

# Special UniCat Colloquium

Wednesday, October 18, 2017 at 4:15 PM

**ATTENTION: earlier starting time**

## Dr. Martin Oschatz

MPI für Kolloid- und Grenzflächenforschung

### *Influence of Pore Structure and Surface Chemistry of Nanostructured Carbons on their Properties as Support Materials in Heterogeneous Catalysis*

The active species of heterogeneous catalysts (most often metal or metal oxide nanoparticles) are frequently dispersed on nanostructured inorganic materials with high specific surface area (the so-called “supports”) in order to minimize particle growth and agglomeration. Nanoporous carbonaceous materials, that is, carbons with pore sizes in the range of only a few nm, are widely applied for that purpose due to their high thermal and chemical stability as well as their tunable pore structure and surface properties. The high surface area of porous carbon maximizes the dispersion of metallic nanoparticles to achieve high activity and stability resulting from small diameters and large distances, respectively. The pore surface of carbon materials can be more or less rich of heteroatoms (e.g., in form of carboxylic groups, phenols, or amines) which will influence the strength of interaction of the active species and the reactants with the support.

The combined effects of the pore structure and the surface properties of carbonaceous support materials will be presented on two heterogeneously catalyzed reactions. On the one hand, iron-based nanoparticles are supported on a series of nanocarbons and their properties in the Fischer-Tropsch synthesis of lower olefins are evaluated as a function of the support porosity and heteroatom content under industrially relevant conditions (CO hydrogenation at 340°C, 10 bar, and a H<sub>2</sub>/CO ratio of 2). On the other hand, the conversion of glucose to gluconic acid with carbon-supported gold nanoparticles is applied as a model reaction for oxidation in aqueous solution. In both cases, the pore structure and surface properties of the supports are having a drastic influence on both the structures and the performance of the resulting catalysts.

## Dr. Bartholomäus Pieber

MPI für Kolloid- und Grenzflächenforschung

### *Continuous Heterogeneous Photoredox Catalysis in Serial-Micro Batch Reactors*

Continuous processing can improve challenging chemical reactions ranging from transformations using gaseous reagents or harsh conditions to photochemistry. Solid materials are typically utilized in packed bed reactors, best suited for heterogeneous catalysis of thermal reactions. Solid reagents, heterogeneous photocatalysts and leaching catalysts complicate continuous flow chemistry and are better suited for batch processes. Continuous systems based on the generation of serial micro-batch reactors (SMBRs) overcome these limitations by combining the strengths of batch chemistry with respect to the use of solids with the advantages of flow synthesis.

The versatility of the SMBR approach is illustrated for visible-light photoredox catalysis using a modified graphitic carbon nitride as a heterogeneous catalyst. The SMBR technology provides a flexible solution for the continuous utilization of solid reagents and catalysts that previously were deemed incompatible with flow. Employing this protocol, common, homogeneous photoredox catalysts can be replaced by a reusable organic polymer for visible-light mediated reactions, here exemplified with different fluorination protocols.

## Dr. Sebastian Matera

Freie Universität Berlin

### *First principles based multiscale modeling of heterogeneous catalysis: error propagation and coupling to the continuum*

First principles based multiscale modeling approaches have gained a lot of popularity in the context of catalysis during the last decade. This popularity originates from the possibility to get an unbiased atomistic reaction mechanism and to derive a predictive kinetic model, e.g. a so-called first principles kinetic Monte Carlo model. An important drawback of the first principles based approach is the necessarily limited accuracy of the employed electronic structure simulation, usually some flavour of Density Functional Theory, for the reaction barriers and adsorption energies.

I will present our recently developed approaches to quantify the propagation of these errors to the kinetic model's output. For the investigated problems, we find that the induced uncertainty of the model predictions might be sizeable, but also that usually only a small subset of all possible errors are responsible for this. These approaches can serve as tools for a hierarchical model construction, where only the most important reaction parameters are determined with highly accurate, but resource-intensive methods. But also computational material screening approaches might profit from our strategies, which can be used to identify suitable descriptors of the catalytic performance.

In the second part of my talk, I will present how first principles kinetic Monte Carlo models can be coupled to continuum level solvers such as Computational Fluid Dynamics for treating macroscopic mass, momentum and energy transport. We have used this approach to shine light into the question of the active phase (site) of a single crystal model catalyst, but also extended the strategy for the modeling of powder catalysts. Finally, I will present our first attempts on coupling of atomistic kinetic models with electromagnetic wave simulations and address the impact of nanoscale field heterogeneities on the photocatalysis on nano-particles.

I will finalize with discussing open issues and possible extensions for problems targeted by UniSysCat.

**Wednesday, October 18, 2017 at 4:15 PM**

**ATTENTION: earlier starting time**

TU Berlin, Institute of Chemistry  
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

**Prof. Dr. Arne Thomas (TUB) and  
Prof. Dr. Peter Hildebrandt (TUB)**  
Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!  
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - [www.unicat.tu-berlin.de](http://www.unicat.tu-berlin.de)