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Benchmark Quantum Monte Carlo Calculations of Optical gaps of carbon Nanotubes FERNANDO REBOREDO, PAUL KENT, Oak Ridge National Laboratory — Optical properties of single wall carbon nanotubes SWCNT have attracted considerable experimental and theoretical attention because they are strongly dependent on the details of the atomic structure (chiral vector). In these systems electronic correlations have been shown to play a dominant role both theoretically [1] and experimentally [2] as electron-electron interactions are increased in low dimensions. In this talk we present ongoing calculations of the optical gaps and quasi-particle energies of SWCNT with an alternative ab-initio technique: Diffusion Quantum Monte Carlo (DMC). We take advantage of a novel algorithm based on non-orthogonal localized orbitals that allows almost linear scaling calculations for $\sim$1000 electrons. DMC is a complementary technique to methods based on the GW approximation and the Bethe-Salpeter equation avoiding strong approximations. While the full absorption spectra cannot be obtained with DMC, we provide accurate benchmark values for the quasiparticle energy gaps and exciton binding energies. Research sponsored by the Division of Materials Sciences and Engineering, U. S. DOE, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. and by the Division of Scientific User Facilities, U. S. DOE. This work used resources of the NCCS at ORNL. [1] C. S. Spataru, PRL **92**, 077402 (2004). [2] Z. Wang PRL 96, 047403 (2006)

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