

## Frontiers in Catalysis Science and Engineering Seminar Series

### Biomass Transformations Over Transition Metals – Unraveling Complex Reaction Networks by Computational Catalysis



#### Biography

Prof. Rösch's research focuses on the development and application of quantum chemistry methods to explain a wide range of chemical and physical questions. His work involves investigating complex systems, such as metal clusters, adsorbates on metal and oxide surfaces and in zeolite cavities, heterogeneous and homogeneous catalytic reaction systems and actinide complexation and sorption.

He has been a professor at TUM's chemistry department since 1980. Prof. Rösch has been Director of TUM's Catalysis Research Center since its foundation in 2008.

#### Prof. Notker Rösch

Technische Universität München and  
A\*STAR Institute of High Performance Computing

**Wednesday, March 9, 2016**

**12:30pm**

**EMSL Auditorium**

We discuss catalytic reaction networks related to aqueous phase processing of biomass derived poly-ols, modeled computationally by mono-ols. In particular, we address reforming and hydrodeoxygenation reactions of propanol on Pt [1-3] and we compare these results to the situation on the more oxophilic transition metal Ru [4]. In addition, we discuss the reaction network of lignin-derived aromatic oxygenates over transition metals on the example of the hydrodeoxygenation of guaiacol over Ru [5,6].

- [1] D. Basaran, A. Genest, N. Rösch, *J. Catal.* **287** (2012) 411.
- [2] D. Basaran, A. Genest, J.A. Lercher, N. Rösch, *ACS Catal.* **3** (2013) 1730.
- [3] C.-c. Chiu, A. Genest, N. Rösch, *ChemCatChem* **5** (2013) 3299.
- [4] C.-c. Chiu, A. Genest, N. Rösch, *Top. Catal.* **56** (2013) 874.
- [5] C.-c. Chiu, A. Genest, A. Borgna, N. Rösch, *ACS Catalysis* **4** (2014) 4178.
- [6] C.-c. Chiu, A. Genest, A. Borgna, N. Rösch, *PhysChemChemPhys* **17** (2015) 15324.

Host: Bob Weber, 372-4748 - Admin POC: Beth Randle, 375-2021