

Abstract Submitted
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Van der Waals density functionals applied to solids JIRI KLIMES,
London Centre for Nanotechnology, University College London, DAVID BOWLER,
London Centre for Nanotechnology and Department of Physics and Astronomy,
University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology,
University College London — Dispersion interactions are ubiquitous in nature and contribute to the binding in biomolecules or to the adsorption of molecules on surfaces. However, due to their non-local nature they are difficult to describe accurately with electronic structure methods. It is now well established that standard density functional theory functionals give misleading results for systems where dispersion is important. The van der Waals density functional (vdW-DF) of Dion et al. [Dion et al., Phys. Rev. Lett. 92, 246401 (2004)] is one of several promising approaches for accounting for dispersion. We have shown that with an improved treatment of the exchange part it can offer much better than chemical accuracy for a range of weakly interacting molecular systems [Klimeš et al., J. Phys.: Cond. Matt. 22, 022201 (2010)]. Here we extend this work beyond the weakly bonded regime and report results for lattice constants of solids (metals, semiconductors, ionic solids) and geometries and atomization energies of molecules. This extensive and rigorous test of vdW-DF shows how to a large extent such properties are dependent on its underlying exchange functional. We use this new insight to discuss prospects for further improvement of the method.

Jiri Klimes
London Centre for Nanotechnology, University College London

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