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Interrogating the strength of the bond between salt and water: a combined DFT and MP2 study BO LI, ANGELOS MICHAELIDES, MATTHIAS SCHEFFLER, Fritz-Harber-Institut der Max-Plank-Gesellschaft —
The interaction of water with salt (NaCl) is of widespread importance and of considerable general interest. Although numerous theoretical studies have been reported [1], none has provided a convincingly reliable estimate of the strength of the bond between water and a flat NaCl surface, such as NaCl(001). Moreover, the computed adsorption energies predicted by DFT vary from 0.2-0.7 eV/H_2O depending on the choice of exchange-correlation functional [2]. Here, we address this issue through an extensive series of periodic Hartree-Fock and post-Hartree Fock [Møller-Plesset perturbation (MP2) and coupled cluster (CCSD(T))] calculations. Periodic Hartree-Fock calculations have been performed for H_2O molecules adsorbed on NaCl slabs, and by evaluating the local dependence of the correlation contribution to the adsorption energy with respect to cluster size, we obtain accurate MP2 and CCSD(T) estimates of the H_2O adsorption energy on NaCl(001). Our computed adsorption energy, which is around 0.6 eV/H_2O, comes close to the experimental value [3] and is at the upper end of the range predicted by DFT. [1] A. Verdaguer, G. M. Sacha, H. Bluhm, and M. Salmeron, Chem. Rev. 106, 1478 (2006). [2] B. Li, A. Michaelides, and M. Scheffler, in preparation. [3] L. W. Bruch, A. Glebov, J. P. Toennies, and H. Weiss, J. Chem. Phys. 103, 5109 (1995).

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