Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Coulomb Effects in DNA-functionalized Single-Walled Carbon Nanotubes BENJAMIN TAYO, SLAVA ROTKIN, Lehigh University — We study how many-body effects (Coulomb effects) affect the optical and electronic properties of DNA-functionalized SWCNTs. Coulomb effects are very strong in one-dimensional systems and hence play a greater role in their optical and electronic properties. Coulomb interactions contribute to the optical and electronic properties of carbon nanotubes in two main ways: band gap renormalization which comes from electron-electron interaction and the formation of excitons due to electron-hole coupling. The procudure for obtaining the optical exitation energies for DNA-SWCNTs involves incorporating Coulomb interaction within the Bethe-Salpeter (BS) equation combined with the tight-binding approximation (with self-energy contributions restricted to the screened Hartree-Fock approximation). The DNA-SWCNT interaction is modelled by applying a perturbation operator of the Coulomb interaction which breaks both translational and rotational symmetry. This lowering of symmetry induced by DNA-wrapping changes the band gap of the nanotube thus modulating its electronic and optical properties. The role of these effects are elucidated.

Benjamin Tayo
Lehigh University

Date submitted: 20 Nov 2009 Electronic form version 1.4