Original paper

Study of functionally modified carbon nanotubes with respect to carbon dioxide

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Abstract: In this study, the sensory properties towards carbon dioxide of nanocomposites, which are carbon nanotubes with metal oxides attached to it, was studied. The study focused on the geometry and stability of adsorption complexes and the changes in the physicochemical properties (the energy gap and charge distribution) of nanostructures caused by adsorption processes. This research was conducted using computer experiments based on calculations performed with density functional theory methods and a quasi-molecular approach. The results of the computer experiment allowed us to estimate the change in the adsorption energy and the band gap. Based on this analysis, presented below, iron oxide was selected as the most effective material for creating the nanocomposite. Being characterized by a sufficiently weak interaction in terms of the adsorption energy (from 0,17 to 0,23 eV), this materials have a sufficiently strong response (in the best case the energy gap decreases from 1,644 to 1,622 eV) and, consequently, a high sensitivity to carbon dioxide. Response in the case of the carbon nanotubes (6,6)-cobalt oxide is significantly stronger (the energy gap decreases from 1,54 to 1,45 or 1,34 eV depending on the adsorption distance), but the strong interaction between composite and carbon dioxide could cause poisoning the sensor. The carbon nanotubes-copper oxide composite is characterized by weak response and, consequently, low sensitivity towards carbon dioxide. The results obtained reveal important physicochemical patterns of interaction between carbon nanotubes and metal oxides composites and carbon dioxide. These findings are significant in terms of the sensitivity and reproducibility of chemical sensors measurements, making them crucial for the development of nanoscale gas sensors.

Keywords: carbon nanotubes, metal oxides, carbon dioxide, gas sensing, density functional theory, energy gap, charge distribution.

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Исследование функционально модифицированных углеродных нанотрубок в отношении к диоксиду углерода

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Аннотация: В данной работе исследовались сенсорные свойства нанокомпозитов, представляющих собой углеродные нанотрубки с присоединенными к ним оксидами металлов, по отношению к молекулам диоксида углерода. Основное внимание уделялось геометрии и

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стабильности адсорбционных комплексов, а также изменениям физико-химических характеристик (ширины запрещенной зоны, распределения заряда) наноструктур, вызванным процессами адсорбции. Исследование проводилось методом компьютерного моделирования с использованием теории функционала плотности и квазимолекулярного подхода. Полученные результаты позволили оценить изменения энергии адсорбции и ширины запрещенной зоны. На основе проведенного анализа в качестве наиболее эффективного материала для создания нанокомпозита был выбран оксид железа. При относительно слабом взаимодействии (энергия адсорбции от 0,17 до 0,23 эВ) этот материал демонстрирует достаточно выраженный отклик (в лучшем случае ширина запрещенной зоны уменьшается с 1,644 до 1,622 эВ) и, как следствие, высокую чувствительность к диоксиду углерода. В случае композита углеродная нанотрубка (6,6)-оксид кобальта отклик значительно сильнее (ширина запрещенной зоны уменьшается с 1,54 до 1,45 или 1,34 эВ в зависимости от расстояния адсорбции), однако сильное взаимодействие между композитом и диоксид углерода может привести к «отравлению» сенсора. Композит углеродная нанотрубка-оксид меди характеризуется слабым откликом и, соответственно, низкой чувствительностью к диоксиду углерода. Полученные результаты раскрывают важные физико-химические закономерности взаимодействия композитов углеродная нанотрубка–оксид металла с диоксидом углерода. Эти данные имеют большое значение для обеспечения чувствительности и воспроизводимости измерений химических сенсоров, что делает их ключевыми для разработки газовых сенсоров наноразмерного уровня.

Ключевые слова: углеродные нанотрубки, оксиды металлов, диоксид углерода, газовое детектирование, теория функционала плотности, энергетическая щель, распределение заряда.

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1. Introduction

The use of traditional fuels has accompanied humanity throughout all its history [1]. Coal, oil, and natural gas are the foundations of modern energy. However, their use has negative consequences: a large amount of greenhouse gases, including carbon dioxide, leads to air pollution depletion of natural resources, and geopolitical tensions due to energy supplies [2]. During the combustion of traditional fuels, carbon dioxide is released into the atmosphere in large amounts [3]. At the same time, the depletion of natural resources leads to an increase in the cost of the batteries themselves, as described in the review [4]. This makes it necessary to combat climate change, for which, in addition to new energy

sources [5], it is proposed to retain carbon dioxide, then decomposing it into components [6]. Compared to other gases, the volumes of carbon dioxide are the largest among those that affect global warming processes [7]. Carbon dioxide does not decompose in the atmosphere for a long time, having a destructive effect on the environment [8]. Switching to hydrogen energy is also not safe, since one of the reaction products is carbon dioxide [9]. It is necessary to optimize technological processes in such a way that the production of new batteries is not accompanied by the release of harmful substances.

Carbon nanotubes, due to their unique properties, such as the dependence of the type of conductivity (metallic or semiconducting) on the geometry of the nanotube [10, 11], flexibility, great strength, and high value of the Young's modulus [12], varying from 1 to 1,8 TPa for single-walled carbon nanotubes (SWCNTs) [13] and from 0,9 to 1,3 TPa for multi-walled carbon nanotubes (MWCNTs) [14], significant adsorption properties [15], and the possibility of modification for specific applications [16], act as the basis for creating carbon dioxide capture and detection devices [17]. When modifying them, a fairly wide range of different substances is considered, including MOs [18]. The paper [19] de-scribes a technology for modifying CNTs with quinines in order to capture carbon dioxide. In [20], an experiment was described on the modification of CNTs with chitosan in order to capture and store carbon dioxide. In the course of the experiments, it turned out that modified carbon nanotubes in any case, even when high pressure was applied, proved to be an insufficiently effective carbon dioxide trap [21]; vertically aligned CNTs achieve carbon dioxide adsorption levels comparable to those of zeolite 13X at a pressure 18 bar [22]. In [23], CNTs are examined before and after carbon dioxide adsorption using electron microscopy methods, which demonstrate the absence of structural damage during adsorption.

Recently, carbon composite nanomaterials based on CNTs with metal oxides (MOs) have attracted research interest. This class of materials has found its application in the creation of nanosensors due to such advantages as a large specific surface area (281,8 m^2/g for MWCNTs-Co_3O_4, 330,3 m^2/g for MWCNTs-Fe_2O_3, 558,0 m^2/g for MWCNTs-CuO [24]) and unique conductive properties (electrical conductivity of the composite is determined by the structure of the carbon nanotubes network while MO specifies functional properties [25]). Therefore, it is recommended to use such sensors to capture trace amounts of toxic gases. These sensors are in high demand in industries such as monitoring electrochemical processes, detecting impurities in water and air, as well as environmental pollutants. Unlike conventional non-dispersive infrared (NDIR) sensors, chemiresistive sensors based on CNTs-MOs composites have distinct practical advantages. They offer room-temperature operation, ultra-low power consumption, and chip-scale miniaturization, making them suitable for nanoscale sensing platforms. However, the performance of these composites can vary

depending on the type of MOs used. For example, while sensors based on a composite consisting of MWCNTs and zinc oxide require higher operating temperatures and have reduced sensitivity compared to sensors based on pure zinc oxide [26], sensors based on MWCNT-iron oxide (III) (Fe_2O_3) material demonstrate improved response and a broader detection range at room temperature [27]. This highlights the importance of heterojunction design in optimizing sensor performance. CNTs modified with nickel oxide were used to detect 4-aminophenol [28, 29]. This nanocomposite was synthesized with the wetchemical process, and then it was assembled onto a glassy carbon electrode for further examinations as a chemical sensor. The selectivity of the obtained device to the 4-aminophenol was defined based on the comparative measurements conducted with other chemicals such as 2-nitrophenol, 3-methoxyphenol, 4-methoxyphenol, acetone, benzaldehyde, ethanol, hydrazine, ammonium hydroxide, n-hexane, pyridine, tetrahydrofuran, xanthine. It was found that such sensor has great selectivity to the 4-aminophenol, good sensitivity at a level of 0,633 nA/(μM·cm^2) and a low limit of detection (15,0±0,1 pM). Carbon structures modified with copper oxide were used as glucose sensors [30]. The pencil graphite electrode was modified with the improving additives such as polymer poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate), CuO nanoparticles and MWCNTs, and obtained structure was investigated as a chemical sensor for glucose detection. This device demonstrates excellent sensitivity of 663,2 nA/(μM·cm^2) and the addition of MWCNTs is crucial for this parameter. The limit of detection for glucose is 0,23 mM, which is one of the most accurate indicators available at the present moment. There are experimental works devoted to the methods of obtaining and properties of CNTs modified with iron oxide. The paper [31] describes the technology of obtaining such a material. CNTs obtained by chemical vapor deposition were treated with concentrated nitric and hydrofluoric acid in order to dissolve the catalyst particles. Composites based on CNTs and iron [32, 33] or cobalt [34, 35] oxides demonstrate great potential for sensors of various gases. In this paper, it is proposed to use CNTs modified with MOs as new materials for detecting and trapping carbon dioxide. To establish the possibility of interaction, computer experiments were conducted using density functional theory. The novelty of this study lies in the systematic comparative theoretical investigation of the adsorption of carbon dioxide on the surface of CNTs that have been modified with iron, cobalt, and copper oxide.

2. Methodology

Density functional theory is currently one of the most proven and reliable methods for conducting model experiments and quantum chemical calculations. It is based on the Kohn-Sham equation. Let's consider the main stages of its solution. The first step is to determine the type of functional for the average energy $E[n]$:

$$E[n] = \left\langle \Psi[n] \middle| (\hat{T} + \hat{U} + \hat{V}_{ext}) \middle| \Psi[n] \right\rangle = T + U + V_{ext} = T_S + V_H + \hat{V}_{ext} + (T - T_S + U - V_H), \quad (1)$$

where $\Psi[n]$ is the wave function, $\hat{T}$ is the electron kinetic energy operator, $\hat{U}$ is the operator of the Coulomb interaction between electrons, $\hat{V}_{ext}$ is the potential energy of an external field, T_s is the kinetic energy of a non-interacting system and V_H is Hartree potential. The last term in this expression is responsible for the contribution of the exchange-correlation energy V_{XC}:

$$V_{XC} = (T - T_s + U - V_H). \quad (2)$$

This expression includes four terms, the pairwise difference of which adds up to the specified energy value. The first difference is between the kinetic energies of interacting and free particles, and the second difference is between the energies of the Coulomb interaction and Hartree. For greater certainty, we will rewrite the Kohn-Sham functional $E_{KS}[n]$ with an indication of the functional dependence of the terms before proceeding to specific calculations:

$$E_{KS}[n] = T_S[n] + V_H[n] + V_{ext}[n] + V_{XC}[n]. \quad (3)$$

To carry out the variation, we will set the appropriate ratios:

$$\frac{\delta E_{KS}}{\delta \Psi_{i\sigma}(r)} = \frac{\delta T_S}{\delta \Psi_{i\sigma}(r)} + \left[\frac{\delta V_H}{\delta n(r)} + \frac{\delta V_{ext}}{\delta n(r)} + \frac{\delta V_{XC}}{\delta n(r)} \right] \frac{\delta n(r)}{\delta \Psi_{i\sigma}(r)} = 0, \quad (4)$$

$$\frac{\delta T_S}{\delta \Psi_{i\sigma}(r)} = -\frac{1}{2}\nabla^2 \Psi_{i\sigma}(r), \frac{\delta n(r)}{\delta \Psi_{i\sigma}(r)} = \Psi_{i\sigma}(r), \quad (5)$$

where E_{KS} is the exchange-correlation energy, $\Psi_{i\sigma}$ is the Kohn-Sham orbital. These quantities are a function of the coordinate. The index σ signifies the transition from a spin-independent (closed-shell) theory to a spin-dependent (spin-polarized) theory. This is known as the Local Spin Density Approximation (LSDA), or a generalization to the case of different spins. The introduction of the Lagrange multiplier (denoted below by $\varepsilon_{i\sigma}$) sets the normalization condition.

Taking into account all the operations performed above, we can write the Kohn-Sham equation:

$$-\frac{1}{2}\nabla^2 \Psi_{i\sigma}(r) + \nu_{KS}(r)\Psi_{i\sigma}(r) = \varepsilon_{i\sigma}\Psi_{i\sigma}(r). \quad (6)$$

This equation coincides in appearance with the single-particle Schrodinger equation, which describes the behavior of a particle in a self-consistent potential, given by the expression:

$$\nu_{KS}(r) = \nu_{ext}(r) + \nu_H(r) + \nu_{XC}(r), \quad (7)$$

$$\nu_H(r) = \int dr' \frac{n(r')}{|r - r'|}, \quad (8)$$

$$\nu_{XC}(r) = \frac{\delta V_{XC}}{\delta n(r)}, \quad (9)$$

$$n(r) = \sum_{i\sigma} \left|\Psi_{i\sigma}(r)\right|^2, \quad (10)$$

where ν is the effective single-particle potential.

The Kohn-Sham equation can be considered as a generalization of the Hartree theory. With a reliable definition of the expression for the exchange-correlation energy, it would be possible to accurately describe the multielectronic effects. Thus, the importance of the role of the exchange-correlation potential in this theory is emphasized.

In this study, the B3LYP hybrid functional was used to calculate the exchange-correlation energy. For the composite containing iron oxide (Fe_3O_4), a 6-31G basis set was selected for the theoretical model. For composites containing cobalt oxide (Co_3O_4) and copper oxide (CuO), a 3-21G basis set was implemented in the model experiment. Additionally the key word SCF = XQC was used for the case of the composite containing Co_3O_4. The investigation of the adsorption processes of the carbon dioxide on the CNTs-MOs composites was conducted in the framework of the quasi-molecular approach. The broken bonds at the edges of the nanotubes were bound with hydrogen pseudo-atoms. Mulliken scheme was used for the partial atomic charges calculations [36].

3. Results and their discussion

Investigation of the sensory properties of the surface-modified CNT(6,6)-Co_3O_4 composite towards CO_2

At the initial stage of the research, the sensory activity of complexes based on CNTs surface-modified with cobalt oxide (CNT-Co_3O_4) in relation to carbon dioxide was studied. The process was modeled by a step-by-step approximation of a CO_2 molecule to an oxygen atom of cobalt oxide, which modifies the surface of the CNT (6,6). The geometry of the CNT (6,6)-Co_3O_4 composite and interaction model of it with a gas molecule is shown in Fig. 1

The performed calculations allowed us to construct energy curves of the interaction of the systems (see Fig. 2). The analysis of the curves revealed the presence of minima. The presence of minima on the profile of the potential energy surface (PPES) of the interaction of CNT (6,6)-Co_3O_4 and CO_2 suggests the possibility of an adsorption process. It should be noted that two minima are observed at each PPES. Accordingly, there are several stable configurations of adsorption complexes. One is located at a distance of 2,8 Å, which corresponds to physical adsorption, and the low adsorption energy confirms this assumption. This is followed by a potential barrier of approximately 1 eV, overcoming which will lead to the formation of a stable chemical bond between the gas molecule and the composite nanomaterial. The obtained data allow us to evaluate the recovery capacity of the nanosensor: after physical adsorption, it will be low; after chemical

adsorption, there may be a need for additional cleaning of the nanosensor. We also give the parameters of the initial CNT (6,6)-Co_3O_4 composite, which is necessary to understand the material described below: the energy gap is 1,54 eV, the charge on the cobalt atom is 0,88 eV. The energy gap was calculated as the difference between the energies of the lowest unoccupied and the highest occupied molecular orbitals.

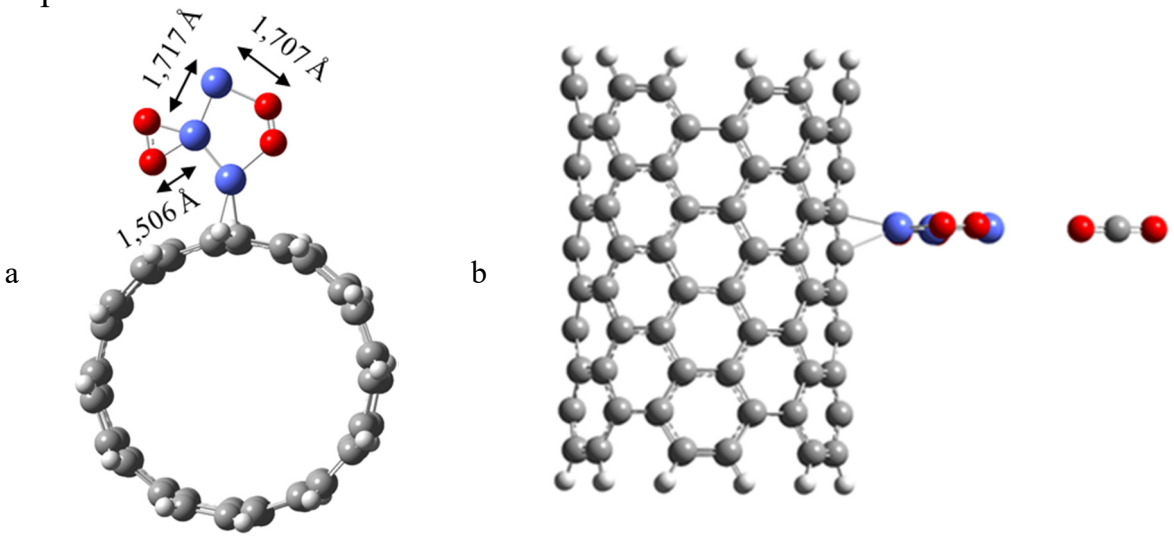


Fig. 1. The geometry of the CNT (6,6)-Co_3O_4 composite when Co_3O_4 is adsorbed at distance of 1,9 Å above the $C-C$ bond (a) and the model of the interaction of CNT (6,6)-Co_3O_4 composites and a CO_2 gas molecule (b).

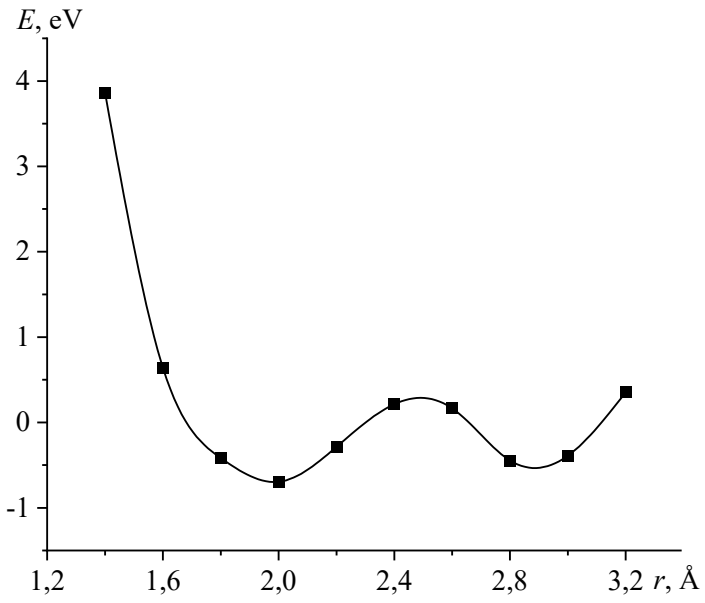


Fig. 2. PPES of the interaction of the CNT(6,6)-Co_3O_4 and CO_2 molecule.

For both configurations of the adsorption complex (with adsorption distances of 2,0 and 2,8 Å), a decrease in the energy gap is observed compared to the initial structure by 13% and 6% for the two configurations, respectively. The electron density shifts from the cobalt atom of the nanostructure to the oxygen

atom of CO_2; the charge on the cobalt atom of the composite is 0,88 before the adsorption and 0,90 (at adsorption distance 2,8 Å) or 0,98 (at adsorption distance 2,0 Å) after the adsorption.

Investigation of the sensory properties of the CNT-Fe_3O_4 composites towards CO_2.

To determine the sensory sensitivity of the constructed CNT-Fe_3O_4 complexes, a step-by-step approach of carbon dioxide molecules to an oxygen atom of iron oxide was simulated. Complexes of CNT (6,0) («zigzag») and CNT(6,6) («armchair») and iron oxide Fe_3O_4 were considered. The interaction between these complexes and carbon dioxide was carried out by step-by-step approximation of a CO_2 molecule to one of the oxygen atoms of these complexes (see Fig. 3). At each stage of the approximation, the energy of the system was recorded to build a profile of the surface of the potential energy of interaction. Based on the data obtained during the model experiment, the potential energy surface profiles were constructed for each case. It was subsequently used to determine the adsorption energy E_a and the distance r_a at which the bond is formed.

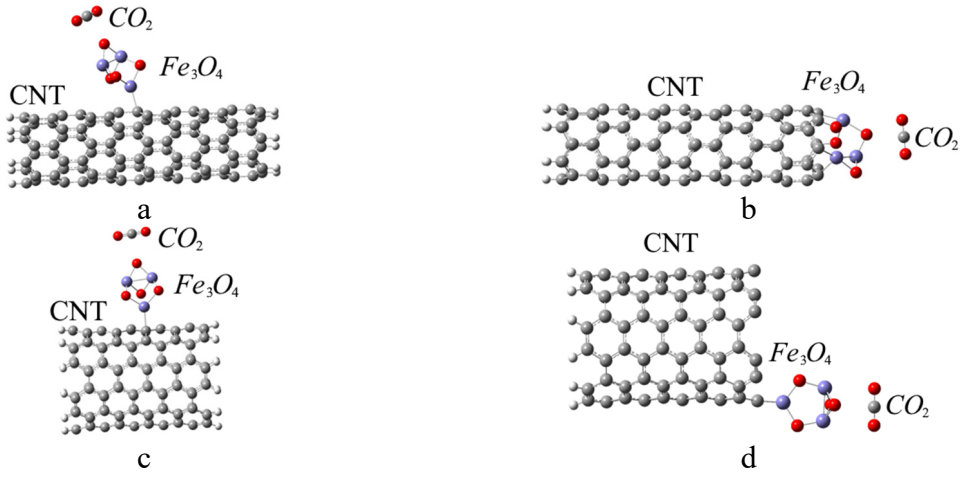


Fig. 3. Interaction models of surface-modified with Fe_3O_4 CNT(6,0): a – edge-modified woth Fe_3O_4 CNT(6,0); b – surface-modified with Fe_3O_4 CNT(6,6); c – edge-modified with Fe_3O_4 CNT(6,6); d – and CO_2 carbon dioxide.

The interaction of CNTs-Fe_3O_4 complexes with a carbon dioxide molecule is characterized by physical adsorption. The energy gap of the CNTs-Fe_3O_4 complexes changes when interacting with gas molecules. In the case of a «zigzag» CNT, there is a slight increase in the energy gap, and for armchair–type CNTs, the energy gap decreases. After the adsorption of CO_2 by the CNTs-Fe_3O_4 composite materials, the charge on the carbon atom of the CO_2 increases from 0,59 to 0,63-0,64 depending on the type of the CNT and the variant of modification.

Investigation of the sensory properties of the CNT(6,6)-CuO composite towards

CO_2.

To prove the possibility of using CNTs modified with copper oxide as a sensor probe material for determining the presence of CO_2 carbon dioxide, a simulation of the interaction of the CNT(6,6)-CuO system with a CO_2 molecule was performed (see Fig. 4).

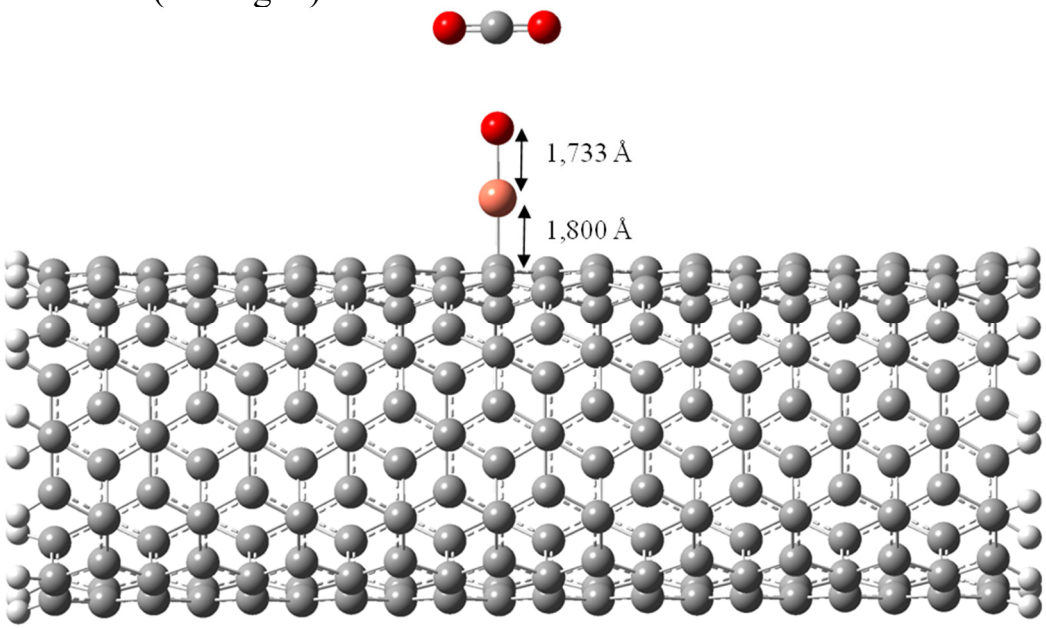
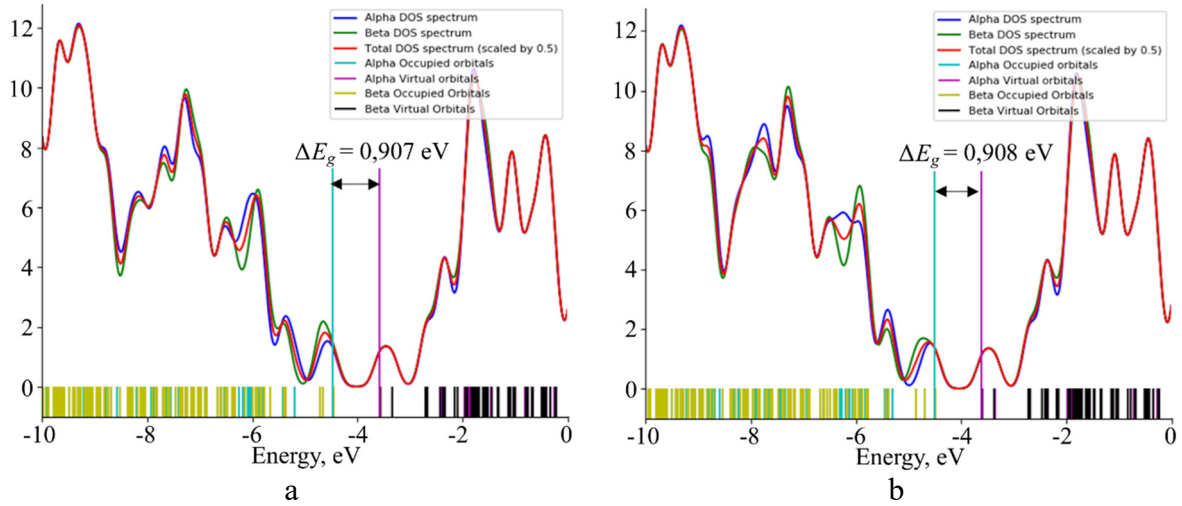


Fig. 4. Model of interaction of surface-modified with CuO CNT(6,6) and carbon dioxide CO_2.



a b

Fig. 5. Densities of states of sensor systems for various variants: a – CNT(6,6)-CuO before the adsorption of the CO_2; b – CNT(6,6)-CuO after the adsorption of the CO_2.

The process was modeled as follows. The gas molecule step-by-step approached to a copper atom of the composite system. The CNT(6,6)-CuO system was considered relatively rigid. The value of the interaction energy was of the order of 0,29 eV. During the interaction, physical adsorption is observed.

The densities of states are shown in Fig. 5. The adsorption of carbon dioxide leads to a increase in the energy gap for surface-modified with CuO CNT(6,6).

Analysis of the results of calculations of the electronic structure of the CNT(6,6)-CuO system with a carbon dioxide molecule showed that the energy gap increases with the interaction of the CNT-CuO system with CO_2 compared with the energy gap of the initial CNT(6,6)-CuO composite. It is 0,907 eV for CNT(6,6)-CuO and 0,908 eV for the composite under consideration after the adsorption of the carbon dioxide molecule.

So, as a result of the calculations carried out, the sensory sensitivity of the CNT(6,6)-CuO composite system in relation to carbon dioxide was investigated. Sorption processes cause a change in the electronic properties of interacting systems. Charge on tЦhe oxygen atom of the composite is -0,428 before the adsorption and -0,454 after the adsorption. The charge on the carbon atom of CO_2 molecule is 0,820 in the isolated state and 0,837 after the adsorption.

Table 1. Characteristics of CO_2 adsorption by CNTs-MOs composites; ra is the adsorption distance, E_a is the adsorption energy, ΔE_g before adsorption is the energy gap before adsorption of the gas molecule (initial composite), ΔE_g after adsorption is the energy gap after adsorption of the gas molecule (adsorption complex), Q(A)CNT-MO is the charge on the atom of the CNT-MO composites, to which the gas molecule was approached (A = Co in the case of the CNT-Co_3O_4 and A = O in other considered cases), Q(B) CO_2 is the charge on the atom of the carbon dioxide molecule, by which the gas molecule was approached (B = O in the case of the CNT-Co_3O_4 and B = C in other considered cases).

Structure	r_a, Å	E_a, eV	ΔE_g before adsorption, eV	ΔE_g after adsorption, eV	$Q(A)_{CNT-MO}$	$Q(B)_{CO_2}$
Surface-modified with Co_3O_4 CNT(6,6)	2,0	0,70	1,54	1,34	0,98	-0,47
	2,8	0,45		1,45	0,90	-0,40
Surface-modified with Fe_3O_4 CNT(6,0)	2,6	0,22	0,665	0,668	-0,693	0,639
Edge-modified with Fe_3O_4 CNT(6,0)	2,8	0,17	0,664	0,667	-0,707	0,630
Surface-modified with Fe_3O_4 CNT(6,6)	2,6	0,23	1,644	1,622	-0,697	0,639
Edge-modified with Fe_3O_4 CNT(6,6)	2,7	0,22	1,506	1,482	-0,626	0,639
Surface-modified with CuO CNT(6,6)	2,5	0,29	0,907	0,908	-0,454	0,837

Table 1 provides a summary of all the cases considered in the work. The largest value of the adsorption energy is observed in the case of the CNT(6,6)-Co_3O_4 composite. Compared to other variants this value is 2-3 times higher depending on the adsorption distance. It can reduce the reproducibility of measurements because of poisoning of the sensor surface. On the other hand relative change in the energy gap is the highest in this case so the CNT(6,6)- Co_3O_4

composite is the most sensitive material for CO_2 sensing of all con-sidered. The adsorption energy in the case of the CNT(6,6)-CuO composite is more than in case of the CNT(6,6)-Co_3O_4, but less than in cases of CNT-Fe_3O_4 composites. Additionally, the relative change in the energy gap in this case is minimal compared to all the other cases considered. The most suitable materials for CO_2 sensing are CNT-Fe_3O_4, characterized by a sufficiently weak interaction with CO_2 in terms of adsorption energy and at the same time a sufficiently high relative change in the energy gap after the adsorption (but smaller than in the case of the CNT(6,6)-Co_3O_4 composite) and, accordingly, a strong response of nanosystems to the adsorption process.

5. Conclusions

Thanks to the analysis of the results of the model experiment, it became possible to estimate the dependence of the sorption characteristics of carbon nanotubes in relation to the carbon dioxide molecule on modifying MOs. Three types of MOs were considered, namely, oxides of iron, cobalt and copper. The performed quantum chemical calculations allowed us to establish that the adsorption of carbon dioxide molecules is possible for all carbon nanotubes modified with MOs. When interacting with cobalt oxide, a potential barrier appears in the path of the carbon dioxide molecule, which reduces the likelihood of the formation of a stable complex. Iron and copper oxides, which modify the CNTs sur-face, activate the process of carbon dioxide adsorption by the nanosystem.

The largest adsorption energy values are observed in the case of the adsorption of CO_2 by CNT (6,6)-Co_3O_4 composite. The smallest adsorption distance also corresponds to this case, but as it was mentioned above, the most stable position (which characterized by the largest adsorption energy) could reached only after the overcoming of the potential barrier. If there are considered cases where there is no potential barrier, the case of the adsorption of CO_2 by CNT-CuO is characterized by the smallest adsorption distance, which may be due to the difference in the dimensional characteristics of the oxides themselves.

In all the cases considered, a change in the energy gap of the studied nanostructure was observed. In the cases of the CNT (6,6)-Co_3O_4 and CNT(6,6)-Fe_3O_4 composites the energy gap increased after the adsorption of CO_2. In the case of the CNT-CuO and CNT (6,0)-Fe_3O_4 composites the energy gap decreased after the adsorption of the CO_2. But for the functioning of the sensors, it is the moment of interaction that is important, at which the volt-ampere characteristics change, on which the action of the sensors is based.

Thus, the use of CNTs modified with MOs is promising for the creation of

nanosensors. Such devices operate on the basis of recording changes in the conductive characteristics of the system when changes in the conduction states of the system occur caused by a change in the energy gap [37]. Of all the options considered, CNTs, modified with Fe_3O_4, have the most optimal characteristics in the context of the reproducibility of the measurements and sensitivity of CO_2 sensing applications. The CNT(6,6)-Co_3O_4 composite is characterized by the strongest response and, consequently, the highest sensitivity, but the gas sensor based on this material is exposed to the influence of the poisoning caused by strong interaction between the composite and CO_2. The weak relative change in the energy gap in the case of the CNT-CuO composite reduces the potential of its applications for CO_2 sensing devices. So, the carbon nanotubes modified with MOs studied can be recommended as materials for nanosensors capable of detecting even a minimal amount of carbon dioxide. The functioning of the sensors is based on the sorption interaction of CNTs decorated with MOs with CO_2 molecules and subsequent detection, possible due to a change in the energy gap of the nanostructure under study and the conductive state of the nanosystems. Potential future research directions in this field include the consideration of larger clusters of MOs with different geometries and the assessment of the selectivity of the materials presented towards CO_2.

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