MAR06-2005-001149

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Excitons in the optical properties of nanotubes[1]

CATALIN SPATARU[2], UC Berkeley and LBNL, Berkeley, CA 94704

We present *ab initio* calculation of self-energy and electron-hole interaction (excitonic) effects on the optical spectra of single-walled carbon and BN nanotubes. We employed a many-electron Green's function approach that determines both the quasiparticle and optical excitations from first principles. We found important many-electron effects that explain many of the puzzling experimental findings in the optical spectrum of these quasi-one dimensional systems, and the calculated spectra are in excellent quantitative agreement with measurements. In carbon nanotubes, excitons can bind by as much as one eV in semiconducting nanotubes[a)]. We discovered that bound excitons also exist in metallic carbon nanotubes with binding energy of many tens of meVs[a)]. Excitonic effects are shown to be even more inportant in BN nanotubes than in carbon nanotubes. Unlike the carbon nanotubes, theory predicts that excitons in some BN nanotubes are comprised of coherent superposition of transitions from several different subband pairs[b)]. We have also calculated the radiative lifetime of excitons in semiconducting carbon nanotubes. Assuming a thermal occupation of bright and dark exciton bands, we find an effective radiative lifetime of the order of 10 ns at room temperature, in good accord with recent experiments[c)].

a) C.D. Spataru, S. Ismail-Beigi, L.X. Benedict and S.G. Louie, Phys. Rev. Lett. **92**, 077402 (2004).
b) C.-H. Park, C.D. Spataru and S.G. Louie, to be published.
c) C.D. Spataru, S. Ismail-Beigi, R.B. Capaz and S.G. Louie, in press Phys. Rev. Lett.

[1]This work was supported by the NSF under Grant No. DMR04-39768, and the U.S. DOE under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NERSC and NPACI.

[2]This work has been done in collaboration with Cheol-Hwan Park, Sohrab Ismail-Beigi, Lorin X. Benedict, Rodrigo B. Capaz and Steven G. Louie.