ωB97M-3c: A small basis composite DFT method for the computation of large systems

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We introduce a new "-3c" composite density functional (DFT) method called ωB97M-3c. Almost 10 years after the release of the first 3c method (HF-3c [1]), we are circling back to the application of a small basis set for a substantial speed-up in computation time. The method is based on the popular ωB97M-V range-separated hybrid density functional [2] together with a fitted D4 dispersion correction [3] and an adaptive polarized minimal basis set, which has been specially optimized in molecular DFT calculations [4]. The savings in expensive polarisation functions must be compensated for the appropriate description of the anisotropic electron density distribution, which is why we employ the idea of atomic correction potentials (ACP) as proposed by DiLabio [5]. These one-electron potentials are very cheap to compute and can be readily used like regular effective core potentials (ECP). With this new method, we make the computation of supramolecular complexes and proteins up to 2000 atoms routinely possible at the range-separted hybrid DFT level.

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