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Bethe-Salpeter and Quantum Monte Carlo Calculations of the Optical Properties of Carbon Fullerenes P.R.C. KENT, M.L. TIAGO, F.A. REBOREDO, Oak Ridge National Laboratory, RANDOLPH Q. HOOD, Lawrence Livermore National Laboratory — We have calculated the low energy optical excitations of the carbon fullerenes C20, C24, C50, C60, C70, and C80. Properties are calculated via the GW-Bethe-Salpeter Equation (GW-BSE) and diffusion Quantum Monte Carlo (QMC) methods. We compare these approaches with time dependent density functional results and with experiment. GW-BSE and QMC have previously shown good agreement for small molecules, but this is the first study of these methods for these larger yet prototypical nanostructures. The first ionization potentials are consistently well reproduced and are similar for all the fullerenes and methods studied. However, electron affinities and first triplet exciton show substantial method and geometry dependence. GW-BSE yields triplet energies around 1eV below the QMC results. We discuss the possible reasons for these differences. Research at Oak Ridge National Laboratory performed at the Materials Science and Technology Division, sponsored by the Division of Materials Sciences, and at the Center for Nanophase Materials Sciences, sponsored by the Division of Scientific User Facilities, U.S. Department of Energy. Research at Lawrence Livermore National Laboratory was performed under Contract DE-AC52-07NA27344.

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