Abstract Submitted
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Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, U. C. Berkeley and LBNL, PAUL TANGNEY, The Molecular Foundry, LBNL, CATALIN D. SPATARU, MARVIN L. COHEN, STEVEN G. LOUIE, U. C. Berkeley and LBNL — The temperature dependence of the band gap of semiconducting single-wall carbon nanotubes (SWNTs) is calculated by direct evaluation of electron-phonon couplings within a "frozen-phonon" scheme. An interesting diameter and chirality dependence of $E_g(T)$ is obtained, including non-monotonic behavior for certain tubes and distinct "family" behavior. These results are traced to a strong and complex coupling between band-edge states and the lowest-energy optical phonon modes in SWNTs. The $E_g(T)$ curves are modeled by an analytic function with diameter and chirality dependent parameters; these provide a valuable guide for systematic estimates of $E_g(T)$ for any given SWNT. Magnitudes of the temperature shifts at 300 K are smaller than 12 meV and should not affect (n, m) assignments based on optical measurements. RBC acknowledges financial support from the John Simon Guggenheim Memorial Foundation and Brazilian funding agencies CNPq, FAPERJ, Instituto de Nanociências, FUJB-UFRJ and PRONEX-MCT. Work partially supported by NSF Grant No. DMR00-87088 and DOE Contract No. DE-AC03-76SF00098. Computer resources were provided by NERSC and NPACI.

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