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Sub-Monolayer Water Adsorption on Alkaline Earth Metal Oxide Surfaces: A First-Principles Study XUNHUA ZHAO, SASWATA BHATTACHARYA, LUCA M. GHIRINGHELLI, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — In the present work, we predict atomic structures of adsorbed complexes that should appear on alkaline earth metal oxide (001) terraces in thermodynamic equilibrium with water and oxygen gases. Density-functional theory with the hybrid exchange-correlation functional HSE06 combined with the self-consistent many-body dispersion approach [1] is used to calculate total energies. The choice of this functional is validated by renormalized second-order perturbation theory [2]. An unbiased search for global minima of H_xO_y adsorption is performed using first-principles genetic algorithm for periodic models. x and y as a function of temperature and pressure are determined using *ab initio* atomistic thermodynamics. We find a range of H_2O chemical potentials where one-dimensional adsorbed water structures are thermodynamically stable on CaO(001). On MgO(001) and SrO(001), such structures are not found. The formation of the one-dimensional structures is explained by the balance between water-water and water-surface interactions.

[1] A. Tkatchenko, R. A. DiStasio, Jr., R. Car and M. Scheffler, Phys. Rev. Lett. **108**, 236402 (2012);
[2] X. Ren, P. Rinke, G. E. Scuseria, M. Scheffler, Phys. Rev. B **88**, 035120, (2013).

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