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Water adsorption on oxygen covered Ru(0001) surfaces SABINE MAIER[1], Lawrence Berkeley National Laboratory, PEPA CABRERA-SANFELIX, Donostia International Physics Center, San Sebastian, Spain, INGEBORG STASS, Lawrence Berkeley National Laboratory, DANIEL SANCHEZ-PORTAL, ANDRES ARNAU, Donostia International Physics Center, San Sebastian, Spain, MIQUEL SALMERON, Lawrence Berkeley National Laboratory — We present a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study of the adsorption of water on a Ru(0001) surface covered with half monolayer of oxygen. The adsorption of water causes a shift of half of the oxygen atoms in the O(2x1) structure from hcp sites to fcc sites, creating a honeycomb structure where water molecules bind strongly to the exposed Ru atoms [1]. The energy cost of reconstructing the oxygen overlayer is more than compensated by the larger adsorption energy of water on the newly exposed Ru atoms. STM images reveal a (4x2) superstructure due to alternating orientations of the water molecules. Heating to 185 K results in the complete desorption of the water layer, leaving behind the oxygen honeycomb structure, which is metastable relative to the original (2x1). This stable structure is not recovered until after heating to temperatures close to 260K.

[1] S. Maier et al. Phys. Rev. B 82, 075421 (2010).

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