

Range-dependence of two-body intermolecular interactions and their energy components in molecular crystals

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Routinely assessing the stability of molecular crystals with high accuracy remains an open challenge in the computational sciences. The many-body expansion (MBE) decomposes computation of the crystal lattice energy (CLE) into an embarrassingly parallel collection of computations over molecular dimers, trimers, and so forth, making quantum chemistry techniques tractable for many crystals of small organic molecules. By examining the range-dependence of different types of energetic contributions to the CLE, we can glean qualitative understanding of solid-state intermolecular interactions as well as practical, exploitable reductions in the number of computations required for accurate energies. We assess the range-dependent character of two-body interactions of 24 small organic molecular crystals using the physically interpretable components from symmetry-adapted perturbation theory. We also examine correlations between the convergence rates of electrostatics and London dispersion terms with molecular dipole moments and polarizabilities, to provide guidance for estimating convergence rates in other molecular crystals.