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GW-BSE, self-consistency, and vertex corrections applied to group IB/IIB atoms and oxide molecules[1] LINDA HUNG, SERDAR OGUT, University of Illinois at Chicago — Time-dependent density functional theory (TDDFT), the GW approximation, and the Bethe-Salpeter equation (BSE) are often used for the first-principles calculation of excited-state properties of materials that contain transition metals. Accuracy is improved compared to mean-field theories such as Kohn-Sham DFT or Hartree-Fock; however, predicted quasiparticle levels and optical spectra can still differ from experiment. We model Cu, Zn, Ag, and Cd atoms and their oxide molecules to assess various approximations in many-body perturbation theory methods that contribute to these differences. In particular, we examine how self-consistent iterations and/or a two-point vertex function affect the predicted excitation energies, compared to "one-shot" G_0W_0 calculations. Experimental measurements of optical spectra and ionization energies for charged and neutral atoms are widely available, and allow us to evaluate excitations from both s and d states. Differences between TDDFT and BSE spectra are also discussed. Calculations are performed with RGWBS, a software suite which uses a basis of transition space and quasiparticle wavefunctions.

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Linda Hung
University of Illinois at Chicago

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