

UniCat Colloquium

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Lecturer: **Prof. Dr. Axel Groß**, Institute of Theoretical Chemistry, University of Ulm

Title: **Modeling reactions in heterogeneous and electrocatalysis on metal surfaces from first principles**

Abstract: In this talk, I will discuss concepts and processes in heterogeneous and electrocatalysis based on first-principles electronic structure calculations. Complex reaction mechanisms in the technologically relevant C1 chemistry on surfaces can nowadays be identified from first principles, as will be demonstrated using methanol oxidation and synthesis on copper substrates as an example. To tailor the catalytic properties of the substrate, the composition and/or structure of bimetallic compounds can be changed, leading to so-called ligand, geometric and ensemble effects. It will be shown that bimetallic surface can in fact exhibit properties that are beyond those of the single compounds.

Finally the study of catalytic reactions at the solid-liquid interface will be addressed which is relevant for electrochemistry and electrocatalysis. Such studies still represent a considerable challenge since in addition to the complexity of the solid-liquid interface the presence of external fields and/or varying electrode potentials have to be taken into account.

Date: **Wednesday, 17 February 2010**

Time: **5:15 pm - around 6:45 pm**

Location: **TU Berlin
Institute of Chemistry, Building C
Straße des 17. Juni 115, 10623 Berlin
room C 243**

Organiser: Prof. Dr. Peter Saalfrank (Uni Potsdam)

Coffee and tea will be served thirty minutes prior to the lecture start. Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat