

Abstract Submitted
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First Principles Real-Space GW+BSE Calculations for Confined Systems LINDA HUNG, SERDAR OGUT¹, University of Illinois at Chicago, JAIME SOUTO, ALEX LEE, CHARLES LENA, JAMES R. CHELIKOWSKY², University of Texas at Austin, FELIPE H. DA JORNADA, STEVEN G. LOUIE³, University of California at Berkeley and LBNL — We investigate the performance of various levels of GW theories for electronic excitations as well as the resulting solutions of the Bethe-Salpeter-Equation (BSE) for optical excitations in a wide range of confined systems including atoms, ions, diatomic molecules, and organic molecules relevant for photovoltaic applications. Starting with solutions of the Kohn-Sham equations for ground state properties computed via the real-space *ab initio* pseudopotential code PARSEC, we perform the GW calculations in the space of single-particle transitions at various levels of theory, and compare the results with photoemission data. The levels of theory include such approximations as G_0W_0 with RPA screening, G_0W_f that includes vertex corrections through the use of a dielectric screening within the time-dependent-local-density approximation (TDLDA), the GW_0 , and the self-consistent GW. The resulting quasiparticle energies and wave functions from the GW calculations are used to solve the BSE for optical excitations, which are then compared with experiments and results from calculations performed within the TDLDA. The effects of the vertex corrections, self-consistency in GW, and core-valence partitioning are discussed.

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