Study of the Sensory Interaction of a Modified Boron-Nitride BN type Nanotube with a Carbon Dioxide Molecule

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Abstract

Recently, the environmental situation in the world has been deteriorating everywhere and there is a need to find new effective means of detecting harmful substances in the air. Every year, the content of carbon dioxide in the air is growing, which in the end can lead to a deterioration in the health of people. Various types of sensor devices are currently used to timely fix the increase in the gas level. As the active material of such a sensor, modern unique materials can be used - nanotubes, which, due to their sorption properties, are able to detect the presence of harmful impurities in the air space of the premises.

It is also possible to use such sensors as detectors of some human diseases by analyzing exhaled air, which makes their use in medicine possible. The results of a theoretical study of the sorption interaction of modified boron-nitride nanotubes with molecules of carbon dioxide and acetone, obtained using the quantum-chemical DFT method, are presented, which prove the possibility of using this type of nanotubes as a sensor material for sensor devices.

Methodology

One of the most proven and reliable methods for conducting model experiments and quantum chemical calculations is currently the density functional theory (DFT, or DFT - Density Functional Theory). It is based on the Kohn-Sham equation.

$$E_{KS}[n] = T_S[n] + V_H[n] + V_{\text{ext}}[n] + V_{XC}[n].$$

Introduction of the Lagrange multiplier ($\varepsilon_{i\sigma}$) sets the normalization condition

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

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Study of the sorption and sensory interaction of the BNNT–NO2 system with a carbon dioxide molecule

The simulation of the process of modifying one of the boundaries of a single-layer BNNT of the zig-zag (6,0) type with a nitro group was performed. The functional group step by step (with a step of 0.01 nm) approached the boron atom of the open boundary of the nanotube cluster containing 96 boron and nitrogen atoms taken in equal amounts, being oriented by the nitrogen atom N. The geometry of the system was optimized at each step. It was found that the nitro group was attached to the nanotube boundary at an angle of 173.4°. The length of the B–N bond between the group and BNNT was 0.14 nm. An analysis of the charge distribution in the system found that the electron density was concentrated on the nitrogen atom of the nitro group. The charge on the N atom turned out to be –0.03, and on the nanotube boron atom +0.026.

Next, we studied the sorption interaction between the resulting BNNT-nitro group nanosystem and a CO2 carbon dioxide molecule (Fig. 1a). The molecule approached the oxygen atom of the group step by step, orienting its O atom towards it.

Next, the simulation of the process of scanning a virtual surface containing a CO2 carbon dioxide molecule was performed to determine the sensitivity of the modified boron-nitride nanosystem to the presence of these molecules. The simulation of the scanning process consisted in the step-by-step movement of a carbon dioxide molecule along a straight line drawn parallel to the nanotube boundary and successively passing by the oxygen atoms of the nitro group attached to the BNNT boundary (Fig. 1b).

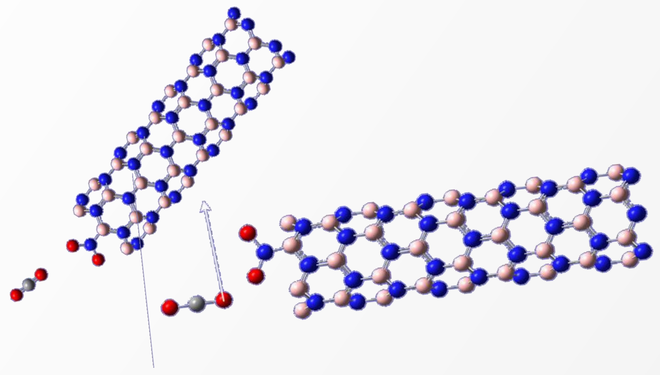

Fig. 1. Model of the process of interaction (a) and scanning (b) a virtual surface containing a carbon dioxide molecule using the BNNT–NO_2 system. The arrow shows the direction of motion of the molecule

As a result of the calculations, the dependence of the interaction energy on the distance between the CO2 molecule and the modified BNNT–NO2 nanotube system was plotted (Fig. 2). Analysis of the curve established the fact of the implementation of the sorption interaction between the boron-nitride nanosystem and the carbon dioxide molecule, the first energy minimum being at a distance of 0.3 nm, the corresponding energy of the sorption interaction is –0.75 eV.

With further approach, the molecule can overcome a small potential barrier with a height of 0.004 eV and find itself in the second minimum at a distance of 0.23 nm. The interaction energy for this minimum was –0.08 eV. Judging by the values of the distances, a weak van der Waals interaction is realized.

The research results are shown in fig. 3. The energy minima shown in the graph correspond to the presence of the CO2 molecule under the oxygen atoms of the nitro group.

Fig. 2. Dependence of the sorption interaction energy of the modified BNNT–NO2 boronitride system with a carbon dioxide molecule on the distance between the CO2 molecule and the oxygen atom of the functional group

Fig. 3. Dependence of the sensor interaction energy on the position of the CO_2 molecule relative to the BNNT–NO_2 nanosystem

Conclusions

On the basis of the conducted model studies, the presence of sorption and sensory interaction between the boundary-modified BNNT nitro group with a carbon dioxide molecule was proved. Since the nature of the interaction is weak Van der Waals, i.e., it is of a physical nature, these active elements of the sensors can be used repeatedly without destruction and chemical contamination.

Thus, on the basis of the conducted studies, it is possible to develop recommendations on the technology for creating new high-performance devices, including sensors, biomedical, nano- and microelectronic devices, filters, etc., based on tubular boron-nitride nanomaterials. The principle of operation of such sensors will be based on a change in the current-voltage characteristics of a nanotube as a result of interaction with molecules of a certain type at its modified boundary.