The research on adsorption of methane on carbon nanotube surface

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High sensitivity of electronic properties to the presence of molecules, sorbed on a surface, as well as the record size of a specific surface area (1300 m_2/g), promoting such adsorption make carbon nanotubes (NT) a perspective basis for the creation of subminiature biochemical sensors [1]. The major part of natural gas is up to 98 % composed of methane (CH_4). Thus, in order to create such a device it is necessary to research the influence of adsorption of methane molecule on the surface of carbon nanotubes on their electronic properties.

The result of the conducted research was the calculation of key parameters of the process of methane atom adsorption on the carbon nanotubes surfaces of various types [2]. It has been shown that adsorption can be performed in four different ways: physical adsorption of methane molecules; adsorption of hydrogen atom on NT and formation of CH_3 radical; adsorption with decomposition into H and CH_3; 2H and CH_2. In all cases there appears a change of the width of the forbidden zone of nanotubes, and all the states are steady.

As a result, it is possible to say that the methane molecule will be adsorbed onto a surface of carbon NT of small diameter. Therefore, it is rational to use the tubes of the diameter of no more than 20 nm for the creation of a gas sensors on the basis of carbon NT. The values of bond energies and top filled and bottom vacant orbitals, the values of the forbidden zones of various carbon nanotubes with the adsorbed methane molecule have been received.

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