A NONEMPIRICAL DENSITY FUNCTIONAL FOR COVALENT AND NONCOVALENT CHEMISTRY

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The exchange-hole dipole moment (XDM) dispersion model of Becke and Johnson combined with the PW86 exchange GGA and the PBE correlation GGA comprise a nonempirical (almost) density functional for covalent and noncovalent chemistry. Only two fit parameters are required in the dispersion damping part. We have fit these two parameters to a comprehensive test set of 65 intermolecular complexes spanning three orders of magnitude in binding energy strength (from the He dimer to the hydrogen bonded uracil dimer) with uniform quality over the entire set. The fit parameters are clearly universal and transferable. Our current efforts are concentrated on obtaining forces and optimized geometries from this functional.