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London Dispersion in Molecular Catalysis[1]

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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. The attractive part of vdW-interactions is an electron correlation effect referred to as *London dispersion*, an interaction that has been underappreciated in molecular chemistry as being key for structures, reactivity, and catalysis. This negligence is due to the notion that dispersion is considered weak, which is only true for pairs of interacting atoms. For 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.[2] 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, both in structural chemistry[3] and, in particular, in catalysis.[4] We will also shed light on the possibilities to use machine learning approaches to improve catalytic reactions[5] and highlight the importance of optimizing for differences in activation free energies (vs. enantiomeric excess).[6]

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