

Abstract Submitted
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Correction to DFT Interaction Energies by an Empirical Dispersion Term Valid for a Range of Intermolecular Distances¹ CHRISTOS DELIGKARIS², JORGE H. RODRIGUEZ, Department of Physics, Purdue University — The computation of intermolecular interaction energies via commonly used density functionals is hindered by their inaccurate inclusion of medium and long range dispersion interactions. Computation of inter- and intra-molecule interaction energies as well as computational design of (bio)materials, requires a fairly accurate yet not overly expensive methodology. It is also desirable to compute intermolecular energies not only at their equilibrium (lowest energy) configurations but also over a range of distances. We present a method to compute intermolecular interaction energies by including an empirical correction for dispersion which is valid over a range of intermolecular distances. This is achieved by optimizing parameters that moderate the empirical correction by explicit comparison of density functional (GGA) energies with distance-dependent (DD) reference values obtained at the CCSD(T)/CBS limit. The resulting GGA-DD method yields interaction energies with an accuracy generally better than 1 kcal/mol for different types of noncovalent complexes, over a range of intermolecular distances and interaction strengths, relative to the expensive CCSD(T)/CBS standard

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²Present address: Department of Physics, Drury University

Jorge H. Rodriguez
Department of Physics, Purdue University

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