Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

The structure of water on the (101bar0) surface of ZnO OLGA DULUB, Department of Physics, Tulane University, New Orleans, LA 70118, BERND MEYER, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany, ULRIKE DIEBOLD, Department of Physics, Tulane University, New Orleans, LA 70118 — The room temperature adsorption of water on the ZnO(101bar0) surface has been investigated with scanning tunneling microscopy (STM), low energy electron diffraction (LEED), low energy He^+ ion scattering spectroscopy (LEIS), and DFT calculations. At low water coverage (0.5 - 1 Langmuir (L)), formation of 2D water clusters with a (2 x 1) periodicity was observed on the well-ordered surface. A mixed state with half the water molecules dissociated and the other half molecularly adsorbed was found to be the most favorable configuration of the water monolayer. At surface saturation, reached at exposures of $\sim$3 L, domains with (2x1) periodicity, as well as domains of (1x1) structure of the similar height, were observed. The (1x1) domain is a minority structure (about 10% of the total water overlayer), localized in the vicinity of surface defects. The influence of defects on water adsorption was also examined on the slightly sputtered surface. In this case, no (2x1) superstructure was observed on the surface by LEED, although LEIS confirmed the presence of water species.

Olga Dulub
Department of Physics, Tulane University, New Orleans, LA 70118

Date submitted: 01 Dec 2004 Electronic form version 1.4