



VAN DER WAALS INTERACTION IN BIOLOGY, CHEMISTRY AND PHYSICS

A TALK BY DR. ALEXANDRE TKATCHENKO,
A MEMBER OF THE FRITZ-HABER-INSTITUTE OF THE MAX-PLANCK-SOCIETY, THEORY DEPARTMENT IN BERLIN, GERMANY

DATE / TIME	17.10.2011, 4:00 p.m. (CEST)
LOCATION	Seminar Room 138C, Vienna University of Technology, "Freihaus"-building, 9th floor, "yellow" – Wiedner Hauptstraße 8-10, A-1040 Vienna, AUSTRIA)

Van der Waals (vdW) interactions are ubiquitous in nature, playing a major role in defining the structure, stability, and function for a wide variety of molecules and materials. Thus, the accurate description of vdW interactions is essential for improving our understanding of many biological, chemical, and (hard and soft) condensed matter.

We have developed an efficient method to obtain an accurate description of the long-range vdW interactions in terms of adding pairwise interatomic $C6[n]/R^6$ terms, where $C6[n]$ is a functional, calculated from ground-state molecular electron density [1].

Recently, we have extended this approach to the calculation of full non-additive many-body vdW energy [2].

We demonstrate that many-body effects play a significant role even for rather small molecules, becoming crucial for an accurate treatment of conformational energies in bio-molecules, and binding of molecular crystals. Our method achieves accuracy close to that of the "gold standard" of quantum chemistry, namely CCSD(T).

However, the computational cost of our method is negligible compared to the underlying DFT calculation, enabling calculations for thousands of atoms.

Examples to be discussed include (hard and soft) bulk crystals [3,4], organic/organic and organic/inorganic interfaces [5], and the unfolding dynamics of polypeptides [6].

In all case it is found that vdW interactions play a noticeable if not crucial role, not just for quantitative values but also for the qualitative behavior.

[1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. 102, 073005 (2009).

[2] A. Tkatchenko, R. A. DiStasio Jr., R. Car, and M. Scheffler, Phys. Rev. Lett., submitted.

[3] G. Zhang, A. Tkatchenko, J. Paier, H. Appel, and M. Scheffler, Phys. Rev. Lett., submitted.

[4] N. Marom et al., Cryst. Growth Des. (2011), <http://pubs.acs.org/doi/abs/10.1021/cg200409d>.

[5] N. Marom et al., Phys. Rev. Lett. 105, 046801 (2010).

[6] A. Tkatchenko, M. Rossi, V. Blum, J. Ireta, and M. Scheffler, Phys.

Rev. Lett. 106, 118102 (2011).