

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

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) Ala₂ and Ala₄, and (iii) infinite polyaniline conformers, comparing to published post-HF results for (i) and (ii). Even though the relative energies are not changed for small H₂O clusters and Ala₂ 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 polyaniline 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.

Alexandre Tkatchenko
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Date submitted: 24 Nov 2007

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