Probing the Surface Heterogeneity of Polycrystalline Zinc Oxide by Static Adsorption Microcalorimetry. 2. The Adsorption of Carbon Monoxide

Xinyu Xia, Jennifer Strunk, Raoul Naumann d'Alnoncourt, Wilma Busser, Lamma Khodeir, and Martin Muhler*

Laboratory of Industrial Chemistry, Ruhr-University Bochum, D-44780 Bochum, Germany

Received: January 25, 2008; Revised Manuscript Received: May 6, 2008

The adsorption of CO on polycrystalline ZnO powder samples was investigated as a function of the pretreatment by applying static adsorption microcalorimetry and temperature-programmed desorption (TPD). Mainly weak adsorption sites were found to be present on the exposed ZnO surfaces but also a minor amount of highly active sites (>0.1 μmol/m^2). On the majority sites, the adsorption of CO is weak, as reflected by the isotherms and the TPD profiles, with a maximum heat of adsorption of about 40 kJ/mol, which decreases with increasing coverage and also with an increasing amount of surface hydroxyl groups. The standard adsorption entropy is derived to amount to -102 J mol^{-1} K^{-1}. These weak adsorption sites are hardly influenced by the pretreatment in flowing oxygen, hydrogen, or helium. On the highly active sites, as probed by small doses of CO in the calorimetric experiments, different exothermic (>100 kJ/mol) and endothermic surface reactions occur in addition to CO adsorption, depending on the gas atmosphere applied during the pretreatment. These results clearly indicate that the small amount of highly active sites accounts for the catalytic properties of ZnO.