

## UniCat – BasCat Colloquium

Thursday, 1<sup>st</sup> December 2016 16:00-18:30 h

at

Gerhard-Ertl Center, Villa Bell, Seminar room BEL 301, Marchstr. 6, 10587 Berlin

**16:00** Dr. Franziska Heß, Justus-Liebig-Universität Gießen, Institute of Physical Chemistry:

***Atomic-scale insight into the surface science of heterogeneously catalyzed reactions from a combined experimental and theoretical approach***

Modern multiscale modeling makes it possible to bridge time and length scales in unprecedented ways. For heterogeneous catalysis such multiscale modeling can be achieved by coupling electronic structure calculations to kinetic simulations, which can again be coupled to continuum models to reach the reactor scale.

The Kinetic Monte Carlo (KMC) method is able to model surface reactions with high accuracy because it takes into account individual sites of the catalyst and can thus describe heterogeneity on the surface induced by defects or spatial correlation. However, to reach this accuracy, KMC requires a considerable number of parameters to properly describe the interactions between the adsorbed reactants. The combination of DFT and KMC is considered as quite promising because DFT offers a reasonable compromise between computational cost and accuracy, both of which are required to determine the parameters necessary for KMC simulations. This talk will explore the possibilities and limits of current atomic-scale simulations of surface reactions using the CO and HCl oxidation reactions over RuO<sub>2</sub>(110) as examples.

**17:00** Coffee / Tea

**17:30** Dr. Sandra Luber, University of Zurich, Graduate School of Chemical and Molecular Sciences:

***Computational investigation and design of bio-inspired catalysts for water splitting***

Solar energy is an inexhaustible energy source for a sustainable solution to the global energy consumption. The storage of large amounts of light energy can be achieved by conversion into chemical energy saved in biomass. Artificial photosynthesis permits the splitting of water into molecular hydrogen and oxygen and is therefore a very promising strategy to meet the increasing worldwide need for clean energy. This requires the development of high-performance water reduction and water oxidation catalysts (WOCs) where the latter is currently the main bottleneck for efficient photocatalytic water splitting. Very recently, the first Co(II)-based cubane WOCs have been presented, which excel through unprecedented structural analogies to the oxygen-evolving complex of nature's photosystem II. We study their properties and catalytic behavior by means of density functional theory (DFT) in combination with DFT-based molecular dynamics. In this talk, I will give an overview about our recent efforts for the study of these biomimetic WOCs and the development of sophisticated methods for condensed phase catalysis. Moreover, structurally simpler Co-based WOCs are investigated in detail, which allows the derivation of important guidelines for smart design of novel efficient WOCs.