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Defect Analysis of High Performance Catalysts: What makes Cu active in Methanol Synthesis?

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$Cu/ZnO/(Al_2O_3)$ composites are active catalysts in methanol synthesis, while bulk-Cu is not. This difference cannot only be attributed to a larger specific Cu surface area, but the presence of ZnO and the promotion by Al_2O_3 seem to be essential and affect the micro- and defect structure of Cu. A comprehensive analysis is difficult due to the nanostructured nature of the catalyst. Establishment of structure-activity-relationships, thus, requires model samples, which are well-defined, but still show a catalytic performance high enough to be measured and compared under relevant conditions. A series of such functional models was prepared from various single phase precursor compounds [1] like $(Cu,Zn)_2(OH)_2CO_3$, $(Cu,Zn)_5(OH)_6(CO_3)_2$, $(Cu,Zn)_{0.67}Al_{0.33}(OH)_2(CO_3)_{0.17}$, $(Cu,Zn)_2(OH)_3HCO_2$ or amorphous phases. Several complementary methods, including neutron diffraction, were used for structural analysis of the resulting catalysts and revealed trends, e.g. in stacking fault density of Cu, which can be related to the intrinsic catalytic activities [2, 3].

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