

Structural and Chemical Study of CuZnO a Model Catalyst in Oxidising and Reducing Environment

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Energy storage is one of science's most pressing concerns of late. How do we store energy produced in excess by renewable sources for later use? Chemical storage in the form of methanol offers one such solution, owing to being a high energy density material that is liquid at room temperature[1]. Currently methanol is, almost exclusively, produced from a syngas mixture of hydrogen and carbon dioxide and/or monoxide under heterogeneous catalytic conditions. The industrial standard is a composite of Cu and ZnO nanoparticles, however although it is well documented that the synergy between the metal/metaloxide increases the catalytic properties of the material[2] the atomistic description of this phenomenon is still uncertain. Currently there are two opposing models, both of which have gained notable recognition. One model claims that the interface between the ZnO and the Cu surface has a strong influence on the synergy between the two materials, enhancing the catalytic properties[3,4]. The other model, which favours the formation of a highly active Cu_{1-x}Zn_x alloy, only arising during reaction conditions where ZnO partially reduces, incorporating the free Zn into the Cu surface[5]. The need for *in situ* measurements to determine the active phase has prompted our study.

Beginning with a bare Cu(111) crystal a model catalyst was created by low level deposition of Zn onto the surface in ultrahigh vacuum (UHV). Synchrotron XPS was performed at ASTRID to ascertain the chemical composition of the surface. Previous work has shown that the core level peaks for both Cu and Zn shift to a higher binding energy upon forming an alloy[6] and as such the 3s and 3p peaks of both metals were tracked throughout the course of the experiment. Exposing to a series of oxidative (H₂O, CO₂) and reductive (UHV, H₂) anneals revealed the reversibility of the transition between the alloy and ZnO island states. The formation of these ZnO islands on the Cu surface was monitored with both STM and spectroscopically by tracking the 3d peaks of Zn, which merge and shift to higher binding energy upon oxidation[7]. Off angles studies showed the penetration depth of the oxide within the CuZn alloy during island formation.

References:

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