

Abstract Submitted
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Formation and stability of surface oxides and oxide surfaces of the O/Cu system: First-principles investigations ALOYSIUS SOON, MIRA TODOROVA, School of Physics, the University of Sydney, Australia, BERNARD DELLEY, Paul-Scherrer-Institut (PSI), CATHERINE STAMPFL, School of Physics, the University of Sydney, Australia — Copper-based catalysts are important for several industrial reactions, e.g., the low-temperature water-gas-shift reaction and for methanol oxidation reactions. Despite this, very little is presently known about the surface structure, about the atomic and molecular processes involved and the associated reaction pathways. As a first step towards a microscopic understanding, we use density-functional theory to investigate chemisorption of oxygen on Cu(111), and the stability of surface oxides and oxide surfaces. Surface oxide structures are found to be energetically favoured over chemisorbed oxygen even at coverages as low as $\frac{1}{16}$ ML. Taking into account the pressure and temperature through the framework of *ab initio* thermodynamics [1,2] however, shows that for the conditions relevant to technical catalysis, bulk oxide structures are the appropriate ones to consider. Our results are compared to the behavior of other O/transition-metal systems.

[1] K. Reuter, C. Stampfl and M. Scheffler, in Handbook of Materials Modeling, Volume 1, Fundamental Models and Methods, Sidney Yip (Ed).

[2] C. Stampfl, Catal. Today 105, 17 (2005).

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