

A Density-Based Basis Set Correction For Wave Function Theory

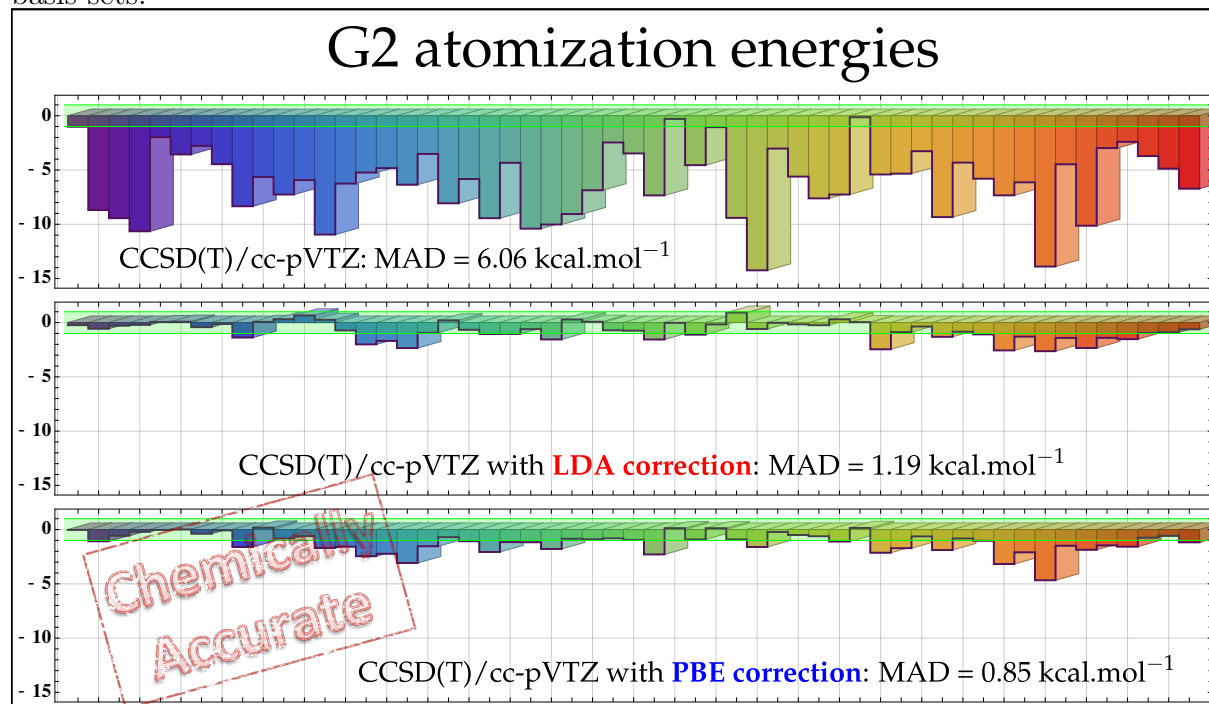
Roland Assaraf^a, Anthony Ferté^b, Emmanuel Giner^a, Pierre-François Loos^c,
Bathélemy Pradines^a, Andreas Savin^a, Anthony Scemama^c, Julien Toulouse^a.

^a: LCT, Sorbonne Université, ^b: LCPMR, Sorbonne Université,

^c: LCPQ, Université Paul Sabatier

emmanuel.giner@lct.jussieu.fr

We report the extension of a recently proposed [1] universal density-based basis set incompleteness correction that can be applied to any wave function method, together with its first numerical application on molecular systems. The present correction, which appropriately vanishes in the complete basis set (CBS) limit, relies on short-range correlation density functionals (with multi-determinant reference) from range-separated density-functional theory (RS-DFT) to estimate the basis set incompleteness error. Contrary to conventional RS-DFT schemes which require an *ad hoc* range-separation *parameter* μ , the key ingredient here is a range-separation *function* $\mu(\mathbf{r})$ which automatically adapts to the spatial non-homogeneity of the basis set incompleteness error. As illustrative examples, we show how this density-based correction allows us to obtain CCSD(T) atomization and correlation energies near the CBS limit for the G2 set of molecules with compact Gaussian basis sets.



References

1. Giner, E.; Pradines, B.; Fert, A.; Assaraf, R.; Savin, A.; Toulouse, J. Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. J. Chem. Phys. 2018, 149, 194301.