

# Basis-set correction based on density-functional theory

JULIEN TOULOUSE<sup>1</sup>

<sup>1</sup>*Laboratoire de Chimie Théorique, Sorbonne Université and CNRS, F-75005 Paris, France*

<sup>2</sup>*Institut Universitaire de France, F-75005 Paris, France*  
toulouse@lct.jussieu.fr

## ABSTRACT

One of the main limitations of standard electronic-structure wave-function computational methods is their slow convergence with respect to the one-electron basis set. This slow convergence is due to the description of short-range correlation in the wave function around the electron-electron cusp condition. The two main approaches for dealing with this problem are (1) extrapolating the results to the complete-basis-set (CBS) limit by using increasingly large basis sets, or (2) using explicitly correlated methods which incorporate in the wave-function a correlation factor reproducing the electron-electron cusp.

In this talk, I will present some of our efforts [1-8] on developing an alternative basis-set correction method based on density-functional theory. It consists in correcting the energy calculated by a correlated wave-function method with a given basis set by an adapted basis-set correction density functional incorporating the short-range correlation effects missing in the basis set, resulting in an accelerated convergence to the CBS limit. I will summarize the results obtained for various properties and systems.

## References

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