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Van der Waals interactions in complex materials: Beyond the pairwise approximation ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, ROBERT A. DISTASIO, JR., ROBERTO CAR, Princeton University, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Despite the well-known fact that van der Waals (vdW) interactions are many-body in nature and the polarizability is a non-local function, popular vdW-DF [1] and DFT+vdW [2] methods are based on (semi)-local approximations for the polarizability and only model the pairwise part of vdW interactions. Here we show how to go beyond the pairwise (semi)-local approximation to vdW interactions by coupling the recently developed TS scheme [2] with the Fluctuating-Coupled-Dipole Model (CFDM) [3]. The TS scheme provides parameter-free input atomic polarizability distributions and the CFDM allows to model both polarizing and depolarizing local fields, and captures the many-body nature of vdW interactions. Results are presented for small and medium-size molecules, as well as solids. We find that the many-body screening plays a major role in modifying the polarizability of large systems. Our results for vdW coefficients in semiconductor clusters and solids are in excellent agreement with TDDFT calculations. [1] M. Dion *et al.*, Phys. Rev. Lett., **92**, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009); [3] M. W. Cole *et al.*, Mol. Simul. **35**, 849 (2009).

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