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Application of vdW-DF Methods to Hydrogen Adsorptions and an Organic Ferroelectric¹

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In recent years, several schemes have been proposed to include van der Waals (vdW) interactions into the framework of density functional theory (DFT). These offer the potential to extend the scope and usefulness of DFT, allowing applications to an entire new class of sparse materials. For finite systems, we validated our non-empirical van der Waals density functionals (vdW-DFs) with respect to very accurate quantum chemical calculations of the potential energy curves (PECs) for small molecular duplexes [1]. For extended systems, however, typical tests focus on comparisons with a few accessible observations, such as binding energy and bond length [1]. In this talk, we present a third approach in which full PECs from accurate experiments are used for the assessment of vdW methods for extended systems [2]. We calculate the PECs of the H₂ molecule and light atoms on the (100), (110), and (111) surfaces of Cu. The gas-surface-scattering experiments provide the rich data bank that covers results for the whole shape of the physisorption potentials. We also present an application of vdW-DF2 to an organic ferroelectric, phenazine-chloranilic acid [3]. In spite of extensive experimental efforts to characterize this rare organic material, the origin of the long-range order is unclear and even the ground state structure is not completely determined yet. We study its structure, energetics, ferroelectric properties, structural instability, and the proton-transfer process in it in comparison with PBE results and experiments wherever possible.

[1] K. Lee, E. Murray, L. Kong, B. I. Lundqvist, and D. C. Langreth, *Phys. Rev. B* **82**, 081101 (2010).

[2] K. Lee, A. K. Kelkkanen, K. Berland, S. Andersson, D. C. Langreth, E. Schröder, B. I. Lundqvist, and P. Hyldgaard, *Phys. Rev. B* **84**, 193408 (2011).

[3] K. Lee, B. Kolb, T. Thonhauser, D. C. Langreth, and D. Vanderbilt, *in preparation*.

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