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Formation of 1D adsorbed water structures on CaO(001) XUNHUA ZHAO, SASWATA BHATTACHARYA, LUCA M. GHIRINGHELLI, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — Understanding the interaction of water with oxide surfaces is of fundamental importance for basic and engineering sciences. Recently, a spontaneous formation of one-dimensional (1D) adsorbed water structures have been observed on CaO(001) [1]. Interestingly, at other alkaline earth metal oxides, in particular MgO(001) and SrO(001), such structures have not been found experimentally. We calculate the relative stability of adsorbed water structures on the three oxides using density-functional theory combined with the *ab initio* atomistic thermodynamics. Low-energy structures at different coverages are obtained with a first-principles genetic algorithm. Finite-temperature vibrational spectra are calculated using *ab initio* molecular dynamics. We find a range of (T, p) conditions where 1D structures are thermodynamically stable on CaO(001). The orientation and vibrational spectra of the 1D structures are in agreement with the experiments [1]. The formation of the 1D structures is found to be actuated by a symmetry breaking in the adsorbed water tetramer, as well as by a balance between water-water and water-substrate interactions, determined by the lattice constant of the oxide.—[1] X. Shao, Y. Fujimori, M. Sterrer, H.-J. Freund, and N. Nilius, to be published.

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