

## Transition metal surfaces under oxygen-rich conditions (abstract only)

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# Transition metal surfaces under oxygen-rich conditions

Nicola Seriani

Computational Materials Physics, Vienna University, Vienna, Austria

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## Abstract

The catalytic oxidation activity of transition metal particles in automobile catalysts is influenced by the superficial oxide phases which form under oxygen-rich reaction conditions. Here we study the thermodynamic stability of ultrathin oxide films on low-index surfaces of transition metals by means of first-principles atomistic thermodynamics calculations based on density functional theory. On Pd(111) a surface oxide with Pd<sub>5</sub>O<sub>4</sub> stoichiometry is stable, which does not correspond to any bulk structure. At the same time, a variety of metastable structures form. On Pd(100) a PdO(101) trilayer is the stable surface oxide. All structures display two-oxygen-coordinated and four-oxygen-coordinated Pd atoms, the difference lying in the spatial arrangement of these basic structural elements. On rhodium surfaces a Rh oxide trilayer forms that corresponds to a bulk oxide structure. On the Pt(111) surface the most stable superficial oxide phase is found to be a thin layer of  $\alpha$ -PtO<sub>2</sub>, which appears not to be reactive to either methane dissociation or carbon monoxide adsorption. On Pt(100) an  $\alpha$ -PtO<sub>2</sub> layer is thermodynamically the most stable, even if Pt<sub>3</sub>O<sub>4</sub> films could grow in a coherent and stress-free manner. Bulk Pt<sub>3</sub>O<sub>4</sub> is found to be thermodynamically stable in a region around 900 K at atmospheric pressure. The enthalpy barrier for the adsorption of CO molecules on oxygen atoms of this surface is as low as 0.34 eV, and desorption of CO<sub>2</sub> is observed in molecular dynamics simulations to occur without any appreciable energy barrier.

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