DSD-DFT – A DOUBLE HYBRID VARIATION

Among the many interesting talks was one by Sebastian Kozuch who reported on an interesting double hybrid methodology.[1,2] Working with Jan Martin, they defined a procedure that Kozuch referred to as "putting Stefan Grimme into a blender". They extend the double hybrid concept first suggested by Grimme that adds on an MP2-like correction functional. Kozuch and Martin substitute a spin-component scaled MP2 (SCS-MP2) model for the original MP2 correction. SCS-MP2 was also proposed by Grimme. Lastly, they add on a dispersion correction, an idea championed by Grimme too. The exchange-correlation term is defined as

$$E_{XC} = c_X E_X{}^{DFT} + (1 - c_x)E_x{}^{HF} + c_C E_C{}^{DFT} + c_O E_O{}^{MP2} + c_S E_S{}^{MP2} + s_6 E_D$$

where c_X is the coefficient for the amount of DFT exchange, c_C the amount of DFT correlation, $c_C$and c_S the amount of opposite- and same-spin MP2, and s_6 the amount of dispersion. They name this procedure **DSD-DFT** for **D**ispersion corrected, **S**pin-component scaled **D**ouble hybrid **DFT**.

In their second paper on this subject, they propose the use of the PBEP86 functional for the DFT components.[2] Benchmarking against a variety of standard databases, including kinetic data, thermodynamic data, along with inorganic and weakly interacting systems, this method delivers the lowest mean error among a small set of functionals. Kozuch reported at the conference on a number of other combinations and should have a publication soon suggesting an even better method. Importantly, these DSD-DFT computations can be run with most major quantum codes including *Orca*, *Molpro*, *Q-Chem* and *Gaussian* (with a series of IOP specifications).

While double hybrid methods don't have quite the performance capabilities of regular DFT, density fitting procedures offer the possibility of a significant reduction in computational time. These DSD-DFT methods are certainly worthy of fuller explorations.

Source: http://comporgchem.com/blog/?p=2444