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Towards a unified description of ground and excited state properties: *GW* vs RPA and beyond

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In the quest for finding an "optimal" first principles electronic structure method, that combines accuracy and tractability with transferability across different chemical environments and dimensionalities (e.g. molecules, wires/tubes, surfaces, solids), the treatment of exchange and correlation in terms of "exact-exchange plus correlation in the random-phase approximation (EX+cRPA)" offers a promising avenue. Likewise one can express the same level of theory in the Green's function context through the *GW* approximation, which has the additional advantage that quasiparticle spectra as measured by direct and inverse photoemission become accessible. In this talk I will contrast both approaches and present the latest results from our continuous assessment. We find that self-consistent (sc) *GW* provides excellent charge densities [1], which is particularly important for charge transfer systems [2]. Spectral properties for closed shell molecules are generally in good agreement with photoemission spectra, although a judicial choice of the starting point in perturbative G_0W_0 calculations can outperform scGW [1,3]. Other ground state properties do not improve over EX+cRPA calculations [1]. EX+cRPA, on the other hand, provides a good description of the ground state [4] even for challenging cases like chemical reaction barrier heights [5] and the *f*-electron metal cerium [6]. The notorious underbinding of EX+cRPA can be corrected by going beyond RPA to renormalised second order perturbation theory (rPT2) [7] that gives the overall most balanced performance. I will also discuss the associated rPT2 self-energy that goes beyond *GW*.

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