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Nonlinear Optical Properties of Carbon Nanotubes from First Principles JACK DESLIPPE, University of California at Berkeley and Lawrence Berkeley National Lab, DAVID PRENDERGAST, Lawrence Berkeley National Lab, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The optical excitation spectra of both semiconducting and metallic single-walled carbon nanotubes (SWNTs) as well as other 1D materials are dominated by exciton states of large binding energy and well defined symmetry in the group of the k-vector along the periodic direction. The optical oscillator strength is transferred almost entirely from the continuum into the excitons and the corresponding exciton-phonon states. Recent experiments have probed the spectral structure of the excited states of various symmetry in SWNTs using nonlinear optics techniques such as ultrafast spectroscopy, multi-photon spectroscopy, and phonon-assisted spectroscopy. We have developed and applied a new method based on the first-principles GW-Bethe Salpeter approach to the study of the nonlinear optical properties of the SWNTs. Supported by NSF Grant No. DMR07-05941, US DOE Contract No. DE-AC02-05CH11231 and DOE CSGF grant DE-FG02-97ER25308 and computational resources from Teragrid and NERSC.

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