

The interaction of water with a model Cu/ZnO catalyst

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The Cu/ZnO catalyst is widely used for the synthesis of methanol and for the production of hydrogen via the water-gas shift reaction. Despite the widespread use of this catalyst, there are still many open questions, especially concerning the role of ZnO in the above-mentioned catalytic reactions. It is believed that the high activity and selectivity of the Cu/ZnO catalyst is

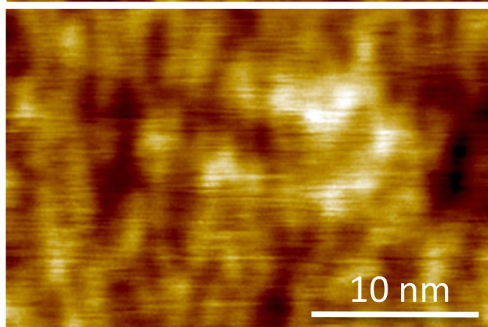
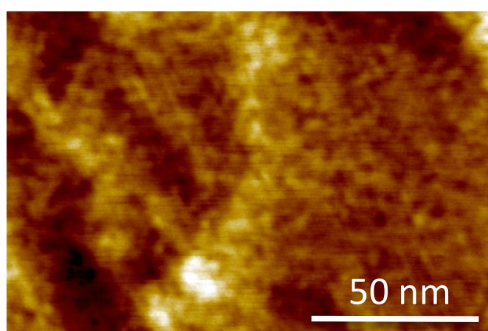


Figure 1: Non-contact AFM images of ZnO(0001)-Zn surface exposed to water vapor at partial pressure of 23 mbar and post-annealed in UHV at 620 K.

largely due to the copper and zinc synergy [1]. By far, the role of ZnO in the catalyst is much more important than that of a support only, having a big impact on the structural, electronic and catalytic properties of the supported Cu nanoparticles (NPs). Therefore, it is very important to study the effect of the ZnO substrate on the properties of the supported Cu NPs. In order to improve our understanding about the processes in real industrial Cu/ZnO catalysts it is also crucial to study model Cu/ZnO catalysts under realistic conditions [2], particularly in the presence of water vapor at high partial pressure.

In the present study we have investigated the interaction of water vapor with polar ZnO surfaces [3] in the wide range of partial pressure from 1×10^{-9} mbar up to 23 mbar. The properties of the water vapor exposed polar ZnO surfaces as well as the sintering of the Cu NPs on these surfaces have been investigated by a combination of nc-AFM, STM, XPS and TPD techniques. It has been found that the ZnO polar surfaces undergo significant structural transformations after the exposure to water vapor. In particular, we have observed a long-range

semi-periodic ordering transformation (with the periodicity of 5.7 nm) after the exposure of Zn-terminated surface to water vapor with the subsequent post-annealing at 620 K (Fig. 1). These surface structural transformations may influence the growth mode and sintering of the supported Cu NPs and have implications on their catalytic properties, which will be discussed in detail.

References

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