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Dielectric screening dependence of excitonic transition energies in single-wall carbon nanotubes PAULO ARAUJO, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, ADO JORIO, Universidade Federal de Minas Gerais, KENTARO SATO, AHMAD NUGRAHA, RICHIRO SAITO, Tohoku University — The measured optical transition energies E_{ii} of single-wall carbon nanotubes are compared with bright exciton energy calculations. The E_{ii} differences between experiment and theory are minimized by considering first, a diameter/chiral angle-dependent dielectric constant and second, a diameter/exciton size-dependent dielectric constant (k). In our description, k is composed of the screening contributions from the tube, represented by k_{tube} , and from the environment, represented by k_{env} . We discuss the main aspects of each approach and show that in the first case, different k dependencies are obtained for $(E_{11}^S, E_{22}^S, E_{11}^M)$ relative to (E_{33}^S, E_{44}^S) which is understood as follows: A changing environment changes the k diameter dependence for $(E_{11}^S, E_{22}^S, E_{11}^M)$, but for (E_{33}^S, E_{44}^S) the environmental effects are minimal. We show that in order to achieve a single dependence for all E_{ii} , the exciton's size should be taken into account, as considered in the second approach. The resulting calculated exciton energies reproduce experimental E_{ii} values within $|50|$ meV for a diameter range $(0.7 < dt < 3.8$ nm) and $1.2 < E_{ii} < 2.7$ eV, thus providing a theoretical justification for E_{ii} and important insights into the dielectric screening in one-dimensional structures.

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