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Assessment of dispersion-corrected density functional approaches for extended systems WISSAM AL-SAIDI, University of Pittsburgh, Chemical and Petroleum Engineering, VAMSEE VOORA, KEN JORDAN, University of Pittsburgh, Department of Chemistry — Standard density functional (DFT) methods are known to fail in describing the long range van der Waals interactions, and currently, there is a great interest in incorporating dispersion corrections in density functionals. Recently, Tkatchenko and Scheffler introduced a new scheme where dispersion corrections are included by a summation of damped interatomic C_6/R^6 terms. However, contrary to the DFT-D2 approach of Grimme, the C_6 coefficients depend on the electron density through a Hirshfeld atom-in-a-molecule decomposition scheme. We have implemented the vdW-TS approach in VASP and applied it to the study of a series of prototype dispersion-dominated systems including layered materials, noble-gas solids and molecular crystals. Full optimization of all degrees of freedom is possible in our implementation because dispersion corrections are computed for the forces acting on the atoms, and also the stresses on the unitcell. Our results show that the vdW-TS method yield good structure, bulk moduli, and cohesive energies of weakly bonded systems in much better agreement with experiment than those obtained with standard DFT approaches.

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