

Abstract Submitted  
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**Chemical accuracy for the van der Waals density functional** JIRI KLIMES, London Centre for Nanotechnology and Department of Chemistry, University College London, DAVID BOWLER, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — Dispersion interactions are ubiquitous in nature and contribute to the binding in biomolecules and molecules on surfaces. However, due to their non-locality and small magnitude, they are difficult to describe accurately by electronic structure methods. For example, density functional theory (DFT) with standard functionals can give misleading results for systems where dispersion is important. Therefore, many schemes have been developed that try to improve the description of dispersion in DFT. Here we show that the accuracy of one scheme, the van der Waals density functional proposed by Dion et al. [Phys. Rev. Lett. 92, 246401 (2004)], can be dramatically improved through the judicious choice of exchange functional. This is demonstrated on various benchmark sets for weak interactions and for surface adsorption energies. Since at least similar accuracy for other important properties of matter such as bulk lattice constants is achieved compared to standard semi-local functionals, this opens a way to even more realistic simulations on the nanoscale.

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