

Catalytic oxidation at surfaces: insight from first-principles statistical mechanics (abstract only)

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2008 J. Phys.: Condens. Matter 20 064240

(<http://iopscience.iop.org/0953-8984/20/6/064240>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 29/05/2010 at 10:33

Please note that [terms and conditions apply](#).

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

Jutta Rogal

Fritz-Haber-Institut der MPG, Berlin, Germany

Received 17 December 2007

Published 24 January 2008

Online at stacks.iop.org/JPhysCM/20/064240

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.