# CARRIERS SPECTRA OF SEMICONDUCTOR CNT WITH CONFORMATION TRANSITION IN FUNCTIONALIZING MOLECULES

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Carbon nanotubes (CNTs) are nano materials with a small diameter of about 1 nm, length of about 1 μm, quantization along the nanotube axis exists [1]. The CNTs novel high-sensitive biosensors, electronic and optoelectronic devices work due to their quantum energy levels positions. Functionalization is new powerful method for tuning CNTs quantum energy and their physical properties [2]. Theory of energy spectra tuning in the semiconductor CNTs as the result of functionalization by enough thick molecular films (DNA or Langmuire–Blodgett films) was developed in work [3].

The aim of this work is to consider the theoretical approach to CNTs spectra tuning as result of functionalization by layers with conformation transition of molecules. We research an effect of interaction of the uncompensated charge carried by an electron or hole in a quantum nanowire with the neighboring medium, which has molecules possessing an intrinsic electric-dipole moment. The selfconsistent system of equations is obtained. The system includes (i) the Schrцdinger equation for a charge carrier in a semiconducting CNT, (ii) equation of the intrinsic electric-dipole moments, (iii) the material equations for interaction an extra carrier in CNT and molecular electric dipoles, (iv) normalization condition for the wave function of a carrier.

The carrier electric charge induces the conformation transition with changing of the intrinsic electric-dipole moments in the molecules. The selfconsistent system of equations is obtained. The system includes nonlinear equation of the intrinsic electric-dipole moments. In semiconductor CNT the hole and electron spectra are symmetric. It is shown, the layer of the adsorbed molecules breaks this symmetry. The molecular dipoles create opposite conditions for a carrier localization or tunneling along CNT in dependence on charge sign and dipole orientation.

It appears that the spectrum is extremely sensitive to the state of the molecular subsystem. Carrier localization, which manifests itself in the experiment as an increase of the resistance, is possible.

1. C. Dekker, Phys. Today 52, 22 (1999).
2. S. Daniel et al. Sensors and Actuators B **122,** 672682 (2007).
3. V. A. Lykakh and E. S. Syrkin. Semiconductors, **39**, 679 (2005).