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Improved Description of Soft Layered Materials with van der Waals Density Functional Theory GABRIELLA GRAZIANO, London Centre for Nanotechnology and Department of Chemistry, University College London, ISIS Facility, Rutherford Appleton Laboratory, JIRI KLIMES, London Centre for Nanotechnology and Department of Chemistry, University College London, FELIX FERNANDEZ-ALONSO, ISIS Facility, Rutherford Appleton Laboratory, Department of Physics, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — The accurate description of dispersion forces with approaches based on density functional theory has long been a coveted goal and is currently one of the most active areas of research in computational physics/chemistry. We have tested two new functionals, the optimized Becke88 van der Waals (optB88-vdW) and optimized PBE van der Waals (optPBE-vdW) [1, 2] to describe materials where van der Waals interactions dominate. Structural (bond length and interlayer distance) and energetic parameters (atomization and interlayer binding energies) of graphite and *hexagonal*-boron nitride have been calculated using these functionals and we show that our calculations are in very good agreement with experiments and higher level theoretical calculations. From these calculations it is possible to conclude that optB88- vdW and optPBE-vdW are promising functionals for the accurate description of systems held together mainly by dispersion forces.

[1] Klimeš *et al.*, J. Phys.: Condens. Matter **22**, 022201 (2010).
[2] Klimeš *et al.*, Phys. Rev. B **83**, 195131 (2011).

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