

## **Comparative study of the interaction of a modified borocarbon nanotube of the BC type with carbon-containing molecules.**

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It is proved that functionalized carbon nanomaterials with a certain structure, optimized affinity and solubility can meet most requirements for use in such industries as energy storage, biology and medicine, environmental improvement, etc. Modification of the carbon nanotube surface involves modification of the  $sp^2$  carbon lattice by introducing heteroatoms (doping) or covalent bonds with certain functional groups or other molecules. This methodology provides an opportunity to establish the necessary chemical composition of carbon nanotubes to impart appropriate new properties or change existing ones, in accordance with the necessary requirements. It has been established that boron (B) and nitrogen (N) are the most suitable candidates based on numerous parameters, such as the redox behavior of heteroatoms, the possibility of including a heteroatom in the CNT network.

This paper presents a comparative study of the interaction between modified functional groups, namely carboxyl (-COON), amine (-NH<sub>2</sub>) and nitro group (-NO) boron-carbon nanotube of the BC type with carbon-containing gas molecules, namely with a carbon dioxide (CO<sub>2</sub>) molecule, as well as with an acetone (C<sub>3</sub>H<sub>6</sub>O) molecule.

Based on the results of the study performed using computer simulation of interaction processes and scanning of a virtual surface containing the studied molecules, the possibility of using boron-carbon nanotubes modified by functional groups in nanoelectronics devices used to determine the micro-quantity of substances has been established.

In the course of studying the mechanism of interaction of the "BC nanotube – functional group" tubular system with identifiable substances, energy values determining the presence of physical adsorption of molecules were obtained. Also, at the stage of conducting a study of sensory activity by scanning a space including CO<sub>2</sub> and C<sub>3</sub>H<sub>6</sub>O molecules with a nanosystem based on a modified boron-carbon nanotube, a high reactivity to the presence of a micro amount of carbon dioxide or acetone was noted. Different energy values when interacting with different molecules indicate the selectivity of the modified boron-carbon system