Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Optical properties of doped semiconducting single-walled carbon nanotubes.** CATALIN D. SPATARU, FRANCOIS LEONARD, Sandia National Laboratories, Livermore, CA 94551 — We studied how the optical response of semiconducting single-walled carbon nanotubes changes upon doping. We performed ab initio calculations of the optical absorption spectrum of the p-doped (10,0) SWCNT, employing a many-electron Green's function approach that determines both the quasiparticle and electron-hole excitations from first principles. We found that the absorption spectrum changes dramatically upon doping, due to both quasiparticle and excitonic effects. In the independent quasiparticle picture, the electron-hole continua are strongly red-shifted with respect to the undoped case due to the metallic character acquired by the electronic screening upon doping. However, the main optical features in the absorption spectrum, including both quasiparticle and electron-hole interaction effects, are only slightly shifted, but qualitatively very different, with respect to the undoped case. Small doping levels (where the Fermi level lies below the valence band maximum by an energy much smaller than the binding energy of excitons in the undoped SWCNT) are sufficient to bleach band-gap absorption. In addition, while resonant excitons associated with the second electron-hole continuum can still exist in the doped SWCNT, their binding energy is much reduced, to a level typical of metallic SWCNTs of similar diameter.

Catalin D. Spataru
Sandia National Laboratories, Livermore, CA 94551

Date submitted: 20 Nov 2008 Electronic form version 1.4