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Modeling of the SWNT-DNA complexes in the water solution
ALEXEY A. TSUKANOV, EUGENE A. GRACHEV, Moscow State University, SLAVA V. ROTKIN, Physics Department and Center for Advanced Materials and Nanotechnology, Lehigh University — It is known that the single-wall nanotubes (SWNTs) may form a hybrid with a single-stranded DNA having a regular helical structure of the DNA wrap around the SWNT cylinder. Such DNA wrapping creates a periodic potential at the NT surface, which results in developing a specific modulation of the NT bands. Numerical self-consistent modeling of these effects requires knowledge of the polarization of the environment. We have shown that the result is very sensitive to what extent the exterior water (and ions in the solution) are polarized to screen the potential of the DNA. Both the NT screening and the response of the environment are important to include self-consistently to obtain quantitative results. We present the Monte-Carlo simulation of the interaction of a NT, a DNA and a solvent and provide heuristic physics interpretation of the results. We show that the NT screening is different from what one expects for a metal or insulator material due to non-local Coulomb correlations. An effective dielectric screening of the water exterior is extracted from the simulations.

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