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Van der Waals Interactions in Density-Functional Theory.

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The application of conventional GGA, and meta-GGA, density functionals to van der Waals complexes is fraught with difficulties. Conventional functionals do not contain the physics of the dispersion interaction. To make matters worse, the exchange part alone can yield anything from severe over-binding to severe over-repulsion depending on the choice of functional. We rectify these problems by - adding a dispersion term with nonempirical C6, C8, and C10 dispersion coefficients (the Becke-Johnson dispersion model), and - selecting a GGA exchange functional (PW86, also nonempirical) that gives excellent agreement with exact Hartree-Fock repulsion curves. The result is a simple GGA+dispersion theory giving excellent noble-gas pair interaction energies for He through Kr with only two adjustable parameters in the dispersion cutoff.