

Influence of the Boron Impurities in Carbon Nanotubes on the Atomic and Molecular Hydrogen Sorption Processes.

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Abstract - In this research interaction of atomic and molecular hydrogen with carbon nanotubes containing boron impurities is considered. Process was modelled by step-by-step approach of atom or molecule of hydrogen to a surface of a nanotube. Calculations were carried out with use of model of a molecular cluster within a method of density functional theory (DFT). The research of the electronic and energy structure of the complex received in a consequence of influence of step-by-step approach of adatom to a surface of a carbon nanotubes containing boron impurities was conducted.

Keywords: Boron-carbon nanotubes, Hydrogenation, Adsorption, Density functional theory, Quantum-chemical research.