The Interaction of Water with the Oxygen-Terminated, Polar Surface of ZnO

M. Kunat, St. Gil Girol, U. Burghaus,† and Ch. Wöll*

Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany

Received: May 30, 2003; In Final Form: September 5, 2003

The adsorption of H_2O on the oxygen-terminated polar surface of ZnO, ZnO(000-1), has been studied by He atom scattering (HAS), low-energy electron diffraction (LEED), adsorption probability measurements, He atom reflectivity measurements as a function of exposure and surface temperature (He atom thermal desorption measurements, "He-TDS"), and X-ray photoelectron spectroscopy (XPS). The clean O−ZnO(000-1) surface is characterized by an ordered (1 × 3) oxygen vacancy structure which converts to a (1 × 1) hydrogen (OH)-terminated structure upon dissociative H_2O adsorption, even at adsorption temperatures as low as T_S = 200 K. The formation of the OH-species is accompanied by the formation of a shoulder in the XPS O 1s line. A detailed investigation of the coverage dependence of the H_2O adsorption probability indicates the presence of a distinct precursor state. The initial trapping probability is $S_0 = 0.8 \pm 0.1$. The most probable microscopic adsorption mechanism which is consistent with the obtained data is a trapping of the molecules in a precursor state and a subsequent dissociation at O vacancy sites, yielding two OH-species per dissociated H_2O molecule on the surface. The binding energy of the OH-species amounts to ∼130 kJ/mol as determined from He-TDS curves.