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Many-Body Dispersion Interactions in Molecular Materials[1]

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In this work, we have developed an efficient method for obtaining an accurate theoretical description of van der Waals (vdW) interactions that includes both long-range Coulomb electrodynamic response screening effects as well as treatment of the many-body vdW energy to infinite order. This method goes beyond the standard C_6/R^6 pairwise additive approximation and can easily be coupled to a wide array of theoretical methods, ranging from classical force fields to higher-level quantum chemical calculations. To demonstrate the increasingly important role played by many-body vdW interactions in large, structurally complex molecular systems, we use this method to investigate several pertinent molecular properties, such as binding energies/affinities in gas-phase molecular dimers and supramolecular complexes, relative conformational energetics in small polypeptides, and thermodynamic stabilities among competing molecular crystal polymorphs.

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