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Investigation of the Gas Atoms Interaction with BC Nanotube

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In this article we represent the theoretical research of the sorption properties for two types of boron-carbon nanotubes (BCNTs) using the scheme of an ionic-built covalent-cyclic cluster model and MNDO quantum chemical method. We investigated the process of Cl, O, F sorption on the surface of single-walled BC nanotubes arm-chair type. The optimal geometry of the sorption complexes and the sorption energy values have been obtained.

Keywords: Boron-carbon nanotubes, Ionic-built covalent-cyclic cluster model, Quantum chemical calculations, Adsorption, Semiconducting superlattice.

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1. INTRODUCTION

The carbon NTs have been discovered in the early nineties and was followed by intensive investigation into their structure and electronic-energy spectrum parameters, physical and chemical properties. Also researchers started researches in the way to improve NTs and get structures having new physical, chemical and other properties. Because of high surface nanotubes activity they can be used as basis for making various types of composites. In particular, it was found that pure carbon nanotubes may be used as Cl, F, O storage because of their good adsorption properties [1-3].

The properties of pure carbon nanotubes are well known, so the researches started to investigate another types of the nanotubular structures. One of the most useful type of the nanotubes is nanotube on the boron carbide basis. Earlier researches have shown that physical-chemical properties of BCNT are better that carbon nanotube's one [4-8].

The nanotube's adsorption processes attract interest in our research group as well as other researches in the world [9-13]. The calculations of the adsorption processes for the oxygen atom and O2 molecule on the BC_3 nanotubes zig-zag type surface have been carried out earlier [14].

2. THE NANOTUBE MODEL

2.1 Boron Carbon Nanotube Clusters

As geometrical models of the studied tubulenes we used clusters with six hexagon boron-carbon cycles located on the tube perimeter and four elementary layers along the tube axis. For the aim of correct model of the nanotube as an infinite structure hydrogen pseudo atoms were used to complete chemical bonds on the nanotube edge. A model of a covalent cyclic cluster built in via ionic bonding in the framework of the semi-empirical quantum chemical MNDO calculation procedure was applied [1]. The possible positions of carbon and boron atoms in respect to an adsorbed atom on the tube external surface in BC-tubulenes clusters are shown in Figure 1.

This article represents investigation of gas phase atoms (GA) (O, Cl, F) interaction with the BC nanotubes (6,6) type [2-10]. The adatoms have been neared to the external surface of the nanotube to explore a possibility of creating nanotube based gas-phase composites.

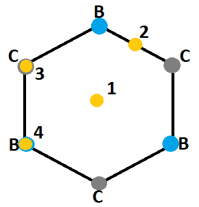

Fig. 1 – BC nanotube (6,6) with an absorbed atom on the nanotube surface: 1. Above the hexagon center, 2. Above the B-C bond, 3. Above carbon atom. 4. Above boron atom

2.2 Calculation Model

In order to eliminate the influence of boundary effects, we modelled the process so that adsorbed at-oms (Cl, F, O) bound either to a carbon or boron atom located approximately in the middle of the boron-carbon nanotube cluster. The adsorption process for gas phase atoms was modeled in increments of 0,1 Å in the direction of the perpendicular to the tube axis passing through the point on which the adsorption takes place.

The geometrical parameters of the system were opti-mized in quantum-chemical calculations. Adsorption energy values were calculated as the difference between the total energy value of non-interacting adsorbent model of a corresponding atom and a related adsorption complex, Formula (1).

$$E_{ад} = E_{ад.к.} - (E_{tub} + E_{GA}) \quad (1)$$

3. RESULTS AND DISCUSSION

The calculations allowed to build profiles of the potential energy surface of the adsorption process of the oxygen atom to the surface of boron-carbon nanotubes. The analysis of the energy curves found that the atom adsorbed on the surface of the boron-carbon tubulene. It should be noticed that the most active adsorption

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takes place, when the oxygen atom is positioned above boron and carbon atoms of the tube. The energy curves for these positions are similar. They have a minimum on the curves (Fig. 2). The distance and energy of the adsorption suggested us, that the type of the adsorption is chemical one.

For the position 1 (connection with the center of the hexagon) the energy minimum is observed at a distance of 1.6 Å. The type of the adsorption is physical. In position 2, namely above the center of the B-C bond, the adsorption of oxygen atoms is also possible. Optimal distance adsorption (Ra) and the corresponding values of the activation energy (Ea), and the energy barrier presented in the table (1).

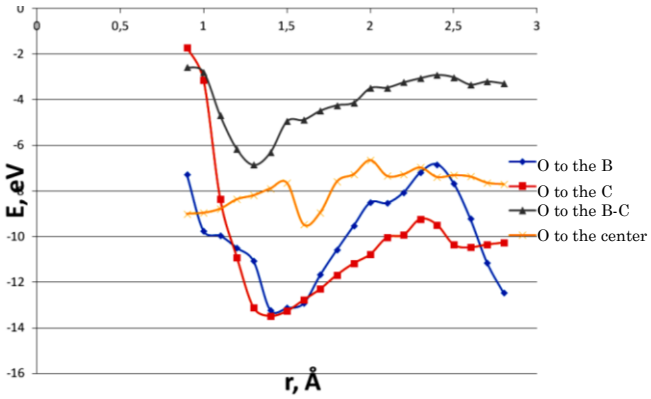

Fig. 2 – Profiles of the potential energy surface of interaction with the surface atoms of the boron-carbon nanotube (6, 6) for four variants of its location relative to boron-carbon tubulene

Table 1 – Basic characteristics of the electron energy of adsorption of oxygen atoms at the surface of the boron-carbon nanotubes: 1) above the center of the hexagon, 2) above the center of the B-C, 3) over a C-atom, 4) on the boron atom; *E*ad – adsorption energy, eV; *R*ad – distance adsorption, Å; *E*a – activation energy

Variants of adsorption	E_a, eV	R_{ad}, Å	E_{ad}, Å
O to the B	5,633	1,4	– 13,213
O to the C	1,039	1,4	– 13,479
O to the B-C	4,242	1,3	– 6,85
O to the center of the hexagon	1,058	1,6	– 9,475

The analysis of the geometry optimization for the case of the oxygen atoms attached to positions 3 and 4. found that during the approximation of oxygen on 2.4 Å atoms to the B and C atom of the tube begins to deflect towards the center of the hexagon and at a distance of 1.4 Å O the surface of the tube forms a bond with two boron atoms, the length of connection RO-B = 1,48 Å (Fig. 3).

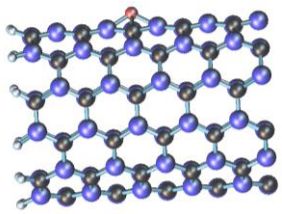

Fig. 3 – The process of interaction of the oxygen atom with a tube BC

By analogy with the oxygen atom, we investigated the possibility of chlorine atoms adsorption to the external surface of a single-layer boron-carbon nanotube (6,6). The calculations were performed using the model of a molecular cluster, using the semi-empirical scheme MNDO. All parameters of the chlorine adsorption have been chosen and the process modeled in the same manner as in the case of an oxygen atom.

As it could be seen in the energy curves of the interaction of chlorine atoms with the surface of BCNT (Fig. 4), for the chlorine atom is realized only physical adsorption (Table 2).

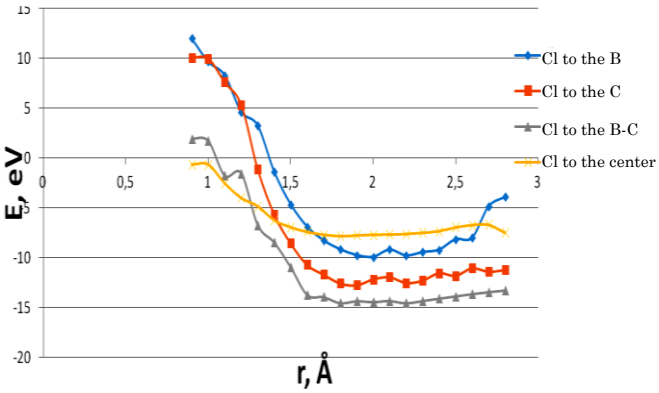

Fig. 4 – Profiles of the potential energy surface of interaction Cl atoms with the boron-carbon nanotube (6, 6) surface for four variants of atom orientation relative to boron-carbon tubulene

Table 2 – Basic characteristics of the electron energy of adsorption Cl atoms on the surface of the boron-carbon nanotube: 1) above the center of the hexagon, 2) above the center of the B-C, 3) over a C-atom, 4) on the boron atom; *E*ad – adsorption energy, eV; *R*ad – distance adsorption, Å

Variants of adsorption	R_{ad}, Å	E_{ad}, eV
1	2	– 9,903
2	1,9	– 12,73
3	1,8	– 14,5
4	1,8	– 7,8

We investigated the possibility of a fluorine atom surface adsorption to the outer surface of a single-walled boron-carbon nanotube (6.6). Four variants of the adsorbed atom location above the nanotube surface have been investigated (Fig. 1). The calculations were performed using the model of a molecular cluster, using the semi-empirical scheme MNDO.

As the figure shows (Fig. 6) energy curves for different positions of the fluorine tube are similar, the adsorption process occurs without a barrier, and in all cases the chemical adsorption of fluoride on the surface of boron-carbon nanotube takes place (see Table 3). From the energy point of view, the adsorption process efficiently occurs at the location of the fluorine atom above the boron atom of the tube. Adsorption of fluorine on the outer surface of the tubulene leads to small deformation. Boron atom to which adsorbed fluorine rises to 0.2 Å relative to the surface of the tube (Fig. 5).

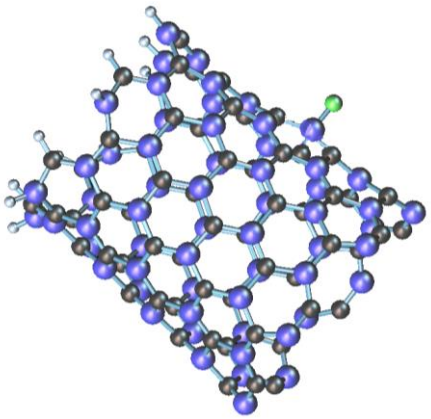

Fig. 5 – The interaction of the fluorine atom with a BC tube

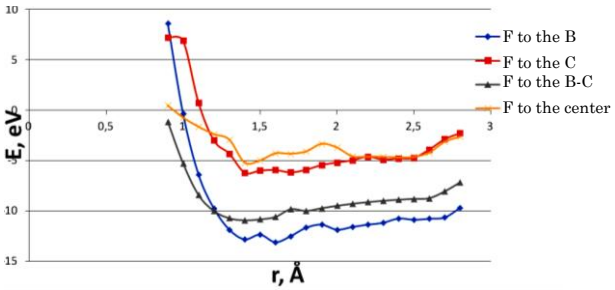

Fig. 6 – The profiles surface of the potential energy of adsorption of the fluorine atom

Table 3 – Basic characteristics of an electron-energy process the F atom adsorption: 1) above the center of the hexagon, 2) above the center of the B-C, 3) over a C-atom, 4) on the boron atom; E_{ad} – adsorption energy, eV; R_{ad} – distance adsorption, Å

Variant of adsorption	R_{ad}, Å	E_{ad}, eV
F to the B	1,6	– 13,101
F to the C	1,4	– 6,2006
F to the B-C	1,4	– 10,92
F to the center	1,4	– 5,19078

4. SUMMARY

The calculations made using the MNDO framework showed, that the adsorption of the gas atoms on the external surface of the BC nanotube is possible and depend on the basic orientation of the adatom.

The energetically favorable location in the case of fluorine atom is above the boron atom of the nanotube

For the chlorine atom the most energetically favorable location is above the B-C bond

For oxygen atom the most probable location is above the carbon atom of the BC nanotubulene.

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