Carrier spectrum in CNT functionalized by molecules with conformation transition

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Carbon nanotubes (CNTs) are nano materials with a small diameter of about 1 nm, length of about 1 μm and the mean free path of the charge carriers exceeds 10 μm[1] which is important for quantization along the nanotube axis[2]. 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[3]. 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[4]. It appears that the spectrum is extremely sensitive to the state of the molecular subsystem.

The aim of this research is to develop theoretical approach to CNTs spectra tuning as result of functionalization by layer of molecule with conformation transition. We consider effect of interaction of the uncompensated charge carried by an electron or hole in a quantum nanowire with the neighboring medium, which has low mechanical rigidity and consists of molecules possessing an intrinsic electric-dipole moment. The molecules' intrinsic electric-dipole moments are considered all to be oriented perpendicular to the CNT axis along radii. The situation is expected when 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 (i) the Schrödinger equation for a charge carrier in a semiconductor CNT, (ii) nonlinear equation of the intrinsic electric-dipole moments, (iii) the material equations for interaction an extra carrier in a nanotube and molecular electric dipoles subsystem. In semiconductor CNT the hole and electron spectra are symmetric. 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.

References

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