Optimized Effective Potential Method based on the Scaled–Opposite–Spin Second–Order Correlation

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The correlated optimized effective potential (OEP) method based on the spin resolved second-order correlation energy (SCS-MP2) is presented. The effect of scaling the same- and opposite- spin components is investigated in detail to determine optimal scaling coefficients for different properties in our new correlated OEP procedure. Special attention is dedicated in particular to the recently proposed scaled-opposite–spin OEP functional OEP2-SOS [1] which is the most advantageous from a computational point of view (*O(N^4)* scaling).

We find that for high accuracy, a careful (but costless), system dependent, selection of the scaling coefficient is required. Proposed new composite approach, named OEP2-SOSh, can yield high accuracy for many properties, being comparable with the most accurate OEP procedures previously reported in the literature but at substantially reduced computational effort.

The performance of the OEP2–SOS method is validated for benchmark atomic and molecular systems and we have found that all the OEP2-SOSh results largely outperform those from second–order Görling–Levy perturbation theory and, additionally, the new method can converge also when quasidegeneracy is present (e.g. in the Beryllium atom case).

The OEP2-SOSh approach is thus an accurate and efficient DFT method to supplement exact-exchange with an *ab initio* correlation and, importantly, with a small additional computational cost *O(N^4)* [2].

[1] I. Grabowski, E. Fabiano, F. Della Sala, *Phys. Rev. B* **87**, 075103 (2013).

[2] I. Grabowski, E. Fabiano, S. Śmiga, A. Buksztel, Andrew M. Teale, F. Della Sala, *J. Chem. Phys.* **141**, 024113 (2014)