vdW-DF3: a more accurate van-der Waals density functional

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Within the vdW-DF framework, the switching function that controls the rollover from long- to short-wavelength plasmons in the non-local correlation term plays a major role in controlling the dispersion interaction at equilibrium separations [PRB 99, 195418, 2019]. We show that tuning this switching function together with the GGA enhancement factor of the exchange functional to a dataset of molecular dimers, we can provide accurate binding energies at equilibrium distances *and* far-separations at the same time, as well as improved lattice constants for layered systems and binding energies for adsorption systems such as benzene on coinage metals. Our new functional is comparable to m-GGA dispersion-corrected functionals, like SCAN+rVV10 and will be called vdW-DF3. This work was funded by NSF grant No. DMR1712425.