

Beyond the Random Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations

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The random phase approximation (RPA) for the electron correlation energy, combined with the exact-exchange energy, represents the state-of-the-art exchange-correlation functional within density-functional theory (DFT). However, the standard RPA practice -- evaluating both the exact-exchange and the RPA correlation energy using local or semilocal Kohn-Sham (KS) orbitals -- leads to a systematic underbinding of molecules and solids. Here we demonstrate that this behavior is largely corrected by adding a "single excitation" (SE) contribution, so far not included in the standard RPA scheme. A similar improvement can also be achieved by replacing the non-self-consistent exact-exchange total energy by the corresponding self-consistent Hartree-Fock total energy, while retaining the RPA correlation energy evaluated using Kohn-Sham orbitals. Both schemes achieve chemical accuracy for a standard benchmark set of non-covalent intermolecular interactions.

Comments: 5 pages, 4 figures, and an additional supplementary material

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