Dispersion through the eyes of local orbital spaces

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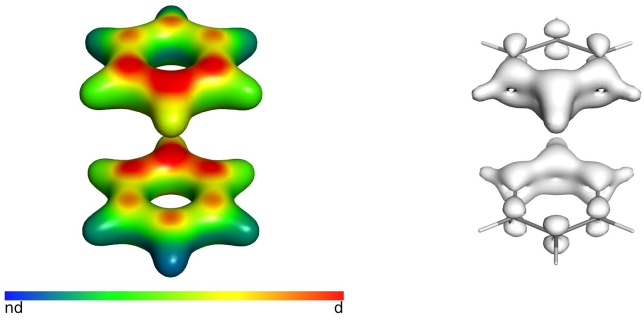
As the saying goes, „one look is worth a thousands words“. This principle can also be applied to the study of chemical phenomena. There are several visualization techniques in chemistry which are used to ease the interpretation of “raw data” (MEP, Orbitalmaps, and so on). Our work is inspired by the idea of MEP´s, which visualize electrostatic potentials of molecules by color coding a predefined electronic density. These images help to design novel compounds or to understand transition state stabilization effects.

London dispersion is a significant driving force for molecular aggregation, ubiquitous in molecular systems. Representations targeting such interactions are definitely warranted. Based on local orbital approaches we are able to restrict electron correlation to a certain region of a molecule.[1] The calculated correlation energy can then be split up in physically meaningful contributions, including dispersion effects.[2,3] These two properties of local correlation methods lead us to the proposal of a straightforward method to represent what could be described as a dispersion interaction density (DID) in molecules. This method will help us to obtain a better understanding of intra- and intermolecular interactions. Examples are given for the benzene dimer, a typical benchmark system for dispersion, as well as selected dispersion-driven aggregation phenomena.



[1] C. Hampel, H. J. Werner, *J Chem Phys*, **1996**, *104(16)*, 6286-6297.
[2] M. Schütz, G. Rauhut, H. J. Werner, *J Phys Chem A*, **1998**, *102(29)*, 5997-6003.
[3] M. Andrejić, R. A. Mata, *Phys Chem Chem Phys*, **2013**, *15(41)*, 18115-18122.