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Investigation of Atomic Adsorption on the Surface of BC3 Nanotubes

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Abstract : Studing of nanotubes sorption properties is very important for researching. These processes for carbon and boron nanotubes described in the high number of papers. But the sorption properties of boron containing nanotubes, susch as BC3-nanotubes haven't been studied sufficiently yet. In this paper we present the results of theoretical research into the mechanism of atomic surface adsorption on the two types of boron-carbon nanotubes (BCNTs) within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme and DFT method using B3LYP functional with 6-31G basis. These methods are well-known and the results, obtained using them, were in good agreement with the experiment. Also we studied three position of atom location above the nanotube surface. These facts suggest us to use them for our research and quantum-chemical calculations. We studied the mechanism of sorption of Cl, O and F atoms on the external surface of single-walled BC3 arm-chair nanotubes. We defined the optimal geometry of the sorption complexes and obtained the values of the sorption energies. Analysis of the band structure suggests that the band gap is insensitive to adsorption process. The electron density is located near atoms of the surface of the tube. Also we compared our results with others, which have been obtained earlier for pure carbon and boron nanotubes. The most stable adsorption complex has been between boron-carbon nanotube and oxygen atom. So, it suggests us to make a research of oxygen molecule adsorption on the BC3 nanotube surface. We modeled five variants of molecule orientation above the nanotube surface. The most stable sorption complex has been defined between the oxygen molecule and nanotube when the oxygen molecule is located above the nanotube surface perpendicular to the axis of the tube.

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