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Ab initio study of the optical properties of carbon nanotubes

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We present an ab initio study of the optical properties of carbon nanotubes. We use state-of-the-art electronic structure methods based on many-body perturbation theory to compute the optical absorption and resonance Raman spectra of large tubes which have up to 200 atoms [1,2]. Our symmetry-based method makes the study of large tubes feasible within the many- body framework and also allows us to understand the symmetry properties of the excitons and selection rules. We include a study of the so-called dark excitons which are crucial for understanding luminescence efficiency in carbon nanotubes. The mechanism that explains the dark-bright splitting can be understood within our symmetry-based approach. Finally, we present an analysis of the two-photon spectra for several carbon nanotubes, a theoretical analysis which, in conjunction with combined one- and two-photon experiments, allows one to measure the binding energy of excitons. We find in all cases that the excitonic binding energy is large, ranging from 0.5 to 0.9 eV depending on the diameter of the tube, and that the excitonic wavefunction is Wannier-like and extended over many atoms. Our studies for the one- and two-photon absorption and resonance Raman spectra have been fruitful for understanding the corresponding experiments. In particular, our theoretical results are in good agreement with one- and two-photon absorption experiments [3-5]. The results for resonance Raman show that such a spectroscopic technique is a good alternative to optical absorption since it allows for the selection of tubes of a given diameter while probing the same excited states. 1. E.K. Chang, G. Bussi, A. Ruini, and E. Molinari, Phys. Rev. Lett. 92, 196401 (2004). 2. E.K. Chang, G. Bussi, A. Ruini, and E. Molinari, Phys. Rev. B 72, 195423 (2005). 3. M. Y. Sfeir et al., Science 306, 1540 (2004). 4. J. Maultzsch et al., to be published in Phys. Rev. B, see also cond-mat/0505150. 5. Z. M. Li et. al., Phys. Rev. Lett. 87, 127401 (2001).