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Nano-ice on Boron Nitride Nanomesh: accessing proton disorder HAIFENG MA, THOMAS BRUGGER, SIMON BERNER, YUN DING, MAR-CELLA IANNUZZI, JUERG HUTTER, JUERG OSTERWALDER, THOMAS GREBER — The adsorption behavior of water and the concomitant proton arrangement have been investigated on a hexagonal boron nitride nanomesh (h-BN/Rh(111) template using variable temperature scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT) calculations. Below 52 K, two distinct phases self-assemble within the 3.2 nm unit cell of the nanomesh that consists of "holes" and "wires." In the 2 nm holes, an ordered and dense phase of nano-ice crystals with about 40 molecules is found. They form a hexagonal bilayer structure and obey the ice rules. On the 1-nm-wide wires, a low-density two-dimensional (2D) gas phase forms, which is characterized by contrast modulations and streaky noise in the STM images. Furthermore, by means of tunneling barrier height spectroscopy (dI/dz) measurements and the simulation of the electrostatic potential above the nano-ice clusters, the individual hydrogen positions in nano-ice clusters have been revealed. Based on the agreement between experiment and theory, the results give new insight into the self-assembly process of water and also indicate that the boron nitride nanomesh template is a good candidate to build artificial structures with new functionalities.<sup>1</sup>

<sup>1</sup>Boron Nitride Nanomesh: A template for Nano-ice, ArXiv: 090875.

Haifeng Ma Institute of Physics, University of Zurich

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