Latest updates on a density-dependent dispersion correction

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Résumé

Since its seminal implementation in 2002 by Yang [1] and its popularization by Grimme in the mid-2000s,[2] the utilization of atom pairwise energy corrections to DFT is known to be of utmost importance and its development has represented a turn in the field of computational chemistry. In this context, the dDsC density-dependent atom pairwise dispersion correction [3,4] was formulated with the aim of improving the performance of standard density functional approximations for both typical intermolecular vdW situations as well as the more subtle intramolecular interactions. In dDsC, both the damping function and the dispersion coefficients depend on the charge distribution within a molecule.
Most of the dispersion correction schemes are generally applied in a post-SCF manner under the assumption that the influence on the density is weak. We have recently established the suitability of using the a posteriori dDsC correction through comparisons with the more computationally demanding self-consistent implementation.[5] We evaluated the impact of self-consistency on final converged density as well as on various chemical properties, such as energies, geometries or frequencies and ab initio molecular dynamics of real-life systems relevant to the field of organic electronics.

The applicability of the -dDsC scheme is currently being extended to the description of excited-states, which are also affected by dispersion forces. The current state the work will be presented as well.

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