

Abstract Submitted
for the MAS16 Meeting of
The American Physical Society

Multiscale Model for Optical Response of SWCNT-based biosensor materials WENXIN HUANG, SLAVA ROTKIN, Lehigh University — Single-wall Carbon Nanotube (SWCNT) hybrids have raised considerable interest as biological sensors, in cancer detecting and other fields. We developed a multiscale Multiphysics model for the electronic structure and response of Single-wall Carbon Nanotube hybrids in complex solutions via combined quantum mechanics and electrodynamics approach. The model allows to investigate the response of SWCNT-hybrids to different environments. In particular, it has been reported that single-stranded DNA (ssDNA) interacts strongly with SWCNTs and forms a stable ssDNA-SWCNT hybrid that effectively disperses SWCNTs in aqueous solution. Here, the electrostatic potential and charge density of ssDNA-SWCNT hybrids in aqueous solution has been modeled. We discuss various level of model approximations that can be used (along with the full solution). One can describe the local SWCNT response function in terms of quantum capacitance and geometric capacitance. Such an approach can be further advanced by using full Greens function, solved here by numerical resolvent method. Example patterns of charge density distributions for external point-like and chain-like potentials are presented.

Wenxin Huang
Lehigh Univ

Date submitted: 16 Sep 2016

Electronic form version 1.4