Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

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.


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Date submitted: 15 Nov 2013    Electronic form version 1.4