

Understanding and Designing Heterogeneous Catalysts from First Principles

Dr. Andreas Heyden (Associate Professor of Chemical Engineering, University of South Carolina (Currently on Sabbatical at the Fukui Institute for Fundamental Chemistry, Kyoto))



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No. 205 in 5th building of the Faculty of Science, Hokkaido University
(理学部5号館205号室)

In the last ~15 years computational catalysis started to significantly impact catalysis research by providing a new tool for testing experimental hypotheses and by screening a large number of materials in silico. In this seminar, I will present two case studies illustrating the strengths and challenges of computational catalysis. In the first part of this seminar, I will illustrate recent progress in understanding heterogeneous catalysis at the three-phase boundary of a gas-phase, a reducible oxide surface, and a noble metal cluster. In particular, I intend to illustrate the specific role of the three-phase boundary in determining the activity and selectivity of TiO_2 supported Pt catalysts for the water-gas shift ($\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$) reaction. We find that for heterogeneously catalyzed reactions with more than one key surface intermediate, multiphase catalysts have a significant advantage over conventional monophasic catalysts since each phase can potentially be adjusted independently to activate a key reaction step. In the second part of this seminar, I present a computational case study for the determination of activity and selectivity descriptors for the hydrodeoxygenation of organic acids to alkanes and olefins on transition metal surfaces relevant for the conversion of triglycerides to green diesel and hydrotreating (upgrading) of bio-oils obtained from pyrolysis of lignocellulosic biomass. I will highlight the importance of solvent effects in catalysis and present recent tools for including solvation effects in computational studies.

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Professor Andreas Heyden is an associate Professor of Department of Chemical Engineering, University of South Carolina. He is now doing a theoretical approach to catalysts especially biomass catalysts. He got PhD in Chemical Engineering in Hamburg University of Technology in 2005. He was Assistant Professor August 2007 and was promoted to Associate Professor in August 2014 in University of South Carolina. He is now on his Sabbatical at Fukui Center in Kyoto University.