The surface chemistry of ZnO nanoparticles applied as heterogeneous catalysts in methanol synthesis

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Abstract

Zinc oxide has a variety of applications in catalysis both as support and as active phase for hydrogenation or dehydrogenation reactions. This review provides an overview of the surface chemistry of ZnO nanoparticles concerning the interaction with small molecules such as CO, CO_2, H_2, H_2O, and CH_3OH, which are relevant for the catalytic synthesis of methanol and the water gas shift reaction. These interactions were studied by combining surface-sensitive methods such as infrared spectroscopy, temperature-programmed desorption, and adsorption calorimetry. A thorough understanding of the processes occurring on the different exposed facets of the ZnO particles in an atmosphere of reactive gases was achieved based on the comparison with results obtained in ultra-high vacuum with single-crystalline surfaces, i. e., under well-defined conditions, and by using first-principles calculations.