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Van der Waals Coefficients between Clusters or Fullerenes: A Simple but Accurate Model beyond the Atom-Pair Interaction Picture[1]
JOHN P. PERDEW, ADRIENN RUZSINSZKY, Department of Physics, Temple U., JIANMIN TAO, Department of Chemistry, U. of Pennsylvania — The van der Waals coefficients of all orders between two spherical objects may be computed from the dynamical multipole polarizabilities of the two objects via the Casimir-Polder formula. We present an analytic model [1] for the dynamical polarizabilities that is exact for a classical conducting sphere or spherical shell, exact in the zero- and nearly-exact in the high-frequency limits, and generally accurate. From this model, we compute the low-order van der Waals coefficients for a variety of atom pairs and pairs of clusters or carbon-based fullerenes. We find that the lowest-order coefficient C6 per atom pair may increase or decrease strongly with cluster size, signaling a failure of the simplest version of the atom-pair interaction picture. [1] J. Tao and J.P. Perdew, J. Chem. Phys. 141, 141101 (Commun.) (2014).

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