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The Cu/ZnO(0001) Surface under Oxidative and Reducing Conditions: A First-principles Study KATAWUT CHUASIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, School of Physics, BERNARD DELLEY, Paul Scherrer Institut, Villigen Switzerland, CATHERINE STAMPFL, University of Sydney, School of Physics — The Cu/ZnO(0001) surface is widely used as a catalyst for the production of H_2-gas from methanol and is thus of considerable relevance to the emergent hydrogen economy. A key to the further development of this catalyst system is a detailed atomic-scale understanding of the relation between surface structure and function versus environmental conditions such as copper content and state of surface oxidation. Towards this goal, we use density functional theory within the framework of ab initio atomistic thermodynamics to conduct a detailed survey of conceivable surface structures under variety of Cu exposures. This produces a surface phase diagram that reveals several distinct regimes of surface reconstruction under oxygen-rich and poor conditions. We correlate our findings with experimental studies, including recent scanning tunneling microscopy results by Dulub et al [1].
References:
[1] O. Dulub, M. Batzill, and U. Diebold, Topics in Catalysis 36 (2005) 65.

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