

Abstract Submitted
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**Morphology of alloy catalysts in an oxidizing environment:
Structure-sensitivity of ethylene epoxidation over Ag-Cu particles** SIMONE PICCININ, CATHERINE STAMPFL, University of Sydney, MATTHIAS SCHEFFLER, Fritz-Haber-Institut — Ag-Cu alloys have been proposed as catalysts for ethylene epoxidation due to their superior selectivity compared to pure silver, the predominant catalyst for this reaction [1]. By means of density-functional theory and atomistic thermodynamics, we study the surface structure and morphology of Ag-Cu particles in thermodynamic equilibrium with an oxygen atmosphere. Contrary to the common assumption of the formation of a 2D surface alloy, we find that at temperatures and pressures of interest for practical applications the particles can display a variety of structures, including thin Cu-surface-oxides in coexistence with clean Ag. At variance with pure Ag in UHV, we find that under reactive conditions the (111) facet is not dominant. We identify different reaction pathways that will compete and/or synergetically interplay in the catalysis. In general, the reaction mechanism is structure-dependent and often the reaction does not proceed through the formation of stable intermediates, in contrast to clean Ag and the 2D alloy. Analyzing the competing reactions, we discuss how the addition of Cu improves the selectivity and stress the overall importance of accounting for the effect of ambient conditions. [1] S. Linic et al. *J. Catal.* 224, 148 (2004)

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