We recently reported a new functional (SSB-D)\(^1\) that combines the best of the non-empirical PBE density functional with the best of the empirical OPBE density functional. It was constructed based on the performance of OPBE and PBE for spin states and S\(_N2\) reaction barriers and how these are affected by different regions of the reduced gradient expansion. A previous study\(^2\) already showed how by smoothly switching from OPBE to PBE at a predefined point P of the reduced density gradient s, we could determine which part of the exchange functional determines its behavior for the different interactions. These prior results allowed us to design a new exchange functional, which was subsequently fine-tuned to give the SSB-D functional. It showed the good results of OPBE for reaction barriers and spin-state energies, and combined it with the good (H-bond, π-stacking) results of PBE for weak interactions. The SSB-D functional includes Grimme’s dispersion correction,\(^3\) a portion of the KT1 functional\(^4\) and the simplified PBE (sPBEc) correlation functional.\(^5\)

The new functional was shown to give good performance for the spin ground-state of iron complexes, transition-metal ligand distances, and small deviations compared to CCSD(T) for S\(_N2\) barriers (2.7 kcal mol\(^{-1}\)), geometries (0.005 Å), H-bond distances (0.012 Å), and weak interactions (S\(_2\)2 set, 0.5 kcal mol\(^{-1}\)).\(^1\) Moreover, it works excellent\(^1\) for two difficult cases for DFT as put forward by Grimme.\(^6\) More recently, it was shown to further improve upon OPBE for NMR shieldings,\(^7\) give good results for magnetizabilities,\(^8\) and work well for the relative stability of water-hexamer isomers.\(^9\)

References