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Van der Waals Interactions in Density Functional Theory: Intermolecular Complexes FELIX KANNEMANN, AXEL BECKE, Dalhousie University — Conventional density functional theory (GGA and hybrid functionals) fails to account for dispersion interactions and is therefore not applicable to systems where van der Waals interactions play a dominant role, such as intermolecular complexes and biomolecules. The exchange-hole dipole moment (XDM) dispersion model of Becke and Johnson [A. D. Becke and E. R. Johnson, *J. Chem. Phys.* **127**, 154108 (2007)] corrects for this deficiency. We have previously shown that the XDM dispersion model can be combined with standard GGA functionals (PW86 for exchange and PBE for correlation) to give accurate binding energy curves for rare-gas diatomics [F. O. Kannemann and A. D. Becke, *J. Chem. Theory Comput.* **5**, 719 (2009)]. Here we present further tests of the GGA-XDM method using benchmark sets including hydrogen bonding, electrostatic, dispersion and stacking interactions, and systems ranging from rare-gas diatomics to biomolecular complexes.

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