

Understanding effects beyond pairwise additivity in dispersion interactions

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We categorize three distinct physical causes for the failure, under certain circumstances [1-9], of the concept of evaluating dispersion (van der Waals) energies by summing contributions from pairs of atoms. Although these causes frequently operate together, we give examples where just one of these three causes is the primary factor in non-additivity. We assess a number of theories and modeling approaches for their success in accounting for these three effects.

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