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The relevance of sub-nanometer thin oxide films in the CO oxidation on Pd(100) JUTTA ROGAL, KARSTEN REUTER, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany — There is an increasing awareness that oxides may form at the surface of transition metal (TM) catalysts under the oxygen-rich environmental conditions of oxidation catalysis. What is, however, still an open question is, if the metal is fully oxidized or if only nanometer thin surface oxide films are formed and which of these different phases are crucial for the catalytic activity of the material. On Pd(100) the oxidation of the surface proceeds through several different stages, including a $(\sqrt{5} \times \sqrt{5})R27^{\mathrm{O}}$ surface oxide structure. The stability of this surface oxide and other oxidation states of Pd(100) in an O_2 gas phase up to ambient pressures was recently analyzed in a combined experimental and theoretical study [1]. We now use density-functional theory and atomistic thermodynamics to also account for the other reactant in CO oxidation catalysis by considering the surface structure and composition in a *constrained* equilibrium with an O_2 and CO gas phase. Under gas phase conditions typical of technological CO oxidation the surface oxide results then as the most stable structure. However, this may be significantly affected by the on-going reactions, which continuously drive the system away from equilibrium. Such kinetic effects under steady-state conditions are discussed on the basis of preliminary kinetic Monte Carlo simulations. [1] E. Lundgren *et al.*, Phys. Rev. Lett. **92**, 046101 (2004)

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