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Predicting noncovalent interactions with nonlocal density functional theory JOE HOOPER, FRANK ZERILLI, Naval Surface Warfare Center, Indian Head Division, NIC ROMERO, BETSY RICE, Army Research Laboratory — We report calculations using a new, nonlocal density functional which explicitly treats long-range van der Waals correlation in a nonempirical way. This method is designed to model complex electron interactions such as dispersion, an area where traditional DFT methods often perform poorly. The functional performs quite well for certain types of noncovalent bonding, producing energies within a few percent of high-level CCSD(T) and MP2 methods at a fraction of the calculation time. The nonlocal correlation scales appropriately under compression, reducing to accurate GGA results at intramolecular length scales. Intermolecular distances are generally overpredicted compared to coupled-cluster results; this is largely an artifact of the GGA exchange component, and can be improved by incorporating exact exchange. This new method appears to be quite promising for treating complex organic molecular crystals at a range of pressures.

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