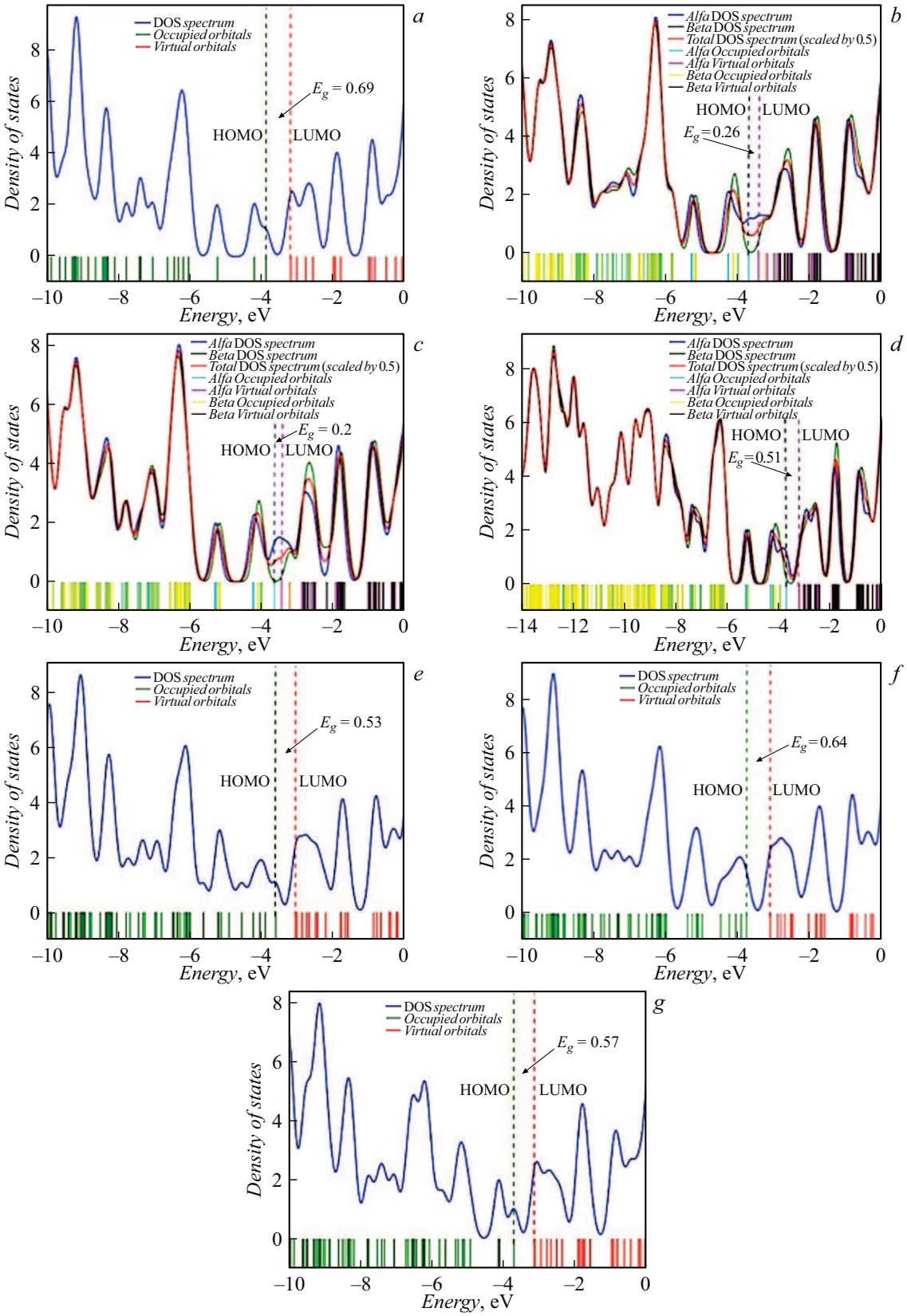


**Figure 4.** Densities of states of the following systems „CNT + Cu and Ni atoms“ for a case of singular adsorption: *a* — CNT (6,0) before functionalization; *b* — CNT + Cu system with the atom located above the carbon atom; *c* — CNT + Cu system with the atom located above the center of the carbon bond; *d* — CNT + Cu with the atom located above the hexagon center; *e* — CNT + Ni system with the atom located above the carbon atom; *f* — CNT + Ni system with the atom located above the carbon bond center; *g* — CNT + Ni system with the atom located above the hexagon atom.

**Table 2.** Charge distribution during single adsorption

| Variant of Cu and Ni atoms adsorption | Charge value on atom metal before attachment | Charge value on metal atom after attachment | Averaged value charge of nearest atom neighbors on to CNT surface before atoms attachment | Averaged value charge of nearest atom neighbors on CNT surface after atoms attachment |
|---|---|---|---|---|
| CNT−Cu above C atom | 0 | 0.631 | −0.010 | −0.298 |
| CNT−Cu above the bond center C−C | 0 | 0.909 | 0.009 | −0.281 |
| CNT−Cu above the center of hexagon | 0 | 0.574 | −0.011 | −0.109 |
| CNT−Ni above the atom C | 0 | 0.888 | −0.010 | −0.672 |
| CNT−Ni above the center of C−C bond | 0 | 0.810 | 0.009 | −0.470 |
| CNT−Ni above the center of hexagon. | 0 | 0.881 | −0.011 | −0.132 |

up to 0.51 eV. When Ni atom is attached allowing for all of its possible locations a similar situation is observed (Figure. 4, *e*−*g*) if it is located above the hexagon center — up to 0.57 eV.

A study of the charge distribution in CNT (6.0) + Cu and Ni atoms systems showed that in all analyzed variants there was a transfer of electron density from metal atoms to carbon atoms of CNT (Table 2). The charge carrier — an electron, is transferred from Cu and Ni atoms to the CNT surface. Due to this, most of the charge carriers are formed there and conduction is realized over its surface.

The data obtained indicate that the most stable of all the analyzed systems are those with the arrangement of metal atoms above the center of CNT hexagon. The interaction distances and adsorption energies of these complexes correspond to the formation of bonds, which, in turn, is evidence of their stability. At the same time, in all the analyzed cases, there is a decrease in the band gap relative to CNT (6.0) before functionalization, and the charge distribution has a positive effect on the sensory properties of the resulting system.

## 2.2. Interaction of CNT (6.0) with Cu and Ni atoms — regular adsorption

Having checked the effectiveness of the functionalization of CNT (6.0) by Cu and Ni atoms during single adsorption, we took the next step, which was to perform a similar operation, but using the mechanism of regular adsorption. We selected the interaction distances of metal atoms with the CNT surface for these complexes based on the best values obtained during single adsorption. 12 atoms of Cu and Ni with various combinations were attached to the CNT surface (Fig. 2). The metal atoms were positioned above the adsorption centers in such a way as to form a metal superlattice above the CNT surface. Various options of alternating copper and nickel atoms were selected to study the effect of atoms arrangement in a crystalline superlattice on the electron-energy structure of a metallic nanocomposite.

The analyzed combinations of Cu and Ni atoms relative to CNT (6.0) surface were as follows:

1) metal atoms above the first and third rows of hexagons were alternating with the formation of Ni−Cu−Ni sequence, above the second and fourth row of Cu−Ni−Cu — with their arrangement above the carbon atom (Fig. 2, *a*), above the center of carbon bond (Fig. 2, *b*), above the hexagon (Fig. 2, *b*);

2) metal atoms above the first and third rows of hexagons formed a ring of Cu atoms, above the second and fourth rows —a ring of Ni atoms, with their arrangement above the carbon atom (Fig. 2, *d*), above the center of the carbon bond (Fig. 2, *e*), over the hexagon (Fig. 2, *f*). The distances between the formed rings were 0.42nm, since the analyzed atoms were quite large.

The theoretical analysis made it possible to plot the densities of states curves for the analyzed systems (Fig. 5). The band gaps for all possible locations of the metal atoms above the CNT (6.0) surface are given in Table 3.

A study of the electron-energy structure of the created CNT + Cu + Ni complexes demonstrated that the molecular orbitals were grouped in the same way as described earlier, i.e. there were valence band and conduction band separated by the band gap.

From the earlier obtained data, it was found that the band gap near CNT (6.0) before functionalization made 0.69 eV, in case of singular adsorption above the CNT hexagon center with Cu atom — 0.51 eV, Ni atom — 0.57 eV. In case of regular adsorption with Cu and Ni atoms the decrease in the band gap is observed compared to both, the „pure“ CNT, and complexes of CNT + Cu, CNT + Ni in case of single adsorption. Among the most stable systems the band gap at regular adsorption was 0.37 eV (Table 3).

The stability of CNT-based complexes during regular adsorption was determined using the following formula:

$$E_{AT} = \frac{aE_c + bE_H + cE_Ni + dE_Cu - E_{\text{CNT+Me}}}{a + b + c + d}, \qquad (2)$$

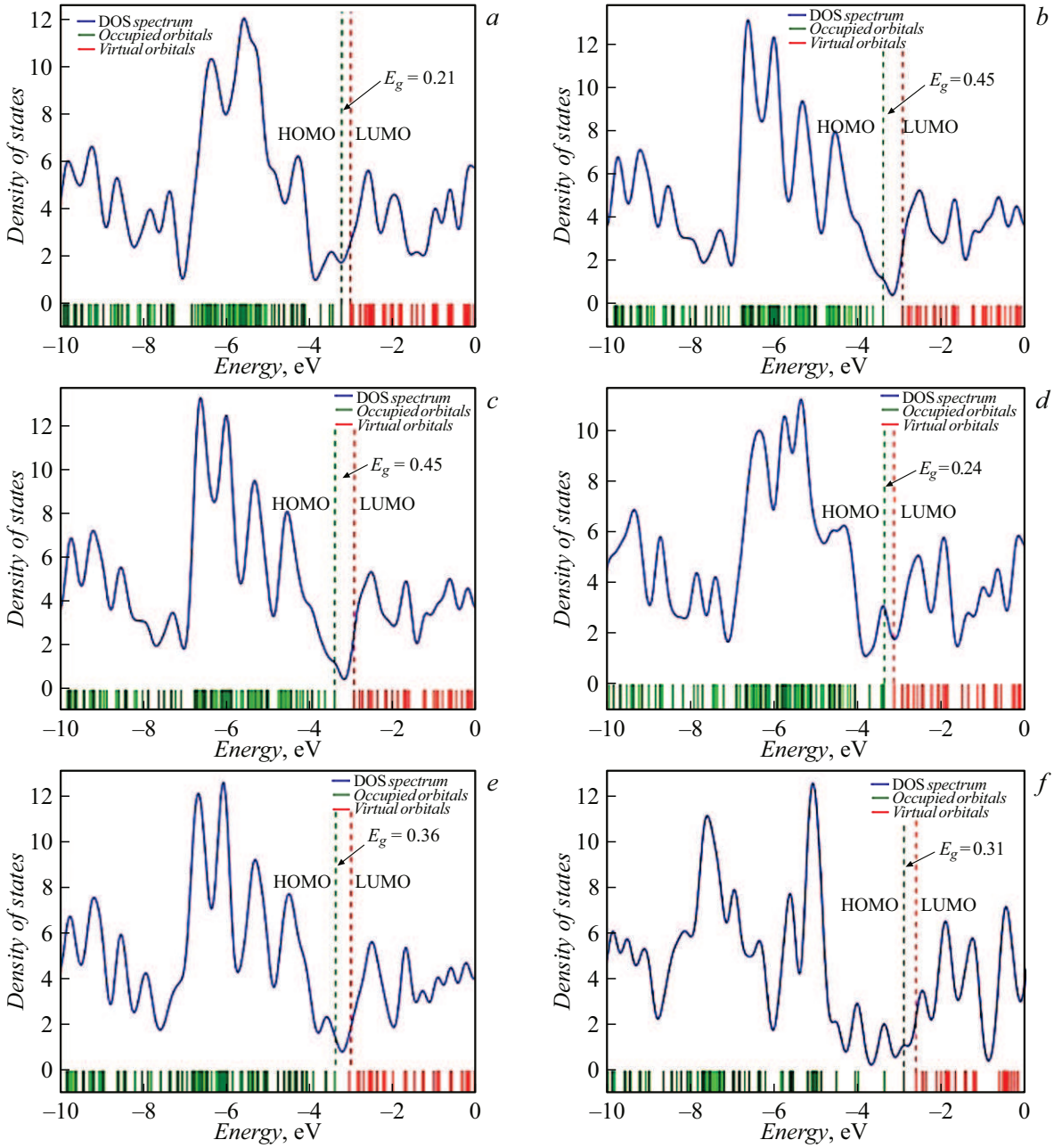


**Figure 5.** Densities of states of the following systems „CNT + Cu and Ni atoms“ for a case of regular adsorption: *a* — CNT + Cu + Ni with the atom located above the carbon atoms; *b* — CNT + Cu + Ni system with the atom located above the carbon bonds centers; *c* — CNT + Cu + Ni system with the atoms located above the hexagon centers; *d* — CNT + Cu + Ni system with the atoms located above the carbon atoms; *e* — CNT + Cu + Ni system with the atoms located above the carbon bond centers; *f* — CNT + Cu + Ni system with the atoms located above the hexagon centers.

where EAT — atomization energy per one CNT atom, EC — energy of carbon atom, EH — energy of hydrogen atom, ENi — energy of nickel atom, ECu — energy of copper atom, *a* — number of carbon atoms in the given CNT, *b* — number of pseudo-atoms of hydrogen, *c* – number of nickel atoms, *d* — number of copper atoms, ECNT + Me — full energy of all atoms of CNT.

The performed studies indicate that the most stable complexes with regular adsorption, as well as with single adsorption, are formed over the centers of CNT hexagons, while the best option is with 1 combination of Cu and Ni atoms (Fig. 2, *c*). The calculation results are provided in Table 3.

The analysis of the charge distribution in CNT (6.0) + Cu + Ni systems showed that with regular adsorption, a similar result is observed with single adsorption, i.e. in all the considered variants, the transfer of electron density from metal atoms to carbon atoms of CNT is noticeable, due

**Table 3.** Comparative table of the electron-energy characteristics of the considered systems during regular adsorption

| Structure | Distance interaction, nm | | Energy atomization, eV | band gap, eV |
|---|---|---|---|---|
| Regular adsorption above C atom (Fig. 2, *a*) | Cu | 0.17 | −7.55 | 0.21 |
| | Ni | 0.16 | | |
| Regular adsorption above C atom (Fig. 2, *d*) | Cu | 0.17 | −7.54 | 0.24 |
| | Ni | 0.16 | | |
| Regular adsorption above the center of carbon bond (Fig. 2, *b*) | Cu | 0.17 | −7.62 | 0.45 |
| | Ni | 0.16 | | |
| Regular adsorption above the center of carbon bond (Fig. 2, *e*) | Cu | 0.17 | −7.62 | 0.36 |
| | Ni | 0.16 | | |
| Regular adsorption above hexagon (Fig. 2, *c*) | Cu | 0.17 | −7.75 | 0.37 |
| | Ni | 0.16 | | |
| Regular adsorption above hexagon (Fig. 2,*f*) | Cu | 0.17 | −7.73 | 0.31 |
| | Ni | 0.16 | | |

to which a large part is formed there. charge carriers and conduction is realized over its surface.

The data obtained indicate that the most stable of all the analyzed systems is the system with the arrangement of metal atoms above the center of CNT hexagon (combination 1, Fig. 2, *c*). The interaction distances and adsorption energies of this complex correspond to the formation of a bond, which is evidence of the system stability. In all the analyzed cases, there is a decrease in the band gap relative to CNT (6.0) before functionalization, as well as its decrease in the most stable system with regular adsorption relative to the system with single adsorption.

## Conclusion

The theoretical study made it possible to determine the effect of functionalization by Cu and Ni atoms on the conductive properties of CNT (6.0), taking into account single and regular adsorptions. The performed quantum-chemical analysis allowed to find the following:

from the configuration stability standpoint, the most optimal position of Cu and Ni atoms relative to the surface of CNT (6.0) for both single and regular adsorption (combination option 1) is their location above the center of the CNT hexagon;

When metal atoms are attached to CNT (6.0) surface, in all analyzed cases, the band gap decreases relative to the CNT before functionalization, while the most stable system with regular adsorption has lower band gap values than a similar system with single adsorption;

The charge distribution of the simulated CNT (6.0) + Cu and Ni systems in all analyzed cases indicates that there is a transfer of electron density from metal atoms to carbon atoms of CNT. The displacement of the electron cloud from metal atoms to the surface of the nanotube will lead to a possible increase in charge carriers. The conductive properties are improved due to a decrease in the band gap.

Thus, it can be concluded that CNT (6.0) can be functionalized with Cu and Ni atoms, while the improvement in the conductive properties of the obtained systems is observed, which is most noticeable with regular CNT adsorption. The data obtained can form the basis for the design of super miniature devices for the needs of nanoelectronics.

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### Conflict of interests

The authors declared that they had not any conflict of interests.

## References

[1] A. Kumar, R.C. Singh, R. Chaudhary. Mater. Today: Proceed., **21**, 1453 (2020). DOI: 10.1016/j.matpr.2019.10.079
[2] A.K. Sharma, R. Bhandari, A. Aherwar, C. Pinca-Bretotean. Mater. Today: Proceed., **27**, 1608 (2020). DOI: 10.1016/j.matpr.2020.03.316
[3] A. Atmakuri, A. Palevicius, A. Vilkauskas, G. Yanusas. Polymers, **12** (9), 2088 (2020). DOI: 10.3390/polym12092088

[4] D.S. Prasad, C. Shoba, N. Ramanaiah. J. Mater. Res. Technol., **3** (1), 79 (2014). DOI: 10.1016/j.jmrt.2013.11.002
[5] A. Kumar, V.P. Singh, R.C. Singh, R. Chaudhary, D. Kumar, A.-H.I. Mourad. J. Mater. Sci., **59** (7), 2644 (2024). DOI: 10.1007/s10853-024-09398-7
[6] S. Suresha, B.K. Sridhara. Mater. Design, **31** (9), 4470 (2010). DOI: 10.1016/j.matdes.2010.04.053
[7] R. Chandel, N. Sharma, S.A. Bansal. Emergent Mater., **4** (5), 1243 (2021).
[8] S.A. Sajjadi, H.R. Ezatpour, M.T. Parizi. Mater. Design, **34**, 106 (2012). DOI: 10.1016/j.matdes.2011.07.037
[9] L. Aryasomayajula, K.J. Wolter. J. Nanotechnol., **2013** (1), 296517 (2013). DOI: 10.1155/2013/296517
[10] N.T. Alvarez, P.Miller, M.R. Haase, R. Lobo, R. Malik, V. Shanov. Carbon, **144**, 55 (2019). DOI: 10.1016/j.carbon.2018.11.036
[11] A. Hoque, C.P. Nawarathne, N.T. Alvarez. Carbon, **235**, 120086 (2025). DOI: 10.1016/j.carbon.2025.120086
[12] M.M.H. Raza, M. Sadiq, M. Zulfequar, S. Husain, J. Ali. J. Phys. Chem. Solids, **178**, 111309 (2023).
[13] M.A.S. Sakr, G.M. Abdelrazek, H. Abdelsalam, O.H. Abd-Elkader, V.A. Saroka, Q. Zhang. Mater. Sci. Eng.: B, **317**, 118160 (2025). DOI: 10.1016/j.mseb.2025.118160
[14] A. Kumar, S. Rathor, S. Singh, R. Kant, H. Singh, M. Vost'ak, S. Houdkova. Tribology Intern., 111249 (2025). DOI: 10.1016/j.triboint.2025.11124
[15] S. Wangchuk, K. Promsuwan, J. Saichanapan, A. Soleh, K. Saisahas, K. Samoson, A. Numnuam, P. Kanatharana, P. Thavarungkul, W. Limbut. Microchem. J., **207**, 112217 (2024). DOI: 10.1016/j.microc.2024.112217
[16] Ya. Wang, J. Chen, W. Tang, D. Xia, Yu. Liang, X. Li. Chemosphere, **214**, 79 (2019). DOI: 10.1016/j.chemosphere.2018.09.074
[17] H. Zhang, J. Dai, H. Zhou, R. Hong, W. Dong, H. Chu. J. Analyt. Appl. Pyrolys., **192**, 107272 (2025). DOI: 10.1016/j.jaap.2025.107272
[18] D. Chu, Ch. Gao, Z. Ji, Y. Li, Q. Jin, Y. He, W. Bai. Mater. Today Chem., **45**, 102616 (2025). DOI: 10.1016/j.mtchem.2025.102616
[19] J. Kang, M. Kang, S. Pyo, K. Park. Composite Structures, **372**, 119614 (2025). DOI: 10.1016/j.compstruct.2025.119614
[20] Sh. Gulati, H.N. Lingam, B.S. Kumar, K. Goyal, A. Arora, R.S. Varma. Chemosphere, **299**, 134468 (2022). DOI: 10.1016/j.chemosphere.2022.134468
[21] V.J. Chakravarthy, C. Thontadari, G.N. Basavaraj, R. Sowndharya, N. Aravindan, V. Sangeetha. Microchem. J., **218**, 115413 (2025). DOI: 10.1016/j.microc.2025.115413
[22] Ch.-Yu. Lin, J.-W. Chang, M.-H. Lin, K.-Ch. Wu, Sh.-H. Hong, J.-M. Lin, Ch.-W. Kung, Ch.-L. Liu. Chem. Eng. J., **521**, 166861 (2025). DOI: 10.1016/j.cej.2025.166861
[23] M. Hamadanian, Z. Tavangar, B. Noori. J. Molecular Structure, **1076**, 49 (2014). DOI: 10.1016/j.molstruc.2014.07.017
[24] N.P. Boroznina, S.V. Boroznin, I.V. Zaporotskova, P.A. Zaporotskov, D.F. Sergeev, G. Murugadoss, N. Venkatesh, Sh.G. Peera. Inventions, **10** (5), 86 (2025). DOI: 10.3390/inventions10050086
[25] S. Ramanathan, W.J. Lau, P.S. Goh, M.F. Omar, M.C. Breadmore, A.F. Ismail, H.H. See. J. Environmental Chem. Eng., **12** (3), 112931 (2024). DOI: 10.1016/j.jece.2024.112931
[26] J. Zhao, X. He, Yu. Wang, Sh. Wang, R.H. Baughman. Microchem. J., **214**, 114086 (2025). DOI: 10.1016/j.microc.2025.114086
[27] S.-W. Choi, B.-M. Kim, S.-H. Oh, Yo.T. Byun. Sensors and Actuators B: Chem., **249**, 414 (2017). DOI: 10.1016/j.snb.2017.04.119
[28] M. Penza, R. Rossi, M. Alvisi, M.A. Signore, G. Cassano, D. Dimaio, R. Pentassuglia, E. Piscopiello, E. Serra, M. Falconieri. Thin Solid Films, **517** (22), 6211 (2009). DOI: 10.1016/j.tsf.2009.04.009
[29] H. Shi, J. Chen, S. Yu. Mater. Today Commun., **37**, 107200 (2023). DOI: 10.1016/j.mtcomm.2023.107200
[30] X. Hao, W. Zhou, Z. Huang, Y. Li, D. Li, J. Xu. J. Colloid Interface Sci., **689**, 137200 (2025). DOI: 10.1016/j.jcis.2025.02.208
[31] R. Li, P. Song, Zh. Ji, H. Zhou, Yi. Xue, L. Kong, X. Shen. Appl. Surf. Sci., **649**, 159188 (2024). DOI: 10.1016/j.apsusc.2023.159188
[32] M.S. Munir, M.I. Alvi, M.A. Saeed, A. Khan, A. Shareef, M. Khan. Mater. Chem. Phys.: Sustainability and Energy, **2**, 100007 (2025). DOI: 10.1016/j.macse.2024.100007
[33] Sh.J. Shetty, T.K. Nanditha, S. Amini, S.M. Rumana Farheen, M.A. Sangamesha, S. Krishnaveni, S.C. Gurumurthy. J. Alloys Compounds, **1041**, 183837 (2025). DOI: 10.1016/j.jallcom.2025.183837
[34] L.S. Elbakyan. *Quantum-chemical analysis using GAUSSIAN software and graphic editor GAUSSVIEW* (Volgograd State University, Volgograd, 2022)

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