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Improving the accuracy of ground-state correlation energies within a plane-wave basis set: The electron-hole exchange kernel[1] DARIO ROCCA, ANANT DIXIT, JANOS ANGYAN, University of Lorraine and CNRS, Nancy (France) — A new formalism was recently proposed to improve random phase approximation (RPA) correlation energies by including approximate exchange effects [1]. Within this framework, by keeping only the electron-hole contributions to the exchange kernel,two approximations can be obtained: An adiabatic connection analog of the second order screened exchange (AC-SOSEX) and an approximate electron-hole time-dependent Hartree-Fock (eh-TDHF). Here we show how this formalism is suitable for an efficient implementation within the plane-wave basis set. The response functions involved in the AC-SOSEX and eh-TDHF equations can indeed be compactly represented by an auxiliary basis set and the explicit calculation of unoccupied states can be avoided by using density functional perturbation theory techniques [2-3]. As shown by several applications to reaction energies and weakly bound dimers, the inclusion of the electron-hole kernel significantly improves the accuracy of ground-state correlation energies with respect to RPA and semi-local functionals.

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