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First principles study of Cu on Zn(0001): Resolution of the ($\sqrt{3} \times \sqrt{3}$)-R30° – Cu/ZnO(0001) surface phase KATAWUT CHUASIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHY STAMPFL, University of Sydney — The Cu/ZnO system is a well known catalyst for methanol synthesis as well as hydrogen production from methanol by the reverse water gas-shift reaction. Despite many years of effort to clarify the characterization and the synergetic mechanisms between Cu and ZnO, there still exists considerable controversy such as the active phase of this combination catalyst. Recently, a ($\sqrt{3} \times \sqrt{3}$)-R30° phase has been reported on the Cu/ZnO(0001) surface (Dulub *et. al.*, Topics in Catalysis, **36**, 65 (2005)). This reconstruction appears in the LEED pattern after annealing the pre-deposited Cu-clusters on the ZnO(0001) surface at 350 °C in a 10^{-6} mbar O_2 environment for 10 minutes. In this work, we perform first-principles total- energy calculations within the framework of *ab initio* atomistic thermodynamics to investigate the atomic geometry and relative stability of this structure. We have extensively surveyed many possible atomic geometries, from which we are able to we propose the atomic structure of this ($\sqrt{3} \times \sqrt{3}$)-R30° phase. To provide an overall understanding of this system, we also construct a two-dimensional phase diagram as a function of the Cu and O chemical potential, thus displaying the most stable surface structures.

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