Accurate orbital-dependent correlation and exchange-correlation potentials from non-iterative ab initio dft calculations

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An approximate non-iterative procedure [1] to obtain accurate correlation and exchange correlation potentials of Kohn-Sham (KS) density functional theory (DFT) is presented. By carrying out only one step of the correlated optimized effective potential (OEP) iterations following the standard iterative exchange-only OEP, one can recover accurate correlation potentials corresponding to the orbital-dependent second-order many-body perturbation theory [MBPT(2)] energy functional that are hardly discernible from those obtained by the more expensive, fully iterative procedure [2]. This new 'one-step' OEP-MBPT(2) algorithm reflects the non-iterative, perturbative algorithm of standard, canonical MBPT(2) of ab initio wave function theory, while it allows the correlation potentials to readjust and include the majority of the MBPT(2) correlation effect. It is also flexible in the treatment of exchange and the Hartree-Fock orbitals may be used in lieu of the exchange-only OEP orbitals, when the correlation or exchange-correlation potential is of interest.

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2. R. J. Bartlett , I. Grabowski, S. Hirata, S. Ivanov, J. Chem. Phys. **122**, 034104, (2005)