THE JOURNAL OF PHYSICAL CHEMISTRY A

ARTICLE

pubs.acs.org/JPCA

dx.doi.org/10.1021/jp200146v | J. Phys. Chem. A 2011, 115, 7180

Combined Theoretical and Experimental Study on the Adsorption of Methanol on the ZnO(10$\bar{1}$0) Surface

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ABSTRACT: The structure, dynamics, and energetics of methanol adlayers on the nonpolar ZnO(10$\bar{1}$0) surface have been studied by He-atom diffraction (HAS), high-resolution electron energy loss spectroscopy (HREELS), thermal desorption spectroscopy (TDS), and density functional calculations. The experimental and theoretical data consistently show that at temperatures below 357 K methanol forms an ordered adlayer with a (2×1) periodicity and a coverage of one monolayer in which half of the methanol molecules are dissociated. The ordering of the methanol molecules is governed by repulsive interactions between the methyl groups of the methanol molecules. This repulsive interaction is also responsible for the formation of a second, low-density phase at higher temperatures with half monolayer coverage of undissociated methanol which is stable up to 440 K.