

GW-BSE: From Atoms to the Nanoscale

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The GW approximation, coupled with the Bethe-Salpeter equation (BSE), allows the first-principles prediction of electronic and optical properties. In this presentation, we examine the efficiency and accuracy of GW-BSE applied to finite systems such as atoms, molecules, or nanocrystals. After a brief introduction of the GW-BSE theory, we discuss how a real-space basis, with wave functions defined on a spherical uniform grid, takes advantage of quantum confinement to improve computational efficiency. We present simulations predicting the excited-state properties of titanium dioxide nanocrystals up to ~ 1.5 nm in size. We also benchmark GW and GW-BSE energies on test sets consisting of transition metal atoms, some of their oxide dimers, and organic molecules, with comparison to other software packages and to experiment. Finally, we explore how a LDA-derived vertex function affects the accuracy of quasiparticle and absorption energies on the same benchmark set.