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When Seeing is Not Believing: The case of O on Ag(111) ANGELOS MICHAELIDES, KARSTEN REUTER, MATTHIAS SCHEFFLER, Fritz-Haber-Institut — A number of recent studies indicate that, under the oxygen rich conditions of oxidation catalysis, some transition metal catalysts are covered in thin oxide overlayers. Moreover, it has been suggested that such 'surface-oxide' layers are catalytically active, and that this role is not performed by the pure metal surfaces as was traditionally assumed. This contemporary picture can be traced back to Ag catalysis, where over 30 years ago it was suggested that the top layer of Ag(111) reconstructed to an epitaxial Ag_2O overlayer upon exposure to oxygen. Extensive experimental work, including scanning tunnelling microscopy studies in which the oxide was apparently imaged with atomic resolution [1], and density functional theory calculations [2,3] largely confirmed this interpretation. However, subsequent density functional theory results, presented here, augmented with thermodynamic calculations, indicate that previous conclusions are significantly incomplete and that the structure of this original surface-oxide must be reconsidered. [1] C. Carlisle *et al.*, Phys. Rev. Lett. **84**, 3899 (2000). [2] A. Michaelides, M.-L. Bocquet, P. Sautet, A. Alavi, and D.A. King, Chem. Phys. Lett. **367**, 344 (2003). [3] W.X. Li, C. Stampfl, and M. Scheffler, Phys. Rev. Lett. **90**, 256102 (2003).

Angelos Michaelides
Fritz-Haber-Institut

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