Beyond RPA and GW: renormalizated second-order perturbation theory for ground-state and excited-state calculations

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We present a renormalized second-oder perturbation theory (rPT2) [1] for the ground-state total energy that combines the random-phase approximation (RPA), second-order screened exchange (SOSEX) [2], and renormalized single excitations corrections (rSE) [3]. These three terms all involve a summation of certain types of diagrams to infinite order, and can be viewed as a renormalization" of the direct, exchange, and single excitation (SE) terms of 2nd-order Rayleigh-Schrödinger perturbation theory based on an (approximate) Kohn-Sham reference state. Extensive benchmarks showed that rPT2 represents a considerable overall improvement over the standard RPA approach [1,4]. Recently we have also extended this concept to quasiparticle energy calculations. While the rSE-type correction to the irreducible self-energy does not exist, a SOSEX-type correction can be formulated rigorously using diagrammatic techniques. We show that such a correction can resolve the difficulties that the GW method encounters for the relative positions of quasiparticle excitations in certain molecules. All these developments and benchmark calculations were carried out in and with the FHI-aims code package [5,6]. Work has been done in collaboration with Patrick Rinke and Matthias Scheffler (FHI-Berlin), Joachim Paier (HU-Berlin), and Gustavo E. Scuseria (Rice Uni., Houston).

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