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Many-Body van der Waals Effects in Advanced Materials
ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, ANATOLE VON LILIENFELD, Argonne National Laboratory, ROBERT A. DISTASIO JR., Princeton University — Van der Waals (vdW) interactions are ubiquitous in molecules and condensed matter. These interactions are inherently quantum mechanical phenomena that arise from concerted correlations between many electrons within a given molecular system. Despite this fact, the vast majority of theoretical calculations include long-range vdW interactions based on a simple effective interatomic pairwise model. We introduce an efficient method that accurately describes the full long-range many-body vdW energy [1,2], and demonstrate that many-body contributions can significantly exceed the highly coveted "chemical accuracy". Cases studied include intermolecular binding energies, the conformational hierarchy of DNA structures [2], the geometry and stability of molecular crystals [1], and supramolecular host–guest complexes [3]. Our findings suggest that inclusion of the many-body vdW energy is essential for achieving chemical accuracy and therefore must be accounted for when studying advanced materials. [1] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012), [2] DiStasio, von Lilienfeld, Tkatchenko, PNAS (2012), [3] Tkatchenko, Alfe, Kim, JCTC (2012).

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