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Unifying Concepts in Catalysis

Vortragsankündigung

- im Rahmen des UniCat-Kolloquiums -

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Es spricht: **Prof. Dr. Alexis T. Bell**
Department of Chemical Engineering
University of California

Zeit: **Freitag, 6. März 2009 14:00 Uhr**

Ort: **TU Berlin**
Institut für Chemie, Franz-Fischer-Bau,
Straße des 17. Juni 124
10623 Berlin
Raum TC 014

Thema: **Controlling the Activity and Selectivity of Catalytically Active Sites - Insights Gained from Experiments and Theory**

Abstract: An ongoing challenge in the field of catalysis is identifying what is meant by an active site and learning how to control its activity and selectivity. While it is well recognized that the composition and structure of a heterogeneous catalyst affect its performance, nonuniformities in site composition and structure make it difficult to define with much precision what is meant by an active site. Similar problems can arise with homogeneous catalysts, if the precursor complex forms a variety of species under reaction conditions. To address this limitation, several groups have recently turned to the preparation of well-defined, single-site catalysts. Such sites can be prepared by grafting molecular precursors onto a support, by supporting well-defined structures such as heteropolyacids, by exchange of metal cations into zeolites. Homogeneous catalysts consisting of a metal cation surrounded by a well-defined set of ligands can also be viewed as single-site catalysts. The advantage of single-site catalysts is that all of the sites are virtually the same, which greatly facilitates characterization of the structure of the site both before and during catalysis, since most spectroscopic techniques used for catalyst characterization provide an average view over all sites. The relative lack of structural diversity also enable the use of theoretical methods to validate the structural interpretations based on experimental methods, as well as the validity of elementary reactions proposed on the basis of experimental studies of reaction mechanism and kinetics. Studies of catalysis over single sites will be illustrated for a number of systems, including N_2O decomposition on iron-oxo centers in Fe-ZSM-5, the oxidation of methanol on isolated vanadate species supported on silica and titania, the oxidative carbonylation of methanol on Cu(I) cations present in Cu-ZSM-5, and the oxidative carbonylation of toluene to toluic acid catalyzed by Rh(III) complexes.

Organisator: Prof. Dr. Schomäcker (TUB)

Gäste sind herzlich willkommen!

Prof. Dr. Matthias Drieß
Sprecher des Exzellenz-Clusters UniCat