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Many-electron effects in the optical properties of single-walled carbon nanotubes CATALIN D. SPATARU, UC Berkeley and LBNL, SOHRAB ISMAIL-BEIGI, Dept.of Applied Physics, Yale Univ., RODRIGO B. CAPAZ, UFRJ, Brazil, UC Berkeley and LBNL, STEVEN G. LOUIE, UC Berkeley and LBNL — Recent optical measurements on single-wall carbon nanotubes (SWCNT) showed anomalous behaviors that are indicative of strong many-electron effects. To understand these data, we performed ab initio calculation of self-energy and electron-hole interaction (excitonic) effects on the optical spectra of several SWCNTs. 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 are in excellent quantitative agreement with measurements. We have also calculated the radiative lifetime of the bright excitons in these tubes. Taking into account temperature effects and the existence of dark excitons, our results explain the radiative lifetime of excited nanotubes measured in time- resolved fluorescence experiments. 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. RBC acknowledges financial support from the Guggenheim Foundation and Brazilian funding agencies CNPq, CAPES, FAPERJ, Instituto de Nanociências, FUJB-UFRJ and PRONEX-MCT.

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