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Two and three-body interatomic dispersion energy contributions to binding in molecules and solids[1] ANATOLE VON LILIENFELD, Sandia National Laboratories, ALEXANDRE TKATCHENKO, Fritz-Haber-Institute, Max-Planck Society — Numerical estimates of the leading two and three body dispersion energy terms in van der Waals (vdW) interactions are presented for a broad variety of molecules and solids. The calculations employ London and Axilrod-Teller-Muto expressions damped at short interatomic distances, where the required interatomic dispersion energy coefficients, C6 and C9, are computed from first-principles. The investigated systems include the S22 database of non-covalent interactions, benzene and ice crystals, bilayer graphene, fullerene dimer, a poly peptide (Ala10), an intercalated drug-DNA model (Ellipticine-d(CG)2), 42 DNA base pairs, a protein (DHFR, 2616 atoms), double stranded DNA (1905 atoms), and molecular crystals from a crystal structure blind test. We find that the 2 and 3-body interatomic dispersion energies contribute significantly to binding and cohesive energies, for some systems they can reach up to 50% of experimental estimates of absolute binding. Our results suggest that interatomic 3-body dispersion potentials should be accounted for in atomistic simulations when modeling bulky molecules or condensed phase systems.

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