

# Catalytic oxidation at surfaces: insight from first-principles statistical mechanics

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## Abstract

Accomplishing a first-principles modeling of heterogeneous catalysis that allows for a quantitative description of the catalytic activity over a wide range of relevant environmental conditions (e.g. elevated temperatures and ambient pressures) poses an enormous challenge. Detailed insight into the elementary processes taking place on a microscopic level can nowadays often be obtained by employing *ab initio* electronic structure theory calculations. The statistical interplay between these processes, however, which is decisive for the functionality of a material only evolves in the mesoscopic to macroscopic regime.

Here we apply a multiscale modeling approach to achieve a predictive modeling of macroscopic material properties on the basis of a microscopic understanding. Within this approach we use density-functional theory to accurately describe the elementary processes in the microscopic regime and we then combine these results with concepts from thermodynamics and statistical mechanics to obtain an appropriate linking to the mesoscopic and macroscopic regimes.

Employing this approach to the field of heterogeneous catalysis we investigate CO oxidation over the Pd(100) surface as an example, particularly focusing on the relevance of the surrounding gas phase as well as the reaction kinetics on the structure and composition of the catalyst surface.