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A Strategy for Finding a Reliable Starting Point for G_0W_0 Demonstrated for Molecules THOMAS KORZDORFER, University of Potsdam, NOA MAROM, University of Texas at Austin — Many-body perturbation theory in the G_0W_0 approximation is an increasingly popular tool for calculating electron removal energies and fundamental gaps for molecules and solids. However, the predictive power of G_0W_0 for molecules is limited by its sensitivity to the density functional theory (DFT) starting point. In this contribution, the starting point dependence of G_0W_0 is demonstrated for several small organic molecules. Analysis of the starting point dependence leads to the development of a non-empirical scheme that allows to find a consistent and reliable DFT starting point for G_0W_0 calculations by adapting the amount of Hartree-Fock-exchange in a hybrid DFT functional. The G_0W_0 spectra resulting from this *consistent starting point (CSP) scheme* reliably predict experimental photoelectron spectra over the full energy range. This is demonstrated for a test set of various typical organic semiconductor molecules.

[1] T. Korzdorfer and Noa Marom, Phys. Rev. B Rapid Communications **86**, 041110 (2012).

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