Conformational hierarchies of weakly bonded systems: Accuracy of dispersion corrected DFT

ALEXANDRE TKATCHENKO, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — It is well known that long-range dispersion interactions, important for stabilization of, e.g., molecular crystals, biomolecules and physisorption, are badly described by state-of-the-art xc functionals in DFT, but naturally included in post-HF methods or empirically in force field simulations. We have implemented a semi-empirical $C_6/R^6$ correction [1,2] in the numeric atom-centered orbital based code FHI-aims [3] and obtained correction parameters by fitting to a database of high quality ab initio calculations [2], improving on previous results due to the more accurate basis set (0.5 kcal/mol average error for binding energies using PBE+$C_6$). We assess the accuracy and impact of the correction on conformational energy hierarchies of (i) $\text{(H}_2\text{O)}_n$ clusters ($n=2-6$), (ii) Ala$_2$ and Ala$_4$, and (iii) infinite polyalanine conformers, comparing to published post-HF results for (i) and (ii). Even though the relative energies are not changed for small $\text{H}_2\text{O}$ clusters and Ala$_2$ compared to DFT-GGA, the impact of dispersion on the conformation hierarchy of larger systems is surprisingly large, reaching $\sim$1-4 kcal/mol for different polyalanine conformers. [1] S. Grimme, J. Comput. Chem. 25, 1463 (2004) [2] P. Jurecka et al., J. Comput. Chem. 28, 555 (2007) [3] V. Blum et al., FHI ab initio molecular simulations (FHI-aims) project.

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