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Single-electron excitations of molecules and solids – reliability and robustness of density-functional theory and GW calculations

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State-of-the-art theory addresses single-electron excitations in molecules and condensed matter by linking density-functional theory (DFT) with many-body perturbation theory. Experimentally such results correspond to measurements by direct or indirect photoemission. In actual calculations it is common to employ the pseudopotential approach, where pseudo-wavefunctions enter the calculation of the selfenergy, and the core-valence interaction is treated at the DFT level. Furthermore, calculations are typically not done selfconsistently but as a first-order perturbation on some starting point. The latter may be DFT with LDA, GGA, LDA+ U , HF, or hybrid functionals. Unfortunately, these different starting points can give noticeably different results. In this talk I will evaluate the various approximations, by comparing and analyzing pseudopotential and all-electron calculations. I will also emphasize the need for selfconsistency either by an iterative solution of the Dyson equation or by properly adjusting the zero-th order exchange-correlation functional.

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