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Using quantum Monte Carlo for the interaction of water with carbon and BN based substrates and assessing exchange-correlation functionals YASMINE AL-HAMDANI, Department of Chemistry, University College London and Thomas Young Centre, DARIO ALFE, Department of Earth Sciences, University College London and Thomas Young Centre, O. ANATOLE VON LILIENFELD, Argonne National Laboratories, Argonne, and Institute of Physical Chemistry, Chemistry Department, University of Basel, ANGELOS MICHAELIDES, Department of Physics, University College London and Thomas Young Centre — The interaction of water with the pure surfaces, graphene and hexagonal boron nitride (h- BN), has received a lot of attention because of interesting phenomena exhibited by these systems and their promising potential applications in clean energy, water purification, hydrogen storage, and bio-sensing. BN doped graphene can also now be made, opening the way to carefully designed hybrid materials. However, much of the fundamental mechanisms regarding the interaction between these surfaces and water is still not well understood. We use quantum Monte Carlo to establish accurate benchmarks for water on a number of carbonaceous and BN based substrates, including 2-dimensional periodic surfaces, for which van der Waals interactions play a key role. The benchmarks are then used to test and understand various exchange-correlation functionals in density functional theory. We find that the physisorption of water is poorly described in terms of the adsorption site and the interaction energy by a range of different classes of exchange- correlation functionals, including some that account for dispersion, and we show where these inadequacies might come from.

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