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

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In the quest for finding an "optimal" 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. For quasiparticle spectra as measured by direct and inverse photoemission the GW approach is on the same level of theory as EX+cRPA for the ground state. For molecules and nanosystems the application of GW has steadily gained in popularity and a full assessment of its performance is emerging. In this talk I will extend the assessment of EX+cRPA and GW to small molecules [1] and molecules on surfaces [2,3]. Based on this I will comment on the prospects of these approaches for nanoscience, address current challenges and present avenues for going beyond RPA/GW.

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