Organic-Inorganic Seminar Series

University of Oregon Department of Chemistry & Biochemistry

Prof. Peter R. Schreiner

University of Giessen, Germany

Tuesday, September 3, 2019

Klamath #331
2:00 pm Reception,
2:30 pm Seminar

London Dispersion Effects in Molecular Chemistry – Reconsidering Steric Effects[1]

The *Gecko* can walk up a glass window because of the adhesion in hydrophobic setae on its toes that convey van der Waals (vdW) interactions with the surface.[2] The attractive part of such vdW-interactions is an electron correlation effect referred to as *London dispersion*. Its role in the formation of condensed matter has been known since the work of van der Waals[3] and London[4] who related dispersion to polarizability. London dispersion has been underappreciated in molecular chemistry as a key element of structural stability, chemical reactivity, and catalysis. This negligence is due to the notion that dispersion is weak, which is only true for *one* pair of interacting atoms. For increasingly larger structures, the overall dispersion contribution grows rapidly and can amount to tens of kcal mol–1. This presentation shows selected examples that emphasize the importance of inter- and intramolecular dispersion for molecules consisting mostly of first row atoms. We note the synergy of experiment and theory that now has reached a stage where dispersion effects can be examined in fine detail. This forces us to re-consider our perception of steric hindrance and stereoelectronic effects, and even the transferability of chemical bond parameters from one molecule to another.

[1] London Dispersion in Molecular Chemistry-Reconsidering Steric Effects, J. P. Wagner, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2015**, *54*, 12274.

[2] Evidence for van der Waals adhesion in gecko setae, K. Autumn, M. Sitti, Y. A. Liang, A. M. Peattie, W. R. Hansen, S. Sponberg, T. W. Kenny, R. Fearing, J. N. Israelachvili, R. J. Full, *Proc. Natl. Acad. Sci.* **2002**, *99*, 12252.

[3] J. D. van der Waals, Leiden University (Leiden, The Netherlands), **1873**.

[4] Zur Theorie und Systematik der Molekularkräfte, F. London, *Z. Phys.* **1930**, *63*, 245.

Hosted by Michael Haley