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Characterizing the copper-based catalyst for the oxygen-assisted water-gas shift reaction at a sub-nano scale. ALOYSIUS SOON, MIRA TODOROVA, CATHERINE STAMPFL, School of Physics, the University of Sydney, Australia, BERNARD DELLEY, Paul-Scherrer-Institut (PSI) — To obtain insight into the structure and surface stoichiometry of copper-based catalysts in commercially important chemical reactions such as the oxygen-assisted water-gas shift reaction, we perform density-functional theory calculations to investigate the stability of oxide surfaces. Taking into account the pressure and temperature through the framework of *ab initio* thermodynamics [1,2] our earlier investigation found that for the conditions relevant to technical catalysis, the bulk oxide is energetically most favourable. Using the same technique, we examine the relative stability of low-index copper oxide surfaces [3], and identify two low energy surface structures that are most stable under such conditions which could be catalytically relevant. These oxide surface structures are found to be non-stoichiometric (with surface defects) and exhibit a metallic character.

[1] A. Soon, M. Todorova, B. Delley and C. Stampfl, *Phys. Rev. B* **73**, 165424 (2006)
[2] C. Stampfl, *Catal. Today* **105**, 17 (2005).
[3] A. Soon, M. Todorova, B. Delley and C. Stampfl, submitted to *Phys. Rev. B.*

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