Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Unified many-body approach to van der Waals interactions based on semi-local polarizability functional JAN HERMANN, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ALEXANDRE TKATCHENKO, University of Luxembourg — Electromagnetic coupling of charge fluctuations leads to van der Waals (vdW) attraction in systems ranging from metal nanoparticles to dielectric materials. In this regard, broadly applicable and accurate description of vdW interactions in complex materials is an elusive and unsolved puzzle. Many promising approaches model various subsets of this general problem, but are limited in scope by the underlying parametrization (atomic models), in accuracy due to missing many-body interactions (nonlocal density functionals), or in efficiency by working with virtual orbital space (e.g., random-phase approximation). Here, we present a unifying method that combines key elements from different theories and accurately describes vdW interactions in covalent, ionic, and metallic systems. In particular, we employ a semi-local polarizability functional of the electron density and its gradient to parametrize material response and its coupling within the many-body dispersion framework, and demonstrate the generality of the method on binding in molecular dimers and crystals, carbon-based nanomaterials, oxides, and salts, as well as on adsorption of molecules on metal surfaces. Our approach allows consistent modelling of a wide spectrum of materials as well as hybrid materials with mixed bond types.

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Date submitted: 09 Nov 2016 Electronic form version 1.4