

# Special UniCat Seminar

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Lecturer: **Dr. Felix Studt**, Stanford University, SUNCAT Center for Interface Science and Catalysis SLAC National Accelerator Laboratory Menlo Park, USA

Title: **Density functional theory in heterogeneous catalysis: Applications in syngas conversion to higher alcohols**

Abstract: Density functional theory (DFT) calculations can be a powerful tool for the understanding of reaction mechanisms in heterogeneous catalysis. Moreover, improvements in the accuracy of DFT calculations and the understanding of trends from one metal surface to the next allows for the screening for new catalyst leads. Here, the conversion of syngas to higher alcohols is used as an example to show how one can use DFT calculations in heterogeneous catalysis.

Syngas, a mixture of CO, CO<sub>2</sub> and H<sub>2</sub>, can be converted to bulk chemicals like methanol and transportation fuels like higher hydrocarbons or higher alcohols. Typically syngas is produced by steam reforming of natural gas, but other feedstocks like biomass can be used as well, representing an interesting route to sustainable fuels.

Based on scaling relations of adsorption energies and transition-states on transition-metal surfaces it was possible to describe both, methane, methanol and higher alcohol formation in terms of the carbon and oxygen binding energy of the transition-metal in question. The combination of these scaling relations with a microkinetic model leads to activity volcanos for methane, methanol and ethanol formation as a function of these descriptors. Having established volcanos for the activity of these three competing reactions allows for the determination of their selectivity. Importantly, to map out the activity and selectivity as a function of only two parameters allows for fast computational screening for new leads of improved catalysts for syngas conversion processes.

Date: **Monday, July 8<sup>th</sup>, 2013 at 2:30 pm**

Location: **TU Berlin, Department of Chemistry  
Straße des 17. Juni 115, 10623 Berlin  
Building C, Lecture Hall C 264**

Organizer: **Prof. Matthias Driess (TUB)**

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