Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Many-body dispersion meets non-local density functionals: A unified approach for van der Waals correlations JAN HERMANN, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft — It is an ongoing challenge to develop an efficient method for van der Waals (vdW) non-local correlation within DFT which would be both accurate and broadly applicable. Current approaches can be loosely divided into the fragment-based ones, two-point density functionals and methods based on the density-density response function. The fragment-based models utilize parameters not derivable from the electron density. Two-point approaches are explicit density functionals, but difficult to generalize to include many-body correlations. Here, we show that these seemingly contrasting approaches can be unified within a single framework based on the adiabatic-connection formalism in the random-phase approximation. We use a local response-function model from the VV09 functional[1] together with the many-body dispersion approach to create an atom-based model with no external parameters. We introduce a consistent correlation-functional-based coupling of the short- and long-range correlation energy. We show that this unification provides new insights into the different approaches, naturally deals with the partitioning of ionic and delocalized states and paves path towards self-consistent description of many-body vdW correlations.

[1]O. A. Vydrov, T. Van Voorhis, Phys. Rev. Lett. 103, 063004

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Date submitted: 13 Nov 2014 Electronic form version 1.4