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Dispersion interactions in Density Functional Theory LAMPROS ANDRINOPOULOS, NICHOLAS HINE, ARASH MOSTOFI, Imperial College London — Semilocal functionals in Density Functional Theory (DFT) achieve high accuracy simulating a wide range of systems, but miss the effect of dispersion (vdW) interactions, important in weakly bound systems. We study two different methods to include vdW in DFT: First, we investigate a recent approach [1] to evaluate the vdW contribution to the total energy using maximally-localized Wannier functions. Using a set of simple dimers, we show that it has a number of shortcomings that hamper its predictive power; we then develop and implement a series of improvements [2] and obtain binding energies and equilibrium geometries in closer agreement to quantum-chemical coupled-cluster calculations. Second, we implement the vdW-DF functional [3], using Soler's method [4], within ONETEP [5], a linear-scaling DFT code, and apply it to a range of systems. This method within a linear-scaling DFT code allows the simulation of weakly bound systems of larger scale, such as organic/inorganic interfaces, biological systems and implicit solvation models. [1] P. Silvestrelli, JPC A 113, 5224 (2009). [2] L. Andrinopoulos et al, JCP 135, 154105 (2011). [3] M. Dion et al, PRL 92, 246401 (2004). [4] G. Román-Pérez, J.M. Soler, PRL 103, 096102 (2009). [5] C. Skylaris et al, JCP 122, 084119 (2005).

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