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EFFECT OF BORON DOPING ON SENSING PROPERTIES OF CNTS FUNCTIONALIZED WITH NITRO GROUP

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ABSTRACT

In this paper, we have examined the effect of impurity boron atoms on the sensory properties of zig-zag type boron -carbon nanotubes (6,0) containing different numbers of boron atoms, namely 50% and 25%. Let's call them BC and BC3 nanotubes. The simulation was carried out using the DFT calculation method, the B3LYP functionality and the basis set of 6-31G.

INTRODUCTION

Currently, carbon nanotubes are attracting increasing attention as potential materials for creating sensors of various types. It can be assumed that their sensory properties can be improved by modifying the surface of CNT with impurity replacement boron atoms. Similar nanotubes can be called boron-carbon nanotubes. Also, to improve the sensory properties of BC and BC_3 nanotubes, their surfaces were functionalized with a NO_2 group, the presence of which can lead to an increase in the sensitivity of nanotubes to various atoms and molecules. Nanotubes can be used as sensors to detect various gases, including explosive and toxic substances, due to their high sensitivity to small environmental changes. In addition, CNTs can serve as the basis for various electronic devices.

STUDY OF SENSORY INTERACTION OF LITHIUM, SODIUM, AND POTASSIUM ATOMS ON THE ARBITRARY SURFACE OF MODIFIED BC AND BC3 NANOTUBES

To evaluate the sensory interaction between the modified boron-carbon nanotubes and alkali metal atoms (Li, Na, and K), an arbitrary virtual surface was scanned on which the presence of these atoms is implied. The scanning was performed along the hydrogen atoms of the amine group.

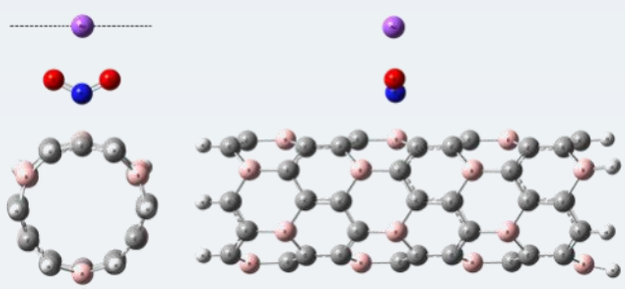

Fig. 1. A) The path by which the surface was scanned; B) BC3-NO2 complex with alkali metal atom Na

CHARACTERISTICS OF SENSORY INTERACTION WHEN SCANNING AN ARBITRARY SURFACE

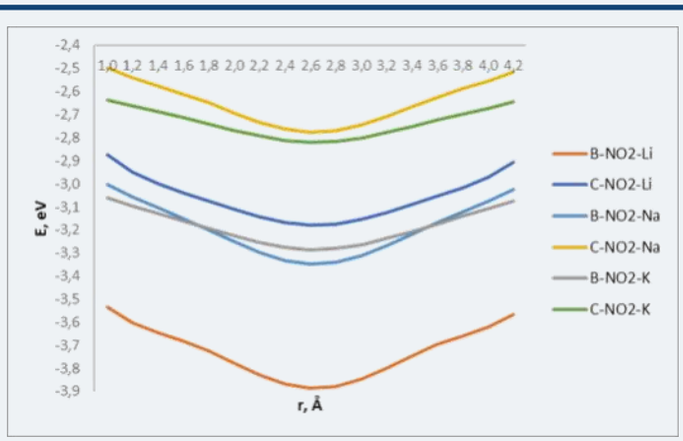

Fig. 2. Energy curves showing the sensory interaction energies of the "BC-NO_2" complex with alkali metal atoms.

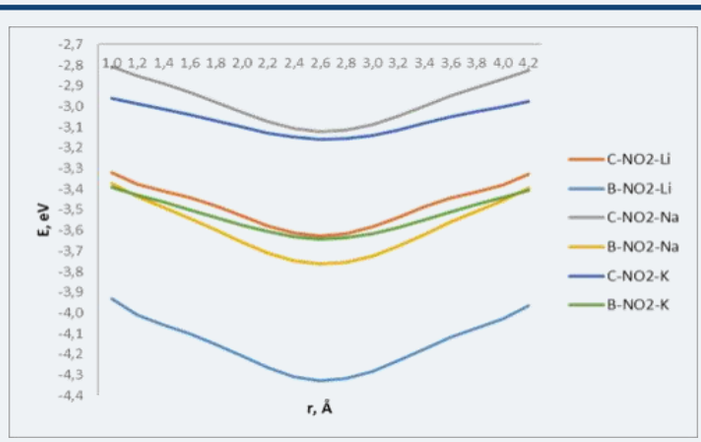

Fig. 3. Energy curves showing the sensory interaction energies of the "BC_3-NO_2" complex with alkali metal atoms.

CONCLUSIONS

Summing up, it can be concluded that all functionalized boron-carbon nanotubes studied can be used to detect the presence of alkali metal atoms. Such systems can act as sensing elements of sensor devices. At the same time, an increase in the number of impurity boron atoms in the obtained systems leads to a decrease in the energy of the sensory interaction of the complexes "BC-NO2", BC3-NO2" with alkali metal atoms Li, Na, K.