DFT-based exchange vertex for the correlation energy and excited states

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Résumé

In order to systematically go beyond the GW and random phase approximation (RPA) we introduce an approximate Hartree-Fock vertex based on the local exact-exchange (EXX) potential of time-dependent density functional theory (TDDFT). In certain limits this vertex is shown to exactly reproduce approximations from many body perturbation theory such as e.g. the SOSEX approximation [1]. It will be demonstrated that this vertex solves fundamental problems of the RPA such as the reliance of error cancellation and the underestimation of the van der Waals forces. The static approximation is for most cases sufficient to obtain good total energies but to a much lower computational cost. Excited states require, however, the inclusion of a dynamical discontinuity also captured by EXX TDDFT [2].

Hellgren, Colonna, de Gironcoli, Phys. Rev. B 98, 045117 (2018) [2] Hellgren Eur. Phys. J. B 9, 155 (2018)

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