

The role of anisotropy in the evaluation of dispersion energy

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The growth of computational capacity over the recent decade has widened the application window of quantum chemical methods to systems of biochemical interest. In particular, DFT has proved to be a popular choice for this sort of applications. The expansive range of data thus produced has, however, not only brought forth the merits of the broad spectrum of available functionals, but also their flaws. A major drawback, for example, is their lack of consistency when it comes to describing dispersion interactions. The abundance of stacking interactions in biochemically active systems requires an immediate, accurate and not overly computationally demanding solution for this problem, if we are to continue applying DFT to these systems.

As one could expect, many suggestions have been made to correct DFT energies for dispersion interactions [1]. A great many of these methods rely on an additive correction scheme, which is rooted in a Perturbation Theory model for long-range interactions, originally proposed by Buckingham [2]. However, an important aspect of this model has been left out by these schemes, namely the anisotropic nature of dispersion. In this work, we propose a method to include anisotropy in a straightforward fashion and demonstrate its impact on a limited yet illustrative set of systems [3–5].

[1] See for example review on Stacking Interactions: *Phys. Chem. Chem. Phys.* **10**, 2581 (2010)

[2] A. D. Buckingham, *Adv. Chem. Phys.* **12**, 107 (1967)

[3] A. Olsaz, K. Vannomeslaeghe, A. Krishtal, T. Veszprémi, C. Van Alsenoy, P. Geerlings, *J. Chem. Phys.* **127**, 244105 (2007).

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[5] A. Krishtal, K. Vannomeslaeghe, D. Geldof, C. Van Alsenoy, P. Geerlings, *in preparation*.