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Re-visiting the O/Cu(111) system - When metastable surface oxides could become an issue! ALOYSIUS SOON, NORINA A. RICHTER, CHANG-EUN KIM, Department of Materials Science and Engineering, Yonsei University, CATHERINE STAMPFL, School of Physics, University of Sydney — Surface oxidation processes are crucial for the functionality of Cu-based catalytic systems used for many industrially important chemical reactions. Based on recent findings in XPS and LEED experiments, we assess the stability and population of the experimentally proposed "8"-structure, a new surface oxide phase, on the Cu(111) surface. Using density-functional theory calculations in combination with *ab initio* atomistic thermodynamics and Boltzmann statistical mechanics, we find that the proposed oxide superstructure is indeed metastable and that the population of the "8"-structure is competitive with the known "29" and "44" oxide film structures on Cu(111). We show that the configuration of O and Cu atoms in the first and second layers of the "8"-structure closely resembles the arrangement of atoms in the first two layers of $Cu_2O(110)$, where the atoms in the "8"-structure are more constricted. $Cu_2O(110)$ has been suggested in the literature as the most active low index facet for reactions such as water splitting under light illumination. If the "8"-structure were to form during a catalytic process, it is therefore likely to be one of the reactive phases.

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