Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

An explicit formula for optical oscillator strength of excitons in semiconducting single-walled carbon nanotubes: family behavior SANGKOOK CHOI, UC Berkeley and Lawrence Berkeley National Lab, JACK DESLIPPE, Lawrence Berkeley National Lab, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, Brazil, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — The sensitive structural dependence of the optical properties of single-walled carbon nanotubes (SWCNTs), which are dominated by excitons and tunable by changing diameter and chirality, makes them excellent candidates for optical devices. Because of strong many-electron interaction effects, the detailed dependence of the optical oscillator strength of excitons on nanotube diameter d, chiral angle θ, and electronic subband index P (the so called family behavior) however has been unclear. Based on results from an extended Hubbard Hamiltonian with parameters derived from *ab initio* GW-BSE calculations, we have obtained an explicit formula for the family behavior of the oscillator strengths of excitons in semiconducting SWCNTs, incorporating environmental screening. The formula explains well recent measurements, and is expected to be useful in the understanding and design of possible SWCNT optical and optoelectronic devices. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and Teragrid.

Sangkook Choi
UC Berkeley and Lawrence Berkeley National Lab

Date submitted: 11 Nov 2012 Electronic form version 1.4