Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Extracting Diameter and Chirality Dependences of Optical and Electronic Properties of Semiconducting Single-Wall Carbon Nanotubes from First-Principles Calculations RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, Brazil, JACK DESLIPPE, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, U. C. Berkeley and Lawrence Berkeley National Laboratory — First-principles methods based on the combination of density-functional theory (DFT) for ground-state properties, GW approximation for quasiparticle properties and Bethe-Salpeter equation (BSE) for optical properties represent the state-of-art for accurate and reliable calculations of optical and electronic properties of solids and molecules. For semiconducting carbon nanotubes (CNTs), they have been applied successfully to selected small-diameter tubes. In this work, we systematically calculate such properties for all zig-zag semiconducting single-wall carbon nanotubes with diameters ranging from (10,0) to (20,0) CNTs, allowing us to extract in a reliable way the diameter and chirality dependence of many properties, such as: (i) optical transition energies; (ii) quasiparticle band gaps; (iii) exciton binding energies; (iv) bright-dark exciton splittings; (v) excited exciton states properties; (vi) transverse-polarized exciton states properties; (vii) electron and hole effective masses (and therefore excitonic reduced masses). All properties are described with good accuracy by diameter- and chirality-dependent analytical formulas, with parameters extracted from the first-principles calculations.

Rodrigo Capaz
Universidade Federal do Rio de Janeiro

Date submitted: 29 Dec 2011 Electronic form version 1.4