Van der Waals Interactions in Molecules, Solids, and Interfaces

Alexandre Tkatchenko

Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195, Berlin, Germany

Van der Waals (vdW) dispersion interactions are essential for determining the structure, stability, and function for a wide variety of molecules and materials [1]. In principle, ubiquitous vdW interactions can only be fully accounted for by high-level wave function methods or by Quantum Monte Carlo (QMC) techniques. In contrast, the correct long-range interaction tail, *e.g.*, for separated molecules, is absent from all popular local-density or gradient corrected exchange-correlation functionals of density-functional theory. To address this problem, we have developed an efficient method to obtain accurate vdW dispersion parameters from first principles [2], and recently extended it to determine the full long-range many-body vdW energy [3]. Our methods can be coupled to DFT calculations and even to quantum-chemical MP2 approach [4]. I will briefly discuss the theoretical underpinnings of the methods and their applications to different cases: intermolecular and intramolecular interactions [5,6], cohesion of solids [7], and the stability of organic/inorganic interfaces [8]. The performance of our approaches will be compared to both the non-local vdW-DF functional of Langreth and Lundqvist [9,10] and the exact-exchange plus correlation energy in the random-phase approximation (EX+cRPA) [11].

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