Implementation and performance of spin-component-scaled double-hybrid density functional theory

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An accurate description of electron correlation is the focus of the development of new quantum chemical theories. Spanning material sciences to biology, the effects of electron correlation are ubiquitous: packing of molecules into solids, self-assembly, molecular recognition, three-dimensional structures of proteins, interaction of substrates with surfaces, homogeneous/heterogenous catalysis, to name but a few.

Among the variety of quantum chemical methodologies, challenges of system size are easily reached, deeming Kohn-Sham density functional theory (DFT) as the theoretical method of choice. Despite the success of standard DFT over the last 20 years, it is widely known that most do not provide an adequate description of non-local dispersion forces. In this regards, dispersion-corrected spin-component-scaled double-hybrid (DSD) methods by Martin have demonstrated high accuracy for correlated chemical systems, but at the expense of large computational cost. As a result, they are limited to relatively small systems (i.e. ca. 100 electrons), warranting efforts to design methods that can bring the computational cost down.

In this talk the development, implementation and performance is reported for (i) a new variety of cost-effective double-hybrid DFT based on the resolution-of-identity (RI) approximation, and (ii) a new family of exchange-correlation functional, which ensures a rigorous contribution of correlation effects with limited empiricism.

With a tolerable error, RI-DSD-DFTs is shown to be suitable for large molecular systems and provide a considerable speed-up over the standard DSD-DFTs. Last, the accuracy of the newly designed family of functionals enable prediction within a targeted accuracy of 0.5 kcal/mol of either experimental values or CCSD(T)/CBS.