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A Benchmark of GW Methods for Azabenzenes: Is the GW Approximation Good Enough? NOA MAROM, The University of Texas at Austin, FABIO CARUSO, XINGUO REN, OLIVER HOFMANN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, THOMAS KÖRZDÖRFER, University of Potsdam, Germany, JAMES CHELIKOWSKY, The University of Texas at Austin, ANGEL RUBIO, MATTHIAS SCHEFFLER, PATRICK RINKE, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Many-body perturbation theory in the GW approximation is a useful method for describing electronic properties associated with charged excitations. A hierarchy of GW methods exists, starting from non-self-consistent G_0W_0, through partial self-consistency in the eigenvalues (ev-scGW) and in the Green's function (scGW_0), to fully self-consistent GW (scGW). Here, we assess the performance of these methods for benzene, pyridine, and the diazines. The quasiparticle spectra are compared to photoemission spectroscopy (PES) experiments with respect to all measured particle removal energies and the ordering of the frontier orbitals. We find that the accuracy of the calculated spectra does not match the expectations based on their level of self-consistency. In particular, for certain starting points G_0W_0 and scGW_0 provide spectra in better agreement with the PES than scGW.

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