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"The microscopic view on the thermally induced interaction of Cu with ZnO(0001)-Zn"

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The Cu/ZnO-based catalysts are used for the synthesis of methanol and water-gas shift reaction on an industrial scale. In spite of their widespread use a number of questions regarding the nature of the active sites, deactivation mechanisms, and the role of Cu-Zn alloying in these catalysts remain unresolved.

In the present investigation, we studied thermally-induced Cu-ZnO interaction using a model Cu/ZnO system where 0.2 ML of Cu was deposited on a UHV-prepared ZnO(0001)-Zn polar surface. The model system has been subjected to cyclic thermal annealing up to 650 K and characterized in-situ by a combination of Scanning Tunneling Microscopy (STM), X-ray Photoelectron Spectroscopy (XPS), and Thermal Desorption Spectroscopy (TDS). The experimental evidence suggests that the thermally activated Cu in-diffusion leads to the pronounced redistribution of the surface and subsurface defects and leads to the complete wetting of ZnO(0001) by Cu. A more detailed discussion about the interplay between the wetting of the polar ZnO(0001)-Zn surface and Cu in-diffusion based on the experimental findings will be presented.