Original paper

Carbon nanotubes with impurity nitrogen atoms as promising filters for harmful gases

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Abstract: Carbon nanotubes modified with nitrogen atoms are one of the promising materials for the development of electronic devices in the modern world. They are characterized by the presence of structural distortions and increased nucleophilicity, which significantly distinguishes them from primitive graphene structures. These facilities exhibit abnormally high stability in aggressive environments and low overvoltage. Their uniqueness lies in the synergy of the mechanical strength of the carbon backbone and the chemical activity of nitrogen-containing centers, which makes it possible to solve the problems of creating effective sorbents and heterogeneous catalysts. To study the interaction of nanotubes with harmful gases and obtain the energy characteristics of adsorption, some semi-empirical calculations using the Gaussian software package were used in the framework of the density functional theory using the B3LYP method with a 6-31G baseline set. The nanotube model was built using GaussView 6.0. Every second carbon atom of the nanotube was replaced by a nitrogen atom. To obtain the adsorption energy, the gas molecule approached the surface of the nanotube perpendicular to the axis of the nanotube with 0,2 nm increments. The energy was calculated at each step, which made it possible to build profiles of the potential energy of interaction of chlorine, fluorine and carbon dioxide. During the theoretical experiment, interaction energies were obtained for each step of the approach of *Cl*, *F*, and CO_2. Based on the results, the potential energy interaction curves were constructed, which made it possible to determine the most effective distance for the sorption of harmful gases onto the surface of a carbon nanotube modified with nitrogen atoms. Sorption occurs at various distances. For chlorine, it is 1,4-1,8 Å, and for fluorine and carbon dioxide, it is 2-3 angstroms. The interaction graphs clearly demonstrate the possibility of sorption of hazardous gases by the nanocomposite. Fluorine forms a stable chemical bond with the carbon atom of the nanotube, while chlorine is physically sorbed onto the nitrogen atom, which indicates the high potential of the material under study for reusable filters. The experiments conducted demonstrate the possibility of using carbon nanotubes with substituting nitrogen atoms as filters. The assessment of the energy properties shows a high potential for application in microelectronic technology.

Keywords: carbon-nitrogen nanotubes, filters, density functional theory, gas adsorption, harmful gases.

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Оригинальная статья

Углеродные нанотрубки с примесными атомами азота, как перспективные фильтры вредных газов

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Аннотация: Углеродные нанотрубки, модифицированные атомами азота, являются одним из перспективных материалов для разработки электронных устройств в современном мире. Они характеризуются наличием структурных искажений и повышенной нуклеофильностью, что существенно отличает их от примитивных графеновых структур. Эти материалы обладают

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аномально высокой устойчивостью в агрессивных средах и низким перенапряжением. Их уникальность заключается в синергии механической прочности углеродной основы и химической активности азотсодержащих центров, что позволяет решать задачи по созданию эффективных сорбентов и гетерогенных катализаторов. Для изучения взаимодействия нанотрубок с вредными газами и получения энергетических характеристик адсорбции были использованы полуэмпирические расчеты с помощью программного пакета Gaussian в рамках теории функционала плотности с применением метода B3LYP с базовым набором 6-31G. Модель нанотрубки была построена с помощью GaussView 6.0. Каждый второй атом углерода в нанотрубке заменен на атом азота. Для расчета энергии адсорбции молекула газа приближалась к поверхности нанотрубки перпендикулярно ее оси с шагом 0,2 нм. На каждом шаге рассчитывалась энергия, что позволило построить профили потенциальной энергии взаимодействия хлора, фтора и углекислого газа. В ходе теоретического эксперимента были получены значения энергии взаимодействия для каждого этапа сближения *Cl*, *F* и CO_2. На основе полученных результатов были построены кривые потенциальной энергии взаимодействия, которые позволили определить наиболее эффективное расстояние для сорбции вредных газов на поверхности углеродной нанотрубки, модифицированной атомами азота. Сорбция происходит на различных расстояниях. Для хлора оно составляет 1,4–1,8 ангстрем, а для фтора и углекислого газа – 2-3 Å. Графики взаимодействия наглядно демонстрируют возможность сорбции опасных газов нанокомпозитом. Фтор образует устойчивую химическую связь с атомом углерода нанотрубки, а хлор физически сорбируется на атом азота, что говорит о высоком потенциале исследуемого материала для фильтров с многоразовым применением. Проведенные эксперименты показывают, что углеродные нанотрубки с замещающими атомами азота можно использовать в качестве фильтров. Оценка энергетических свойств демонстрирует высокий потенциал их применения в микроэлектронике.
Ключевые слова: углерод-азотные нанотрубки, фильтры, теория функционала плотности, адсорбция газов, вредные газы.

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1. Introduction

Air pollution remains one of the major problems in the world due to its impact on climate change and human health, which has led to an increase in morbidity and mortality. Human activity (anthropogenic), such as industrial processes, power plants, internal combustion engines, vehicles, ships, oil refineries, the use of fertilizers, and metallurgical processes, combined with natural phenomena such as volcanic activity, the breakdown of rocks and minerals, forest fires, soil erosion, and dust storms, are among the many factors that have significantly contributed to the increase in air pollution. Air pollution resulting from anthropogenic activities remains the main cause of public health problems worldwide. It leads to 9 million deaths per year, and 91% of the world's population lives in areas where air quality exceeds the levels

recommended by the World Health Organization [1].

Air pollution caused by chlorine, fluorine, and their compounds is among the most dangerous. Prolonged or widespread exposure to such harmful gases affects almost all systems in the body [2], causes serious physiological changes, weakens the immune system, and leads to cardiovascular diseases [3]. Greenhouse gases, including CO_2, have a widespread impact on humans, which largely depends on the duration of exposure[4]. The effects on the body range from mild ones, such as coughing and difficulty breathing, to severe ones, such as pulmonary failure and chronic asthma [1].

Over the past decade of nanotube research, numerous organized nanotube structures have been produced. The idea of using nanotube structures in separation technology was proposed in works [5-7], but the creation of macroscopic structures with controlled geometric shapes, density, and dimensions for specific applications remains a challenging task. These cylindrical structures are used as filters. The exceptional thermal and mechanical stability of nanotubes, as well as their large surface area, simplicity, and cost-effectiveness in manufacturing [8-10], may enable them to compete with separation membranes based on ceramics and polymers used in industry.

Due to the fact that pure carbon nanotubes have a strong aromatic character, they aggregate strongly and form dense conglomerates due to van der Waals interactions, which makes them completely insoluble in most solvents in their unmodified state. Functionalization of carbon nanotubes will make it possible to create new hybrid composites capable of changing the properties of many materials [11]. Based on the published literature, it is worth paying attention to several types of doping additives used as elements for heteroatomic doping. Such additives may include atoms of boron, lithium, sulfur, fluorine, nitrogen, etc. However, boron and nitrogen appear to be the most suitable candidates for doping, which is confirmed by numerous studies of such parameters as the redox behavior of heteroatoms and the possibility of incorporating a heteroatom into the carbon nanotube network [12, 13].

Carbon nitride has a unique electronic band structure and high chemical and thermal stability. Due to these properties, it is widely used in photoelectrochemistry, photocatalysis for the production of hydrogen from water, catalysis of important reactions, and electrochemical sensors [14]. Among the large number of carbon nitride nanostructures, CN nanotubes are currently attracting increasing interest due to their attractive properties and geometric advantages. Nanotubes have a unique one-dimensional hollow structure and provide a large surface area, a high aspect ratio, electron mobility in the axial direction, and the quantum confinement effect. In this regard, carbon nanotubes modified with nitrogen atoms are widely used in many fields related to energy and the environment [15]. However, there is still a need for further research to

reduce the size of modern devices for capturing harmful gases, and new materials play a significant role in this task [16]. Based on this, research is needed that can shed light on the potential of this fascinating nanomaterial.

2. Methodology

Currently, the density functional theory (DFT – Density Functional Theory) method is one of the most popular and well-tested approaches for conducting quantum-chemical calculations and model experiments. This method is also characterized by its convenience for calculating systems based on carbon nanotubes [17].

To achieve high calculation accuracy, it is most effective to use a calculation method that has semi-empirical features. B3LYP is currently the most popular density functional in chemistry. Despite the progress in this field and the emergence of several new functionals every year, B3LYP continues to dominate this field, accounting for 80% of the total number of density functionals described in the literature [18]. The basis of the calculations is the Kohn–Sham functional. Several stages can be identified in solving this equation. The first is determining the form of the 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 the equation takes into account the contribution of exchange-correlation energy V_{XC}:

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

This term includes 4 addends, and by subtracting them pairwise, the specified energy value is obtained. The first difference is between the kinetic energies of the particle interactions, and the second is between the Coulomb interaction energies and Hartree. For greater clarity, we can rewrite the Cohn-Shem theorem, indicating the functional $E_{KS}[n]$ 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 corresponding 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:

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

The resulting equation is similar in form to the single-particle Schrödinger equation, which describes the behavior of a particle in a self-consistent potential defined by the expression:

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

where

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

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

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

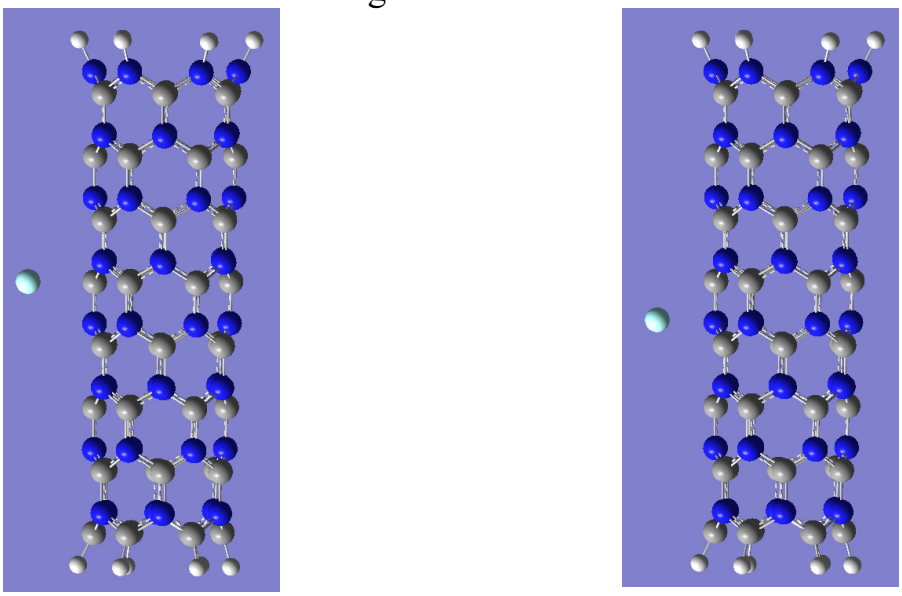
ν is the effective single-particle potential.

The Kohn-Sham functional is a generalized case of Hartree theory. The complexity of determining the expressions for exchange-correlation energy hinders an accurate description of many-electron effects. That is, it plays the main role in the theory under consideration.

3. Results and their discussion

To determine the effectiveness of using CN-type nanotubes as filters for harmful gases such as Cl, F, and CO_2, an analysis was carried out of the interaction between carbon nanotubes and boron impurity atoms of the (6,0) type, as well as the atoms of the aforementioned gases. To establish the localization of adsorption centers for F, CO_2, and Cl on the surface of the carbon nanotube, several models were created for each of the gases under study. The models used to describe the interaction between the nanotube and the gas represented various adsorption centers for chlorine, carbon dioxide, and fluorine, including a nitrogen atom, a carbon atom, a hexagonal center, and a bond center between carbon and nitrogen (see Fig. 1). In the constructed models, the studied nanotubes had a length of 1,54 nm. The ends of the tubes were capped with hydrogen atoms to eliminate edge effects at the boundaries of the nanocomposite. During the experiment, harmful gases approached the nanotube perpendicularly to the axis of the nanocomposite, with a step size of 0,02 nm to each of the adsorption centers. The possible arrangements of adsorption centers

for a fluorine atom are shown in Fig. 1.



a b

Fig. 1. The interaction model CNT type (6,0) with atom F : a – the adsorption center on the carbon atom; b – the adsorption center on the nitrogen atom.

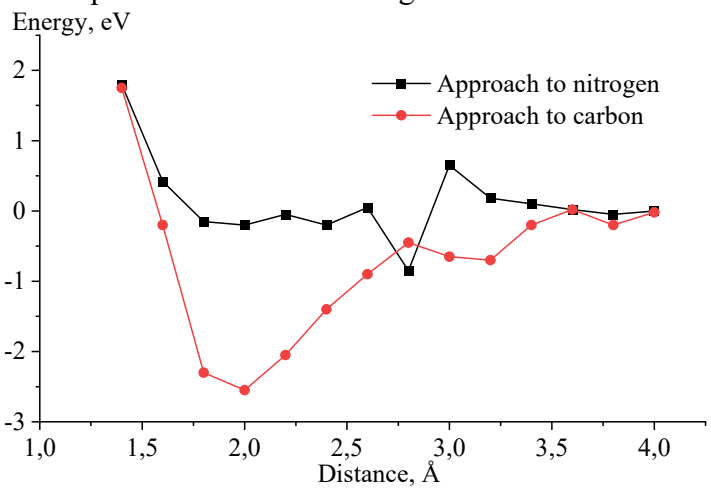


Fig. 2. Energy curves of interaction of fluorine and carbon nanotube with various adsorption centers.

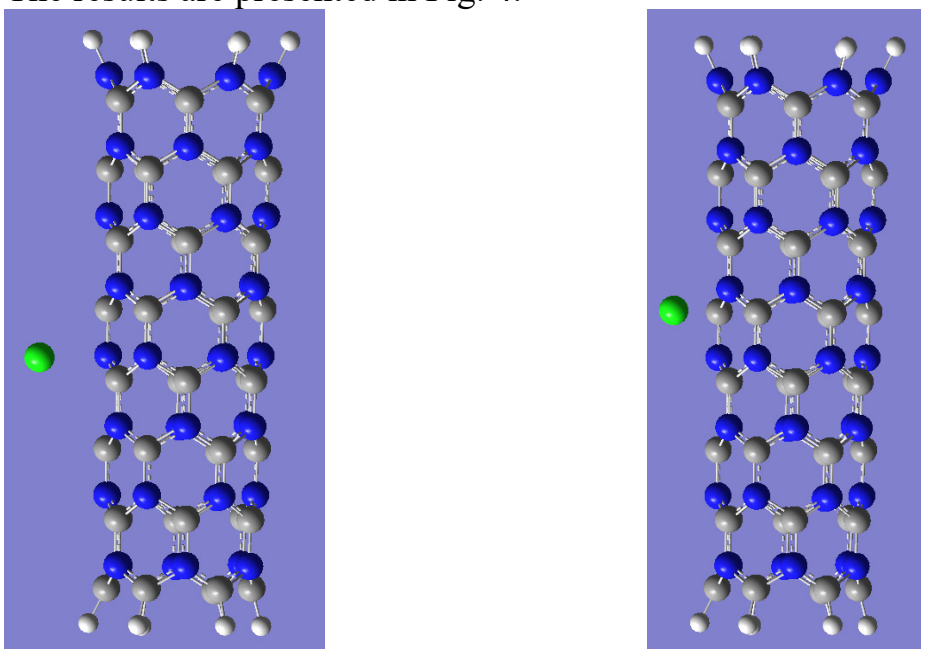
To determine the distance and adsorption energy, the potential energy of interaction between a CN-type (6,0) nanotube and a fluorine atom was calculated at each of the performed steps. The interaction energy was calculated using the formula:

$$E_{ad} = E_{tube+F} - (E_{tube} + E_F), \quad (11)$$

where E_{ad} is the adsorption energy, E_{tube+F} is the total energy of the nanocomposite and the gas, E_{tube} is the energy of the nanocomposite, and E_F is the energy of the gas.

The results made it possible to construct graphs showing the potential energy profiles of the interaction between fluorine and the nanocomposite (see Fig. 2), from which the most likely sorption distances with the corresponding

energy were determined. The possible arrangements of adsorption centers for a chlorine atom are shown in Fig. 3. To determine the distance and adsorption energy, the potential energy was calculated in a manner similar to the case of fluorine. The results are presented in Fig. 4.



a b

Fig. 3. The interaction model CNT type (6,0) with Cl atom: a – the adsorption center on the carbon atom, b – the adsorption center on the nitrogen atom.

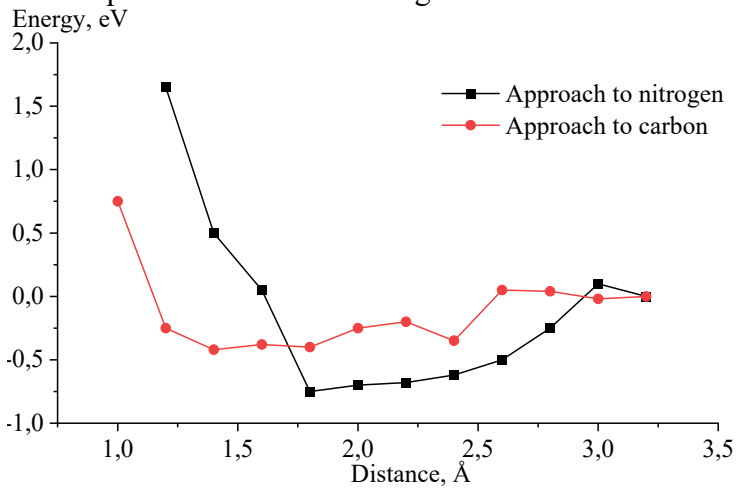
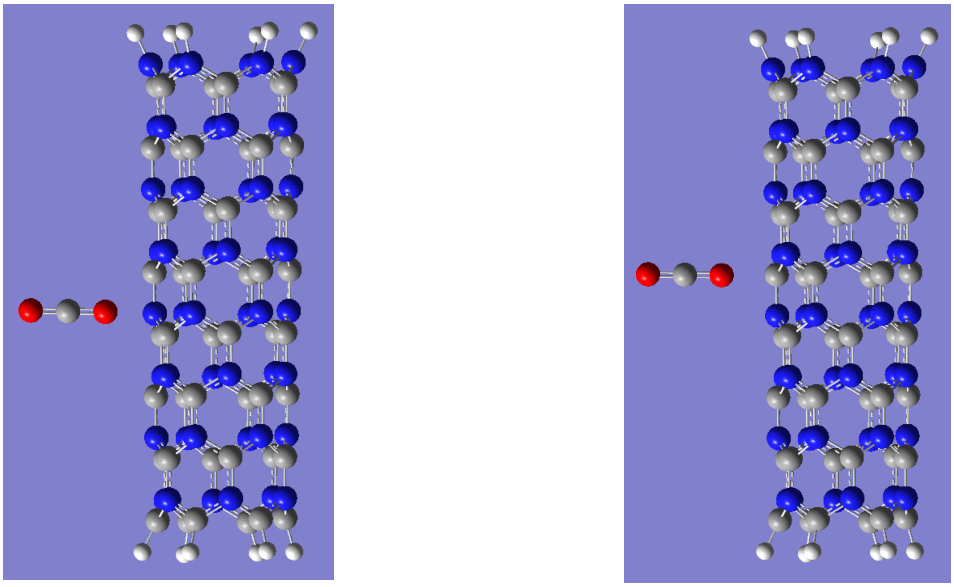


Fig. 4. Energy curves of interaction of chlorine and carbon nanotube with various adsorption centers.

Similarly to the study of the interaction between a CN nanotube of type (6,0) and F / Cl, theoretical studies were conducted for CO_2. The adsorption sites were also selected on the carbon atom and the nitrogen atom of the nanotube (see Fig. 5). The graphs showing the potential energy profiles of the interaction between nanotube and carbon dioxide are presented in Fig. 6.

All the obtained results regarding adsorption energy and distances to adsorption centers are presented in Table 1.



a b

Fig. 5. The interaction model CNT type (6,0) with CO_2: a – the adsorption center on the carbon atom; b – the adsorption center on the nitrogen atom.

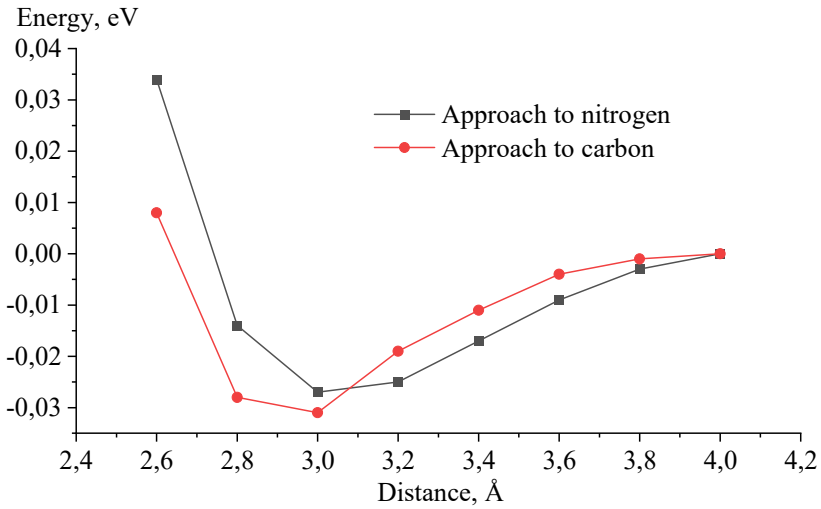


Fig. 6. Energy curves of interaction of carbon dioxide and carbon nanotube with various adsorption centers.

In the case of a fluorine atom, a more interesting scenario is the approach to a carbon atom on the nanotube surface. Fluorine is the most electronegative element, and it forms a chemical bond with it that is more stable than the $C-F$ bond. In the case of a chlorine atom, nitrogen turns out to be more preferable as an adsorption center. This indicates the selectivity of functionalization depending on the adsorbed atom. And in the third scenario, the interaction energies are virtually identical, which indicates the absence of selectivity and that the adsorption centers are equivalent to each other. Furthermore, the interaction energy values indicate weak physical adsorption, and the carbon dioxide molecule will be weakly adsorbed by the composite under study.

Table 1. Summary table of electronic energy characteristics of the studied systems. r_a is the adsorption distance, E_a is the adsorption energy.

Structure	r_a, Å	E_a, eV
F to atom C in CNT(6,0)	2	-2,5
F to atom N in CNT(6,0)	2,8	-0,86
Cl to atom C in CNT(6,0)	1,4	-0,4
Cl to atom N in CNT(6,0)	1,8	-0,76
CO_2 to atom C in CNT(6,0)	3	-0,028
CO_2 to atom N in CNT(6,0)	3	-0,03

5. Conclusions

Computer modeling of the interaction of harmful gases – fluorine, chlorine, and carbon dioxide – using the density functional theory is an integral stage in the development of nanoscale electronics. Such studies make it possible to assess the potential of a nanocomposite as a filtering material for harmful gases.

Thus, the studies conducted have shown that CN-type nanotubes are extremely interesting as a filter for harmful gases. The results made it possible to evaluate the possibility and quality of sorption of F, Cl, and CO_2 by carbon-nitrogen nanotubes. It is a new attractive material for creating gas filters for fluorine and chlorine, with which stable bonds are formed. Fluorine forms a covalent chemical bond with the carbon atom on the nanotube surface. Fluorination is selective for carbon. Chlorine, in turn, is bound by physical sorption to the nitrogen atom, which makes it possible not only to filter this gas but also to easily remove it by heating for the purification of the composite. When considering carbon dioxide, one can judge the weak sorption with the composite in the form of a CN nanotube. Sorption will be possible only under high pressure or low temperature. In this case, it is worth considering modifying the nanotube by doping it with metals or introducing defects.

The experiments conducted show that carbon nanotubes with substituting nitrogen atoms can be used as filters. The assessment of their energy properties demonstrates a high potential for their application in microelectronics.

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