Electronic structure of carbon nanotubes in benzene solution

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In this work the single-walled nanotubes (n, n) type (n = 5, 6) are considered. As the geometrical models of nanotubes the clusters (fragments) containing n six-member cycles (hexagons) on a tube perimeter and 8 - 10 elementary cells along an axis of a tube are chosen. The boundary broken off chemical bonds became isolated atoms of hydrogen. The calculations of an electronic structure of the structures are carried out within the frameworks of the simple molecular cluster model [1] with the use of quantum-chemical semi-empirical schemes MNDO [1].

Studied three variants of the orientation of benzene molecules on the surface of carbon nanotubes: I) over a center of the hexagon (the plane of the molecule perpendicular the plane of the hexagon); II) over the center of the hexagon (the molecular plane parallel the plane of the hexagon); III) plane of the benzene molecule parallel the nanotube. In each of the three cases the molecule was located in the center of the cluster to reduce the influence of boundary conditions.

The analysis of quantum-chemical calculation results has shown that the the highest occupied molecular orbital energy (E_{HOMO}) increases with the tube diameter growth and the lowest unoccupied molecular orbital energy (E_{LUMO}) decreases. Change of E_{HOMO} and E_{LUMO} sizes testifies the change of nanotube properties caused by adsorption, namely the increase in reactionary ability of the given systems. I.e. the tubes of a particle adsorbed on a surface increase affinity carbon nanotubes to other particles.

The analysis of the length of the adsorption of chemical bonds has shown that in cases (I) and (III) between the benzene molecule and the atoms of carbon nanotubes form only hydrogen bonds. And in case (II) formed covalent chemical bond type 6 +6 between the carbon atoms of the molecule and the tube. The latter case seems unlikely, since the formation of both 6 bonds need only possible mutual orientation of the particles, the steric factor which in solution is very low compared to other options.

The analysis of results has shown that due to the adsorption of the benzene molecule the band gap of the nanotube increases slightly. This indirectly leads to a slight change in the physical properties of carbon nanotubes, in particular, the conductivity and transparency. This effect can be used to develop chemical sensors [2], aimed at registering considered in the particles, and the creation of optically active medium based on carbon nanotubes solutions in benzene.

[1] Stepanov N.F. Quantum mechanic and quantum chemistry. Moscow: MSU, 2001. 519 p.
[2] Aggins B. Chemical and biological sensor controls. Moscow: Technosphere. 2005, 336 p.