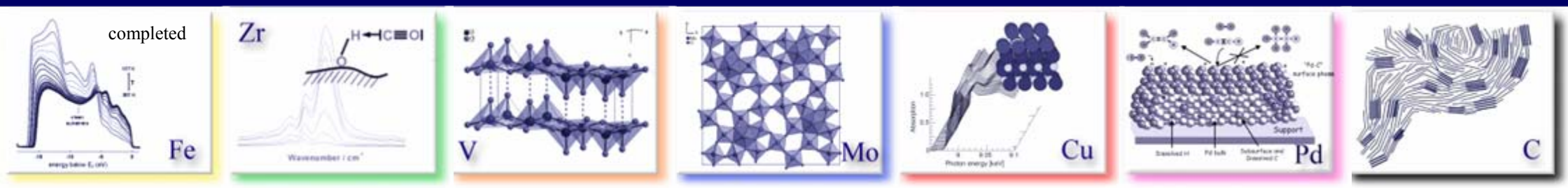
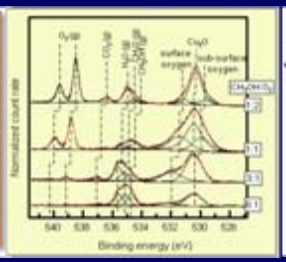
DEPARTMENT OF

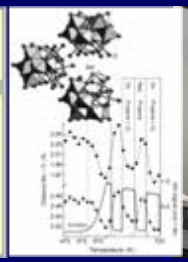
INORGANIC CHEMISTRY

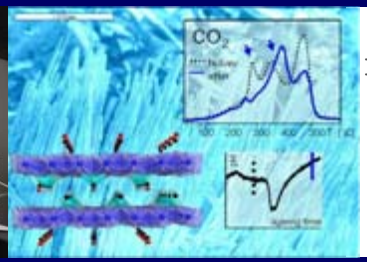
FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT

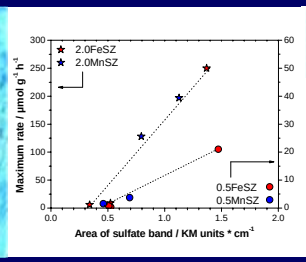
October 2007 / 3rd Edition

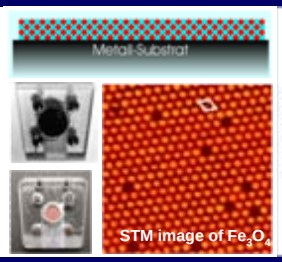


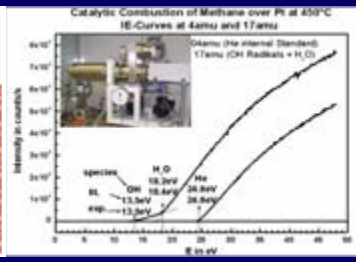




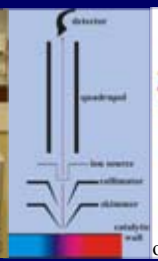


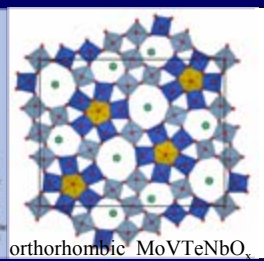


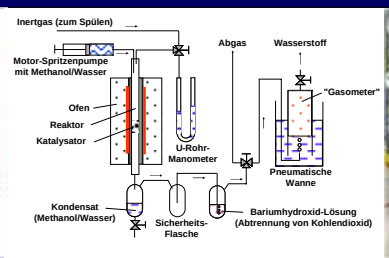


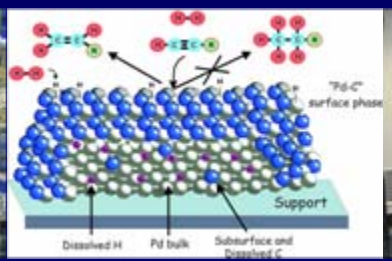


http://www.fhi-berlin.mpg.de









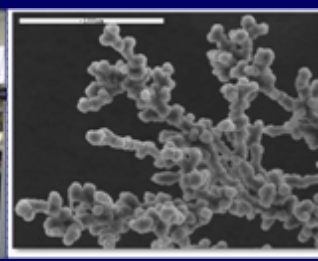


Table of Contents

History of the Fritz-Haber-Institut

MAX-PLANCK-GESELLSCHAFT

http://www.fhi-berlin.mpg.de/history

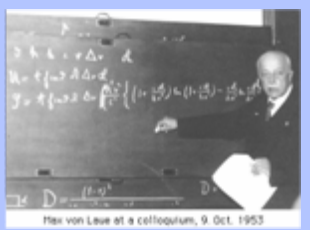
The Kaiser-Wilhelm Institutes for Chemistry (left) and for Physical Chemistry and Electrochemistry (right) --(1913).

What is now called the Fritz-Haber-Institut of the Max-Planck-Gesellschaft was founded in 1911 as the Kaiser-Wilhelm-Institut for Physical Chemistry and Electrochemistry, together with the Kaiser-Wilhelm-Institut for Chemistry. These were in fact the first two institutes of the Kaiser-Wilhelm Society (Kaiser-Wilhelm-Gesellschaft, KWG).

Fritz Haber (left) and Albert Einstein (right) at the "Fritz-Haber-Institut" (1915).

Fritz Haber was appointed director of the institute following the recommendation of the famous Swedish physical chemist Svante Arrhenius. Haber's personality and his previous scientific achievements were considered particularly appropriate for a leader of this new institute, focusing on basic research in the field of physical chemistry, which was expected to give new momentum to the development of the German chemical industry, at that time regarded as a world leader.

In 1951, at the age of 71, Max von Laue became chief director of the institute. This started a new period of consolidation in which Max von Laue applied all his influence and his great scientific reputation to the task of rebuilding the institute.



Max von Laue at a colloquium, 9 October, 1953

1955 **Max von Laue**, director of the institute

1953 Rename in Fritz-Haber-Institut of the Max-Planck-Gesellschaft

1954 **Ernst Ruska**, Scientific Fellow of the institute

1957 "Institute for Electron Microscopy of the Fritz-Haber-Institut".

1959 **Rudolf Brill**, director of the institute, *catalytic properties for heterogeneous reactions, XRD, kinetic measurements*

1969 **Heinz Gerischer**, Dept. of Physical Chemistry, *studies of solid surfaces under ultra-high vacuum conditions and their interaction with gases*

1969 **Jochen H. Block**, *kinetic processes on metal surfaces were studied using field electron and field ion microscopies*

1974 The institute was restructured to consist of three sections which were to combine their collaborative efforts: Physical Chemistry (directors: J. H. Block, H. Gerischer, K. Molière), Structure Research (directors: R. Hosemann, Kurt Ueberreiter), and Electron Microscopy (director: E. Ruska until 1974).

1976 **Elmar Zeitler**, Electron Microscopy

1980 Second reorganization introduced a collaborative structure for the institute with stronger emphasis on surface and interface science.

1980 **Alexander Bradshaw**, Dep. of Surface Physics, *spectroscopy of solid surfaces and the study of chemisorbed molecules*

1981 A. Bradshaw, Scientific Director of BESSY I, 1999 BESSY II, 1997 IPP

1985 **Gerhard Ertl**, Dept. of Physical Chemistry, *structure and chemical reactions on solid surfaces*

1986 Ernst Ruska was awarded the Nobel Prize in Physics

1988 **Matthias Scheffler**, Theory Dept., *surface theory, solid state research, quantum chemistry, computational physics*

1994 **Robert Schlögl**, Dept. of Inorganic Chemistry, *heterogeneous reactions on inorganic surfaces*

1995 **Hans-Joachim Freund**, Dept. of Chemical Physics, *adsorption and reaction on solids, in particular, on oxide surfaces*

2002 **Gerard Meijer**, Dept. of Molecular Physics, *molecular physics using the free-electron-laser*

2007 Gerhard Ertl was awarded the Nobel Prize in Chemistry

How to reach the Institute

By Train from Bahnhof Zoologischer Garten:

Take U-Bahn U9 direction Rathaus Steglitz. Change at Spichernstrasse. Take U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 30 min. Costs are about Euro 2,00. Taxi takes about 20 minutes outside rush hours. Costs are about 15 Euro.

By Air from Flughafen Tegel:

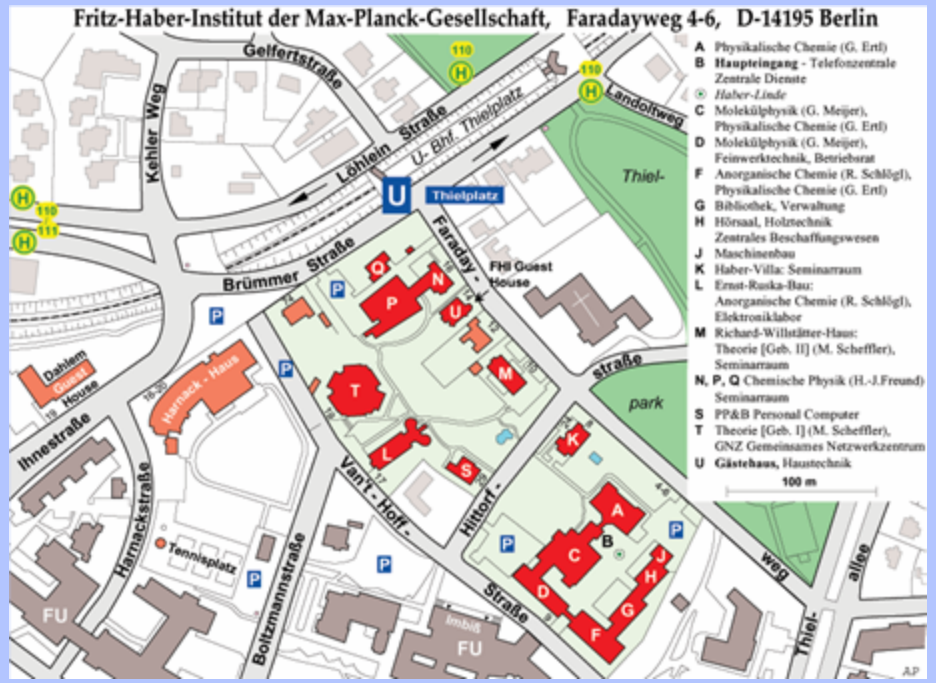
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs are about 20 Euro.

By Air from Flughafen Tempelhof:

Take subway U6 direction Alt-Tegel, change at Mehringdamm, take U7 direction Rathaus Spandau. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 30 min. Costs are about Euro 2,00. Taxi takes about 20 minutes outside rush hours. Costs are about 15 Euro.

By Car:

On the freeway (Bundesautobahn) Potsdam-Berlin take exit Hüttenweg. Follow Hüttenweg to the end (about 3km), two crossings with traffic lights. (Königsallee/Onkel-Tom-Str. and Clayallee). At the end of Hüttenweg turn right into Gelfert Straße, and take the second street to the right, Kehler Weg. At the next crossing, turn left (over the U-Bahn bridge) into Brümmer Straße. Take the next street to the right Faradayweg.



Fritz-Haber-Institut der Max-Planck-Gesellschaft

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Germany

Preface

Director:
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The department AC in the Fritz-Haber-Institute aims to gain a generalized understanding of heterogeneous catalysis as a multi-scale phenomenon. To achieve this goal the department develops and applies in situ methodology and combines the obtained information with kinetic data. The rationale behind this approach is the realization that catalysts are dynamic materials whose active centres are formed or transformed under reaction conditions.

The FHI contributes within all departments towards the understanding of heterogeneous catalysts defined as the prediction of the macroscopically observable performance of a kinetically demanding reaction over a given catalyst system and under given reaction conditions.

This level of understanding being pre-requisite for a rational design of technologically important processes has only be achieved so far for kinetically non-demanding reactions, which exhibit no branching of reaction pathways and/or occur with an adsorption step as rate-determining process. Examples for this are isotope exchange reactions, ammonia synthesis, CO oxidation, decomposition of methanol, total oxidation of hydrocarbons.

Kinetically demanding reactions of interest to the department AC are currently: selective oxidations of un-functionalized or weakly functionalized hydrocarbons, selective hydrogenations of various functionalities, dehydrogenations, skeletal rearrangements of small organic molecules and C1 chemistry. All these reactions exhibit complex selectivity patterns and multiple reaction steps with intermediates. The diversity is seen as important to achieve a generalized understanding. However, links between these reactions exist through common elementary steps.

For example, a typical oxidation requires C-H activation, oxygen activation, oxygen insertion and oxygen addition reactions. Large bodies of phenomenological experience both from applied and fundamental studies exist, but neither the real mode of operation nor the nature of the working catalysts is known in sufficient detail. This lack in knowledge has led to the formulation of empirical concepts (such as: remote control of oxygen activity, synergy of catalyst phases, Mars-van Krevelen formal kinetics, radical-initiated reactions) none of which were as rigorously examined as the ammonia synthesis reaction. The necessary tools and methods to handle the enormous complexity of kinetically demanding chemical transformations are being developed world-wide under substantial participation of the FHI to which the department AC contributes its share in synthesis and development of analytical methodology.

The department AC studies a selection of reactions using materials and conditions typical of technical applications. These efforts and the model and theoretical studies carried out in the other departments are complementary.

The strategy of AC involves monitoring the synthesis of catalytically active materials by in situ techniques. Through understanding and ultimately controlling the processes of inorganic synthesis occurring during all unit operations of catalyst preparation an optimization is achieved resulting in reproducible and homogeneous active materials. The active centres are

envisaged as unique configurations of one or more atoms at or near the surface whose existence is enabled by a surrounding matrix, which is ideally homogeneous. For chemically and structurally complex systems simplified models are generated that exhibit the essential catalytic characteristics. Suitable specimens (e.g. polycrystalline thin films) are tailor-made for in-situ functional studies aiming at verifying the nature of the active ensemble and adsorbates.

Physical chemistry is the key discipline in the interdisciplinary effort of the department. The choice for experimental structure-function relationships requires quantitative kinetic and spectroscopic investigations. The in-situ analytical capability where the department holds a widely recognized position of competence forms the methodical core of the department. Instrumentation development (example: pressure-dependent surface analysis) and creation of novel coupled experiments are features enabling the investigation of working catalysts with an increasingly more complete suite of complementary methods describing geometric and electronic structural details. Physical chemistry is also the target of kinetic competence currently being expanded. Process development and technical implementations are outside the scope of the department.

Kinetic data and intermediate concentrations present input for theory and kinetic modelling. The model systems allow the comparison of fundamental material properties and of structural dynamics of the always metastable catalyst with those from rigorously defined models from surface science and cluster chemistry approaches typically studied in the other departments of the FHI.

A project is completed within the scope of the AC department when the scaling of chemical and structural complexity is defined and when a series of observable surface properties are described amenable to experimental and theoretical modelling. An example for such a completed project is the dehydrogenation of ethylbenzene to styrene over iron oxide catalysts. Although the development of novel systems is not a primary goal, the department seeks to verify and implement its knowledge by the rational synthesis of improved catalysts (example Pd-Ga intermetallic compounds).

Co-operations are essential for the department. The many competencies required for the integral approach to heterogeneous catalysis described here cannot be assembled in one department and not even in one institute. Theory and modelling as well as all the rigorously defined model systems and alternative synthetic concepts are incorporated into the projects through our partners inside and outside of FHI. With industrial partners the verifications of insight und functional understanding are performed.

The department is closely related in its activities to the other departments in the FHI. Outside the FHI and within the MPG strong and project-supported links exist with the MPI Mülheim (F. Schüth), Golm (Antonietti), Dresden (Grin, Steglich), Mainz (Müllen) and Stuttgart (Maier). The department is well connected to local universities (TU Berlin, HU Berlin), is active in a center of excellence program (SFB) and in several EU activities, where it coordinates the activities of the MPG in a NOE on catalysis (IDECAT). A European laboratory on catalysis (ELCASS, with Univ. Strasbourg and U. Messina) and participation in an IP (CANAPE) complete prominent EU activities.

Prof. Robert Schlögl

Internal Structure

The core competence of the Department is focused into the in situ metrology of synthesis and function of heterogeneous catalytic systems. The Scheme represents the current structure indicating its GL, PL, TR and main methodical activities.

PREPARATION

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Molybdenum-PL: Dr. A. Trunschke
Copper-PL: Dr. M. Behrens
20 members

Synthesis, Raman, UV-vis, Reactor design, Elemental analysis, BET, XRD, TG, DSC

FUNCTIONAL CHARACTERIZATION

GL: Dr. F. C. Jentoft (Habilitation)

Tel: 49 30 8413 4408
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Zirconia-PL: Dr. F. C. Jentoft
MBMS-PL: Dr. R. Horn
12 members

IR spectroscopy, UV-vis-NIR spectroscopy, Calorimetry, Gas phase reactions, Sorption methods, Elemental analysis

SURFACE ANALYSIS

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Palladium-PL: Dr. A. Knop-Gericke
Vanadia-PL: Dr. C. Hess
Silver-PL: Dr. M. Hävecker
15 members

Photoelectron spectroscopy, TP desorption, TP reaction, BESSY II

MICROSTRUCTURE

GL: Dr. D. S. Su

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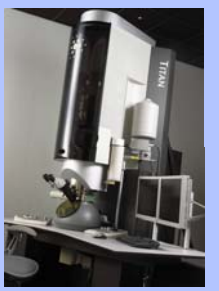
E-mail: dangsheng@fhi-berlin.mpg.de

Carbon-PL: Dr. D. S. Su
Reactions / TR: J. P. Tessonniere
TEM / TR: Dr. T. Hansen
TEM service group: Dr. D. S. Su
19 members

TEM, SEM, ELNES, RFA, Nanoreaction

Group leader: GL Project leader: PL Technical responsibility: TR

Miscellaneous

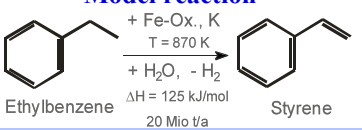


FEI Titan 80-300 aberration corrected TEM:

For Sub-Ångstrøm resolution work, an aberration-corrected FEI Titan 80-300 is available. This microscope has an information limit of ca. 0.8Å.

The completion of the dedicated beam line at BESSY for high-pressure photoemission experiments (ISIS) in April 2007 was a major event resulting already in a multitude of fruitful insights.

Model reaction



The iron oxide project was completed with a conclusive kinetic study linking the mechanistic insights of 10 years of work on single crystalline thin oxide films to well-defined macrokinetic observations of the dehydrogenation (DH) of ethylbenzene to styrene. A consistent picture emerged containing a wealth of insight into structures and dynamics of the active phase. The investigation of the spin-off process of oxidative dehydrogenation (ODH) of ethylbenzene over nanocarbon materials will be continued until the emerging kinetic differences between DH over iron oxide and ODH over carbon are either substantiated or resolved. A functional picture of the industrial DH process was developed; the addition of a large excess of steam supported by the reactivity of the iron oxide may create the same active sites on deposited carbon as occurring under ODH conditions over nanocarbons.

Instrumentation

FUNCTIONAL CHARACTERIZATION

Dr. F. C. Jentoft **(Habilitation)**

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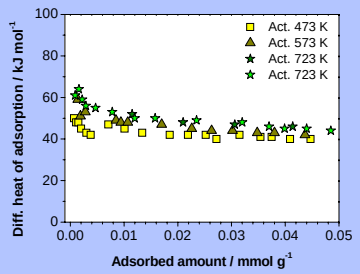
jentoft@fhi-berlin.mpg.de

One of the most important questions in heterogeneous catalysis is the nature of the catalytically active sites on the surface of the solid. Such sites can be identified by their interaction with the reactant or a chemically closely related molecule. We adsorb different "probe molecules" to study the type, number, accessibility and reactivity of surface sites:



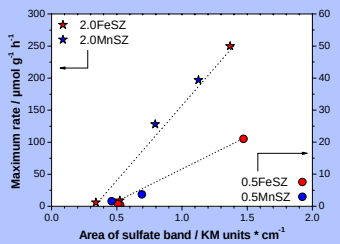
Measurement of adsorption isotherms

Measurement of the differential heats of adsorption by microcalorimetry

SETARAM MS80 and HT1000 Calvet-type microcalorimeters with all-metal cells connected to vacuum and gas-dosing systems (figure above shows propane adsorption on differently activated sulfated zirconia)

Infrared spectroscopy of adsorbates

Perkin-Elmer System 2000 and Spectrum 100 FTIR spectrometers with MIR and FIR options; custom-design transmission cells for batch or flow operation from 77-623 K connected to vacuum and gas-dosing systems



Catalysts change under reaction conditions. In order to investigate their actual state, the nature of surface species and reactive gas phase intermediates while the catalytic process is ongoing, we perform spectroscopy „in situ“. Ideally, we find structure-activity correlations such as shown to the left.

Diffuse reflectance FTIR spectroscopy

Bruker ifs 66 FTIR-spectrometer with Graseby-Specac “Selector” diffuse reflectance accessory with “Environmental Chamber” (to 823 K)

Diffuse reflectance UV-vis-NIR spectroscopy

PerkinElmer Lambda 650 and 950 UV-vis-NIR spectrometers with Harrick Praying Mantis diffuse reflectance accessories DRP-P72 and reaction chambers HVC-VUV and CHC-VUV-2 for applications from 77 to 873 K (see photo)

Molecular Beam Mass Spectrometry

Custom-design, HIDEN HAL IV EPIC Low Energy

SURFACE ANALYSIS

Dr. A. Knop-Gericke

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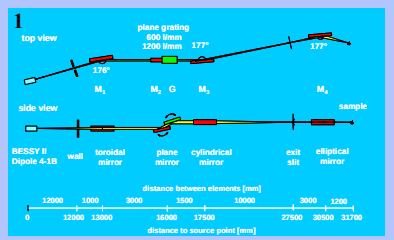
Dr. M. Hävecker, mh@fhi-berlin.mpg.de

ISISS: Soft X-ray station at BESSY :

Obviously, the understanding of the interaction of a catalysts surface with the reactants plays a key role in a detailed description of catalytic processes. However, a spectroscopic characterisation of the reacting surface under ambient conditions is challenging. The FHI in collaboration with the group of M. Salmeron (Berkley) developed a set-up suitable to record XP spectra in the presence of a reacting gas.

1



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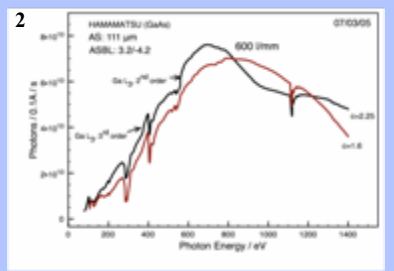

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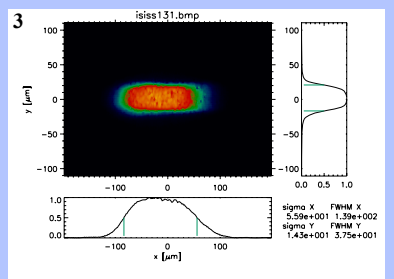

The ultimate surface and element sensitivity on the one hand and the possibility to vary the information depth on the other hand adds an extra quality to XPS when operated at the synchrotron. In addition, X-ray absorption spectra (XAS) can be taken at a synchrotron.

Thus, BESSY and the FHI recently installed the facility ISISS (Innovative Station for In Situ Spectroscopy). ISISS consists of 3 main parts: a) the in situ XPS endstation, b) a state of the art soft X-ray beamline, and c) a permanent infrastructure on site for experiments with a chemical background.

The optical layout of the beamline is shown in fig. 1. The ISISS beamline is designed following the principle of a plane grating monochromator working in collimated light. The beamline is optimised to deliver photons in the energy range between 80eV - 2000eV with a high photon flux of up to $6*10^{10}$ photons/ sec/ 0.1A ring current (fig. 2). The photon beam is re-focused after the exit slit to ensure a high brilliant X-ray spot at sample position. The spot size is typically 150µm x 80µm (h x v) as shown in fig. 3.

Instrumentation

PREPARATION

Dr. A. Trunschke

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The sophisticated formulation and complexity of current heterogeneous catalysts requires the application of controlled synthesis conditions and well-defined chemicals for their reproducible preparation. The work of the Preparation Group is targeted on a deeper understanding of catalyst synthesis ranging from the assembly of molecular building blocks in solution to phase transformations during thermal pretreatment procedures. New synthetic concepts are developed using the following equipment for preparation and characterization:

- Automated **laboratory reactor** system (Mettler-Toledo Labmax, Photo right) **for precipitation** equipped with probes for measuring pH, conductivity, turbidity, and UV-Vis spectra
- 300 ml **autoclave** (Parr) / 400 ml automated high pressure autoclave HPM-PT-040 (Premex Reactor GmbH) equipped with pH probe and two HPLC pumps for controlled dosing
- Büchi Mini **Spray Dryer** B-191 / pilot plant scale spray dryer Niro Mobile Minor 2000H
- Rotating **furnace** (Xerion) for thermal treatments under controlled gas flow
- Zetasizer nano ZS / MPT-2 (Malvern) for **particle size measurements** by dynamic light scattering and for **zeta-potential measurements**
- AUTOSORB-1-C (Quantachrome) **physisorption/chemisorption** analyzer
- STA 449C Jupiter® thermobalance (Netzsch) for **thermal analysis** combined with gas phase analysis by mass spectrometry (OmniStar™, Pfeiffer)
- Temperature programmed desorption/reaction (TPDRO 1100, CE Instruments)
- HP DSC 827e (Mettler-Toledo) modified for in situ measurements

- STOE Theta/theta Bragg-Brentano diffractometer (Photo left) equipped with an Anton Paar XRK 900 reactor chamber (**in situ XRD measurements**)
- Buker AXS D8 Advance diffractometer equipped with a HTK 16 High-Temperature Chamber (Parr)
- STOE STADI P transmission diffractometer with autosampler for routine measurements

- High-throughput, parallel fixed-bed screening unit for **propane oxidation** (ILS)
- Single-tube fixed-bed reactor for gas phase oxidation equipped with GC-MS (Agilent)

MICROSTRUCTURE

Dr. D. S. Su

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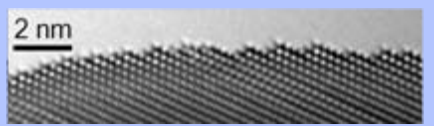
For microstructural investigations, 5 electron microscopes are available.

Morphological studies in vacuum or at low pressures are carried out in a FEI Quanta 200 FEG scanning electron microscope (SEM). This machine is capable of operating at pressures up to 4000Pa and has a resolution of ca. 1.2nm at 30kV acceleration voltage. The Quanta FEG SEM features a heating stage for conducting experiments at elevated temperatures. For morphological studies, a Hitachi S-4800 scanning electron microscope is used. This machine has a resolution of approx. 1.4nm/0.8nm at 1kV/30kV and features various types of detectors. For structural studies, transmission electron microscopy (TEM) is applied. For general studies a Philips CM200 LaB6 with an information limit of ca. 2Å is used. For higher resolution work, a Philips CM200 with a field emission gun is available. This microscope has an information limit of about 1.4Å.

For Sub-Ångstrøm resolution work, an aberration-corrected FEI Titan 80-300 is available. This microscope has an information limit of ca. 0.8Å. The CM200 FEG and the Titan are both equipped with a Gatan Tridiem energy filter (GIF) for acquiring energy-loss spectra (EELS) and energy-filtered images, with an energy resolution <1eV and <0.8eV respectively. All electron microscopes are equipped with EDAX Genesis energy-dispersive X-ray spectrometers (EDS). A well-equipped laboratory is available for preparation of TEM and SEM samples. For the quantitative chemical analysis of macroscopic bulk materials, powders and fluids, wavelength dispersive X-ray fluorescence spectrometry (WDXRF) is used.

FEI Titan 80-300 aberration corrected TEM.



Surface of a silver particle imaged using an aberration corrected TEM.

Understanding catalysis

Why in-situ analysis ?

The department AC has continued its activities centred on heterogeneous catalysis at the interface between fundamental studies of model systems and applied catalysis involving technical systems, practical catalyst synthesis and „real“ reaction conditions. In this large field of scientific activity the department concentrates on in-situ functional analysis and defined material synthesis.

A **concept** of heterogeneous catalysts is developed linking the surface chemistry of the substrate (the desired process) with the material chemistry of the catalyst (an „invisible“ process).

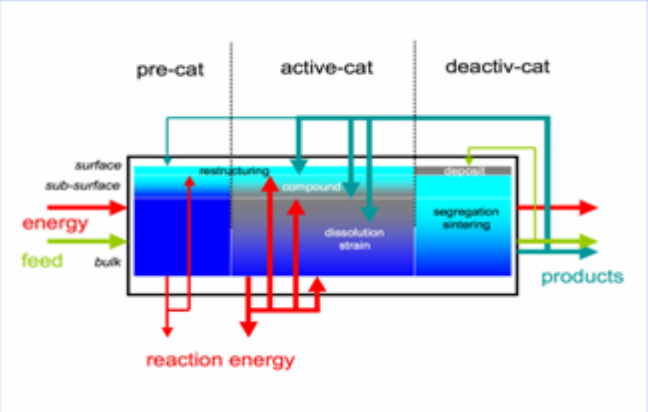
The **key** feature in the concept is the acknowledgement of the essential role of structural dynamics of an active catalyst (has been evidenced by numerous phenomena) under high performance operation conditions.

The essential role of structural dynamics is scientific justification for the use of **in-situ methods** and for the enormous experimental resources required for this kind of catalysis research.

The **aims** of this research are a generic definition of structural dynamics as well as the evolution of synthesis concepts for suitable materials (inorganic target synthesis). A core point is the confirmation of the observation that the optimal function of a catalyst is linked to one well-defined material as opposed to intended or unintentional mixtures of systems.

Working catalyst

alter the structure of the operating catalyst



Schematic representation of a catalyst operating at low performance (model) conditions (pre-cat), at high performance conditions and in deactivated forms. The arrows indicate feedback processes to different compartments of the catalyst. The scheme applies to bulk systems. Similar feedback structures can be constructed for supported systems.

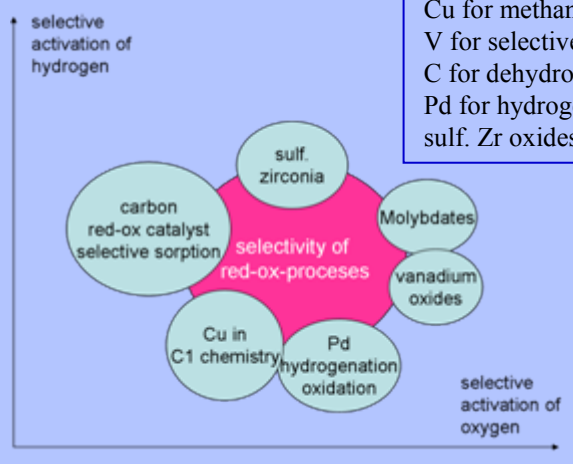
The working catalyst is characterized by the conversion of a low-active precursor phase into a highly active metastable active state through processes of restructuring. These processes are driven by sub-surface chemistry of reactant fragments being incorporated into the catalyst material, a process fuelled by the excess energy liberated during substantial transformation of the educts. The metastability induced by operation in the active mode is expression of the fact that highly reactive systems are far apart from their thermodynamic equilibrium. The price for this evolution is the propensity of the active phase to deactivate through phase transformations (redox processes, segregation or sintering). It is the “art” of catalyst synthesis to select composition and real structure such, that the transformation of the pre-catalyst into the active phase is as facile as possible during the process of “activation“ and that the subsequent equilibration into the thermodynamically stable situation through „deactivation“ occurs as slowly as possible.
The extent to which surface science at low conversion and high structural definition can describe a catalytic reaction depends on the strength of coupling of the feedback loops into structure and stability of the material. A strong coupling will be the more needed, the more demanding the catalytic reaction is, i.e. the more other elementary steps than sorption of molecules control the reaction. Highly specific catalysts of complex chemical composition or delicate geometric structure (such as mixed oxides or nanoparticles) will react strongly on the changes in energy throughput and modification of the reactants chemical potential and thus exhibit strong coupling constants in the feedback loops shown above.

Scientific Progress

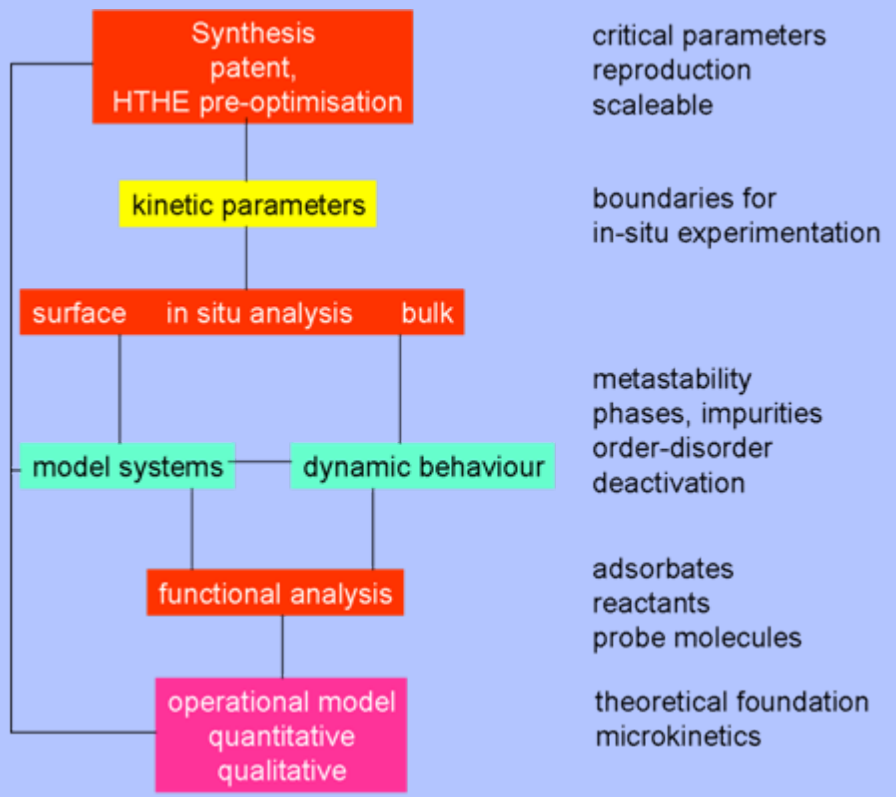
The Department AC is uniquely positioned at the crossroads of synthetic inorganic chemistry and metrology augmented by method development capabilities. Using these elements it seems possible to arrive at the development of truly rational synthesis procedures of nanostructured (defined in several dimensions of size) catalytic materials that can be used as intermediate systems to build the experimental bridge between complex technical and the present model systems. It will be necessary to develop in addition to the bare materials also suitable handling forms for in-situ experimentation such as thin films or nanocrystals. Such catalyst forms require the adaptation of testing environments to allow the novel systems to be used for static model experiments with validated functional performance.

The schemes indicate the target of the Department that will be pursued in six of the research areas:

Mo oxides for selective oxidation
Cu for methanol reactions
V for selective oxidation
C for dehydrogenations
Pd for hydrogenation/dehydrogenation
sulf. Zr oxides for isomerization

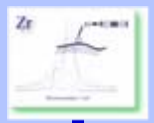


The target of the Department is the rational development of complex model systems. The current profile of the Department allows defining the choices of systems to be synthesized on the basis of in-situ observations of technical systems rather than on pragmatic arguments of nominal catalyst composition or availability of equilibrium phases of a compound catalyst.

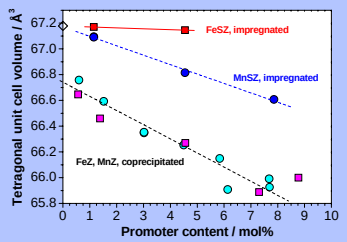


Scientific Progress

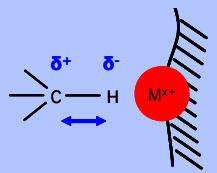
Zirconia in hydrocarbon activation



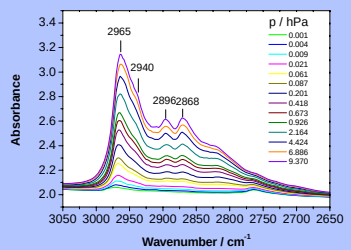
Sulfated zirconia materials are attractive catalysts for the *low temperature skeletal isomerization of alkanes*. We are interested in the role of the zirconia bulk and surface structural properties and how they can be tuned through cation doping and variations in thermal treatment. Looking at the reaction mechanism, the ability of sulfated zirconia surface sites to dehydrogenate and oxidize alkanes is in focus. These reactions may be important for isomerization but may also be responsible for a loss in activity with time. In this context, we also investigate Pt-doping, which in combination with addition of H_2 to the alkane feed stabilizes the catalytic activity.



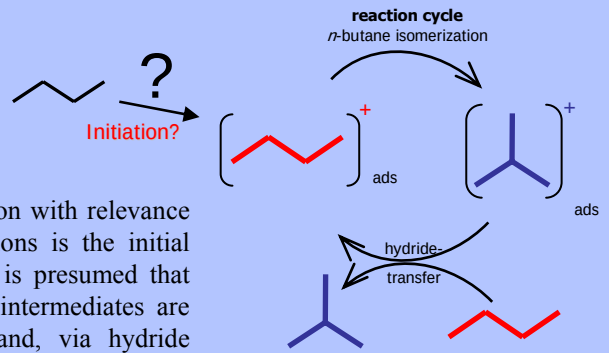
Sulfated zirconia can be promoted through addition of small amounts of manganese or iron cations. Shrinkage of the unit cell of the tetragonal zirconia phase with increasing promoter content (analyzed by XRD, Fig. 1) indicates that these promoters are incorporated into the zirconia lattice, to an extent that depends on the preparation method. We are investigating which types of defects are induced by different lower-valent cations (relative to Zr^{4+}) and whether they play a role for the isomerization. First in-situ EPR experiments indicate variations in the number of paramagnetic centers with promotion and a dynamic nature of these sites.



$$I \propto \left(\frac{\partial \mu}{\partial r}\right)^2$$

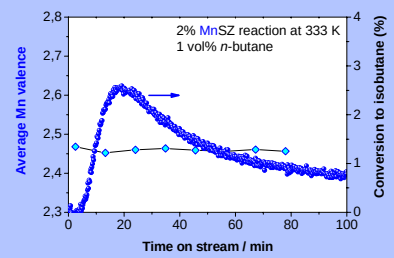


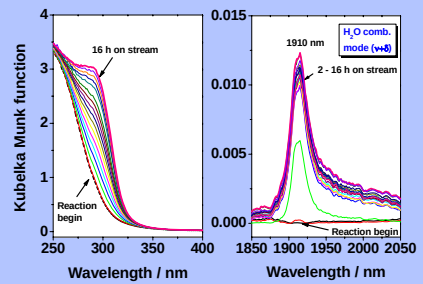
Surface reactivity is probed through the adsorption of small alkanes. We are developing the analysis of IR intensities as a new criterion for the polarization and activation of molecules on surfaces. A high band intensity indicates an activated bond in an adsorbate (Fig. 2). Extinction coefficients are derived from series of spectra (CH vibrations of adsorbed neopentane, Fig. 3) and simultaneously recorded isotherms.

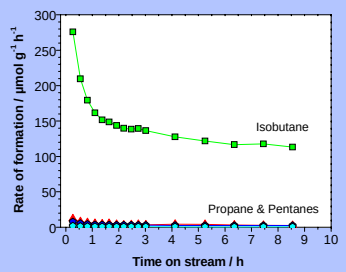


An intensely debated question with relevance beyond isomerization reactions is the initial activation of the alkane. It is presumed that carbenium-ion like surface intermediates are formed, which isomerize and, via hydride transfer from fresh reactant molecules, form the product and new intermediates (Scheme).

Originally, sulfated zirconia was believed to be a solid superacid able to protonate alkanes. However, particularly for promoted sulfated zirconia it has been suggested that the first step is an oxidative dehydrogenation (ODH) to alkenes, which are then protonated. We checked for ODH products, namely water, alkenes, and reduced catalyst species. In situ X-ray absorption (Fig. 4) and UV-vis spectroscopic data reveal that Mn is not reduced during catalysis. In situ UV-vis-NIR spectra of sulfated zirconia indicate water formation only during the first two hours on stream (Fig. 5, right), consistent with ODH initiation. Unsaturated species, which were also found using model films and NEXAFS analysis, accumulate continuously (Fig. 5, left) and are believed to be responsible for the long-term deactivation seen in the catalytic data (Fig. 6). Current work addresses the function of Pt in suppressing deactivation of alkane isomerization catalysts based on sulfated zirconia as well as on zeolitic materials.







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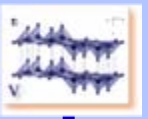
Scientific Progress

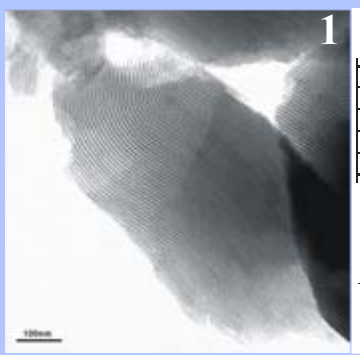
Vanadia in selective oxidation

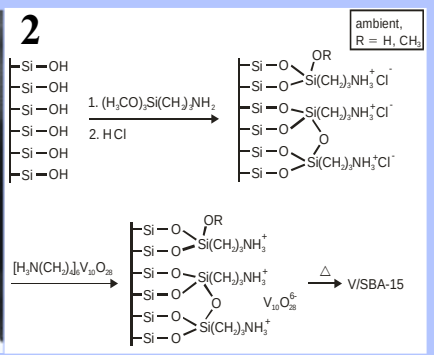


The synthesis, structure and reactivity behavior of nanostructured vanadia model catalysts for propane partial oxidation has been studied. Using a novel synthesis approach based on controlled grafting/ion exchange, highly dispersed vanadium oxide can be deposited homogeneously within the pores of mesoporous SBA-15 (Fig. 1). The individual steps of the synthesis, which consist of surface functionalization, ion exchange and calcination, were elucidated using X-ray photoelectron spectroscopy (XPS) and vibrational techniques (DRIFTS, Raman) allowing for a detailed description of the reaction mechanism (Fig. 2). Interestingly, the functionalization of the surface during synthesis leads to a strong increase in the mechanical stability of SBA-15. As this procedure can be readily applied to other mesoporous silica materials it might be of importance regarding their commercial application.

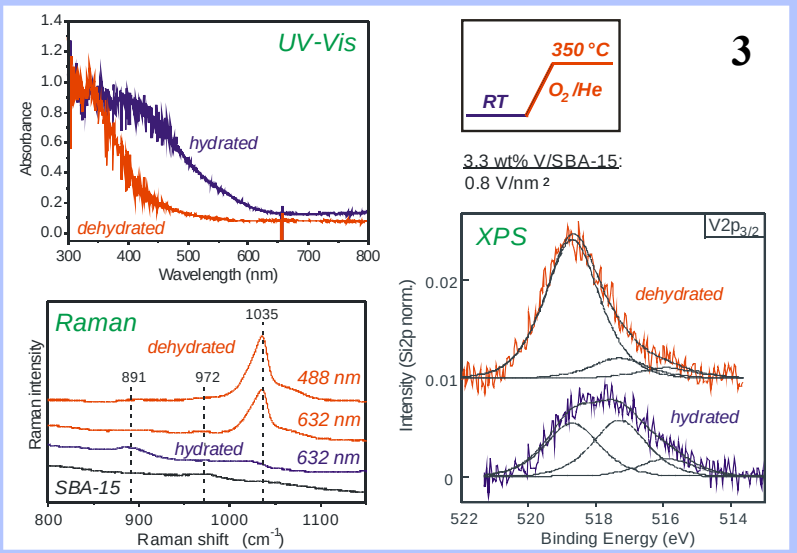
The reactivity behavior of the synthesized vanadia catalysts was tested in the selective oxidation of methanol and propane. High selectivities were observed towards formaldehyde at 300°C (96% at 8% conversion) and towards acrylic acid at 400°C (84% at 8% conversion) in the presence of steam.

To gain a deeper understanding of the role of steam on the selective oxidation of propane, the influence of water on the structure and dispersion of highly dispersed vanadia was investigated.





For these studies a new multiple in situ spectroscopic experiment (Fig. 3) was set up, which for the first time combines UV-Vis, Raman and XPS. The UV-Vis and XP spectra show that the fully hydrated vanadia catalyst is slightly reduced but consists mainly of V5+ species. The corresponding Raman spectra are in excellent agreement with those of the water containing V_2O_5 gel (xerogel) $V_2O_5 \cdot 1.2H_2O$, which consists of polymerized pyramidal VO_5 units similar as in V_2O_5. Upon catalyst dehydration by treatment in oxygen flow at 300°C dramatic changes in all spectra are observed (UV-Vis, Raman, XPS). A highly dispersed V5+ species is formed, which consists of tetrahedrally coordinated vanadium with significantly smaller ensemble size. By combining XPS with optical methods it is shown that changes in the structure and dispersion of highly dispersed vanadia during interaction with water are correlated.



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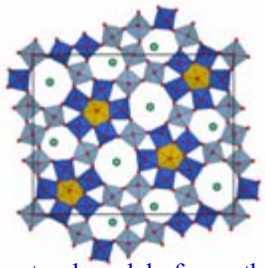
Sonderforschungsbereich 546 (SFB 546): „Struktur, Dynamik und Reaktivität von Übergangsmetalloxid-Aggregaten“

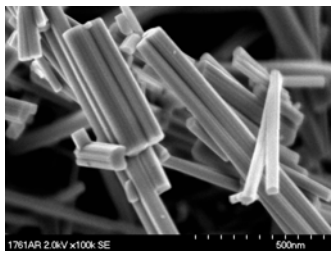
Financial support:
Athena
Deutsche Forschungsgemeinschaft

Scientific Progress

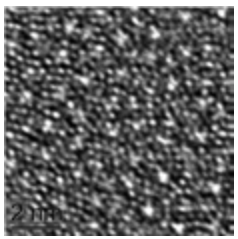
Molybdenum oxide based catalysts in C3 selective oxidation



1 Structural model of an orthorhombic $MoVTeNbO_x$ phase



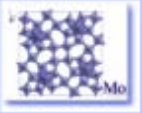
2 SEM image of phase-pure M1



3 HRTEM image of M1 viewed along the <001> zone axis

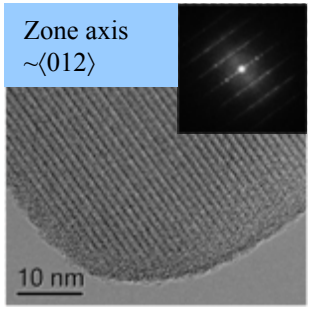
Background and objective

Selective oxidation of light alkanes with molecular oxygen to aldehydes or acids provides alternative access to chemical intermediates by utilization of natural gas or renewable feedstock as a replacement for olefin-based petrochemistry. However, the catalytic activation of C-H bonds in alkanes requires higher temperatures or more active catalysts. Furthermore, the increased reactivity of partially oxidized reaction intermediates is particularly challenging and accounts for high chemical and structural complexity of the catalytically active oxides. The direct oxidation of propane to acrylic acid proceeds with exceptional performance over crystalline MoVTeNb mixed oxides. Propane activation and high selectivity are attributed to the presence of an orthorhombic phase denominated as M1 (ICSD 55097) (Fig.1). The high degree of long-range order with respect to the metal constituents seems to be an important requirement for the development of active and selective metal-oxygen arrangements on the surface of the crystalline material under reaction conditions. With regard to the chemical complexity, phase-pure synthesis of such complex mixed oxides is a basic pre-requisite for understanding the mode of operation of the catalyst.

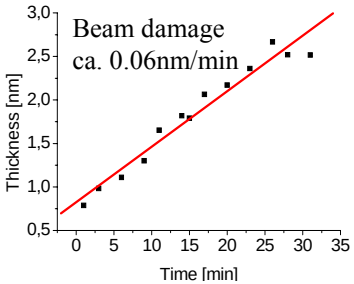


Results

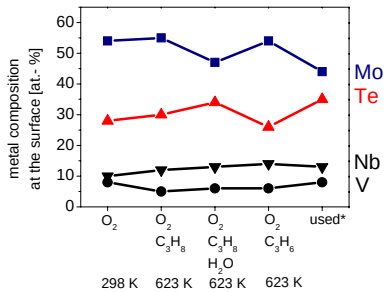
Propane conversion and formation rate of acrylic acid normalized to the total surface area increase with increasing content of M1 in the crystalline catalyst. Hydrothermal synthesis under optimized conditions results in nano-structured M1 that crystallizes in inert atmosphere at high temperatures (873-923 K) into phase-pure M1 crystals with needle-shape morphology (Fig.2-3). SEM based shape analysis of a series of phase-pure M1 catalysts reveals that the diameter of the needle-like crystals depends on the conditions of the thermal treatment. However, such studies have not shown a clear correlation between the catalytic activity and the occurrence of a certain crystal plane, e.g., the (001) plane. Independent of the crystal facet, the M1 surface is terminated by a structurally disordered surface layer roughly 0.7 nm thick, as evidenced by HRTEM (Fig.4-5). This observation is in accordance with the tellurium enrichment of the M1 surface to an extent incompatible with the M1 stoichiometry, as found by in-situ photo-electron spectroscopy in the presence of propane, oxygen, and steam at reaction temperature (Fig.6). The open channel structure of M1 is, apparently, responsible for considerable dynamics observed in the topmost surface layers.



4 Surface termination of M1



5 Effect of irradiation time on the thickness of the damaged region



6 Surface composition of M1 measured by in-situ XPS

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Financial support:
Südchemie AG

Scientific Progress

Copper catalysts in methanol chemistry

1

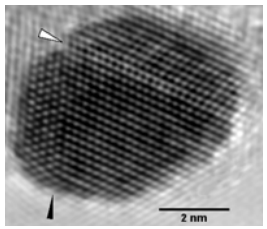
Methanol steam reforming

$CH_3OH + H_2O \rightarrow CO_2 + 3H_2$

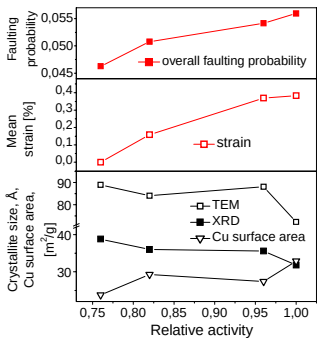
Methanol synthesis

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

2 Defect-rich Cu particle



3 Structure-function correlation



Introduction

Methanol is one of the most important basic chemicals and employed e.g. as source for other chemicals such as acetic acid, formaldehyde, and MTBE. Moreover, it might serve as a future CO2-neutral energy carrier for mobile applications either by fuel generation via dimethyl ether or as a hydrogen source for fuel cell applications. Copper zinc oxide catalysts are industrially used for methanol synthesis and are also active for the steam reforming of methanol (1). The worldwide increasing demand for methanol requires highly active and stable catalysts.

Understanding of the catalyst's "real" structure and its relation to catalytic activity is a prerequisite for knowledge-based catalyst design. This is tackled by detailed characterisation of active catalysts and their precursors to identify relevant features for good catalytic performance. Furthermore, synthetic tools have to be optimised or newly developed to tailor the structural properties in the desired way.

Results

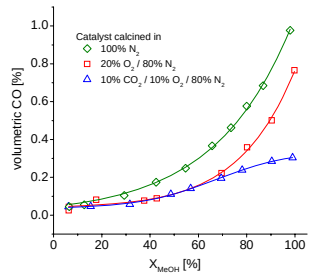
Investigations of a series of catalysts of technical relevant composition and structure by in-situ XRD and HRTEM (2) suggest a correlation of the defect density and lattice strain of Cu particles with the catalytic activity in methanol synthesis (3).

According to these results, the non-equilibrated nature of the Cu surface in "real" catalysts greatly enhances the catalytic performance.

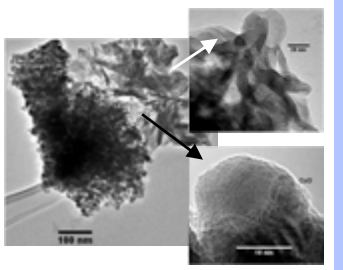
The microstructure of the final Cu particles is controlled by the preparation process. The partial pressure of CO_2 during calcination was identified as a parameter to increase the structural disorder of the Cu particles as well as the amount of residual carbonate in the catalyst, which might serve as a buffer layer at the Cu-ZnO interfacial contact. The presence of CO_2 and O_2 during calcination significantly improves the selectivity of the methanol steam reforming reaction (4).

Many structural properties of the final catalyst are pre-determined already at the stage of the precursor material. CuZnAl hydrotalcite-like layered compounds are a component of typical Cu/Zn/Al hydroxy-carbonate precursor mixtures. These materials were prepared in phase pure form and comprehensively studied. It was shown that the hydrotalcite phase alone yields two different types of Cu species for technical relevant Al poor compositions (5) and should be avoided in order to obtain a homogeneous microstructure. Precursors were prepared in an automated laboratory reactor system (6) allowing a high level of control and reproducibility.

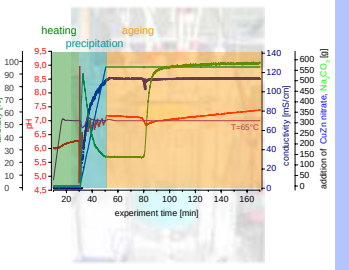
4 Steam reforming selectivity



5 Cu microstructure



6 Precursor preparation



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Financial support:
BMBF (FKZ 01RI05029)

H

Scientific Progress

Palladium based catalyst (Athena Project)

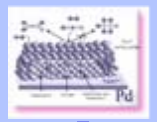


Fig.1 1-Pentyne hydrogenation on Pd foil

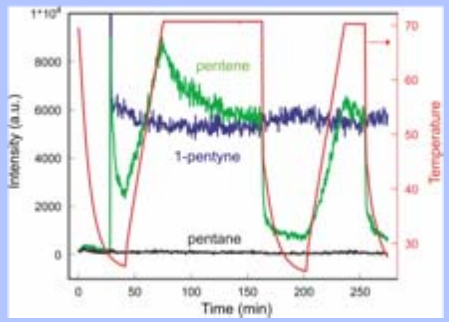
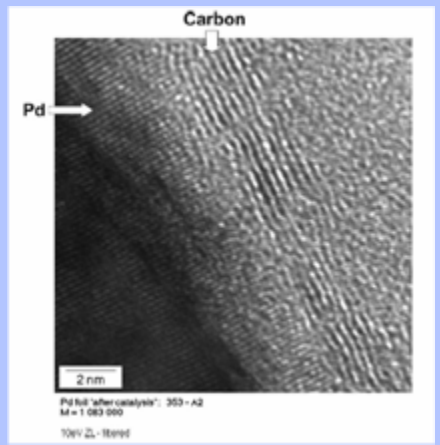


Fig.2



Pd based catalysts are applied for many hydrogenation and oxidation reactions. The hydrogenation of C5 compounds like trans-2-pentene or 1-pentyne over model and real catalysts, the oxidation of carbon monoxide and ethylene and methane combustion over Pd(111) were studied. The correlation between the electronic structure of the surface and the catalytic activity is the main focus of these investigation. High-Pressure X-ray photoelectron spectroscopy (HPXPS) combined with mass spectrometry is applied to unravel such correlations. Hydrogenation of both triple and double C-C bond was observed on supported Pd catalysts at 1 mbar conditions during XPS experiments. However the C=C hydrogenation on bulk palladium (Fig. 1) – especially on Pd(111) – was hindered. There are indications, that subsurface carbon can influence reaction selectivity, via blocking the way of energetic hydrogen emerging from the palladium bulk to the surface. HRTEM (Fig.2) indicated carbon on the surface of palladium, but also significant expansion of Pd lattice was calculated near the surface. Depth profiling XPS experiment during hydrogenation supported the HRTEM results that a massive amount of carbon was localized in the subsurface region (Fig.3).

Isothermal measurements of the sticking coefficient of ethylene on Pd(111) indicate the formation of subsurface carbon as well. In situ XPS measurements proved the existence of a non metallic highly active Pd phase during the ethylene oxidation.

A further aspect of the project is the improvement of the selectivity of Pd based hydrogenation catalyst. The project follows the approach of the site isolation concept. Intermetallic compounds like PdGa and Pd_3Ga_7 have been prepared by mixing the two molten metals followed by milling of the intermetallic compound. The surface of the obtained powder is rather low (1 m^2/g), however selectivity and long-term stability were enhanced compared with the Pd/Al_2O_3 catalyst. (Fig.4). The next step in the project will be the preparation of intermetallic compounds with much higher surface area by the polyol process.

Fig.3 Model of Pd surface during 1-pentyne hydrogenation

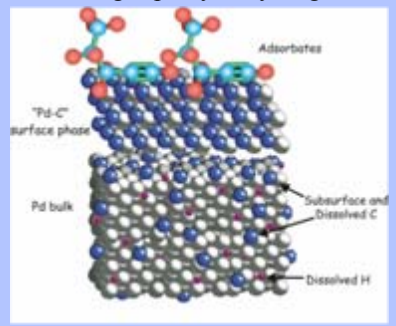
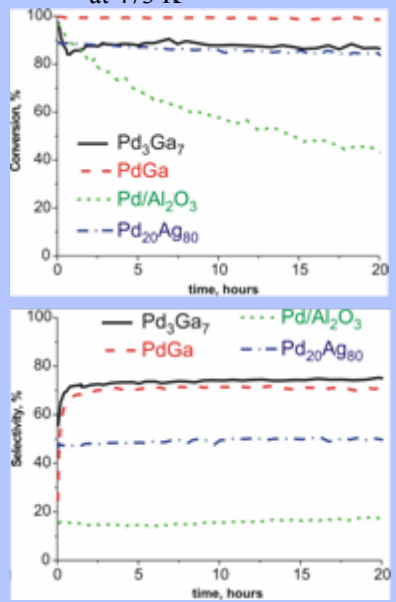


Fig. 4 Acetylene Hydrogenation at 473 K



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Scientific Progress

Carbon in catalysis

Synthesis and functionalization of carbon nanotubes for catalysis:

Figure 1 shows the CNTs grown on Etna lava in a chemical vapor deposition process. In this work, minerals are used both as support and as catalyst; no additional preparation of support and its wet chemical treatment are required. The method is cheaper, can be easily scaled-up and therefore opens new horizon for the application of CNTs/CNTs on a large scale, for instance, in water purification and in catalysis in which tones of immobilized CNTs/CNFs are needed.

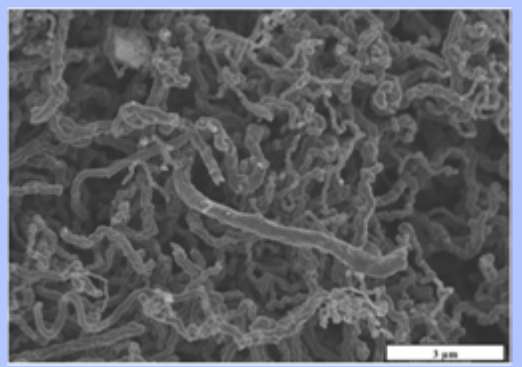

Fig.1

Carbon nanotubes grown on Mount Etna lava

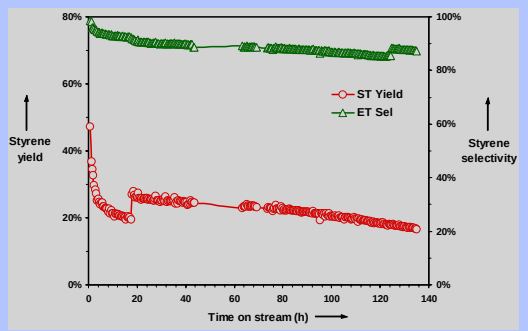

Fig. 2

Long-term test using CNTs as catalyst for oxidative dehydrogenation of ethyl benzene to styrene.

Nanocarbons as catalyst for gas phase reactions:

Nanocarbons (carbon nanotubes and nanodiamonds) show excellent catalytic performance in scale-up reactions for styrene production by means of oxidative dehydrogenation of ethyl benzene. In a scale up (up to 10g) and long-term test of the reaction in a mini-plant reactor, we showed that CNTs can exhibit a performance as good a the conventional industrial metal oxide catalyst, but at a temperature 300°C lower than that of the current industrial process and without used of excess steam. CNTs are extremely active and stable during long-time test, as it is shown in Fig. 2.

Synthesis and functionalization of carbon nanotubes for catalysis:

Mo_xO_y supported on functionalized multiwalled carbon nanotubes (Fig. 3) has been prepared and tested for selective oxidation of butane to maleic anhydride. Whereas bulk MoO_3 and Mo_xO_y supported on oxides like SiO_2 and Al_2O_3 are known to be inactive for such a complex reaction, MoxOy/MWCNT shows a stable catalytic activity. Mo_xO_y was shown to form a thin film on the surface of the carbon nanotubes without any formation of bulk molybdenum oxide. The observation is of generic relevance for the discussion about the necessary chemical complexity of selective oxidation catalysts and of the relevance of an oxide bulk as reservoir of lattice oxygen.

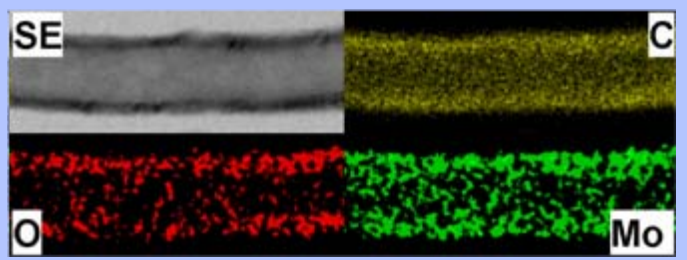

Fig.3

Element mapping shows homogenous dispersion of MoO_x on a CNT.

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further collaborations under L „External Funds“

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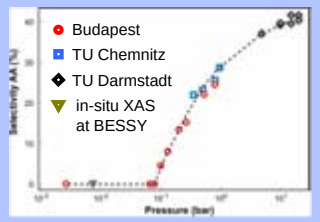
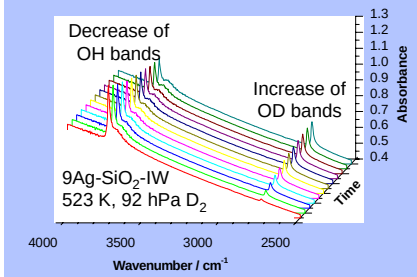
Deutsche Forschungsgemeinschaft

Scientific Progress

Silver as catalyst for selective hydrogenation and oxidation





Supported silver catalysts are active for selective hydrogenation of α,β-unsaturated aldehydes to alcohols. The role of silver, the reasons for the high selectivity, and support effects (SiO_2, ZnO) are not yet understood. The selectivity to allylic alcohol is nil at low pressures (Fig. 1). Angle-resolved in situ X-ray absorption spectra reveal variations in the acrolein adsorbate structure, which permit selective reaction of the CO bond at high coverage. IR spectra of Ag/SiO_2 or SiO_2 exposed to D_2 (Fig. 2) show isotopic exchange of Si-OH to Si-OD groups. Silver acts as accelerant, indicating it provides sites for hydrogen cleavage. Currently, we (i) investigate the enhanced catalyst activity after oxidative treatments and (ii) follow the reaction of acrolein and model compounds by in situ IR spectroscopy.

The unique ability of silver to selectively catalyze the partial oxidation of ethylene to ethylene oxide has attracted scientific interest in this system for several decades. Recently it was shown that copper-silver bimetallic catalysts offer improved selectivities compared to pure silver in the direct epoxidation of ethylene. Based on theoretical calculations and *ex-situ* photoelectron spectroscopy results it was claimed that the superiority of Ag-Cu compared to pure Ag is due to the formation of a Ag-Cu surface alloy. Such an alloy will favor the production of EO by increasing the difference between the activation barriers for the production of selective and not selective products of the reaction. Although the concept of designing new catalyst by computational screening is very attractive in catalysis, we have demonstrated by using a combination of *in-situ* techniques and first principle electronic structure calculations under oxygen atmosphere, that the stability of the structure under operational conditions is essential.
Due to the low adsorption enthalpy, ethylene epoxidation is impossible to study under UHV conditions. Therefore in situ XPS in the mbar pressure range was applied.

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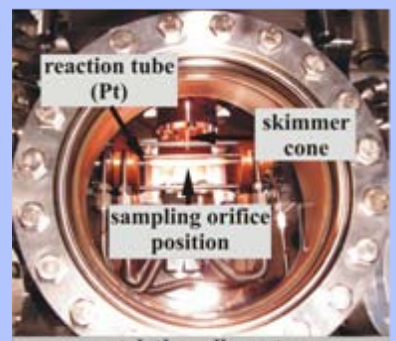
Scientific Progress

In situ molecular beam mass spectrometry for high temperature catalysis research

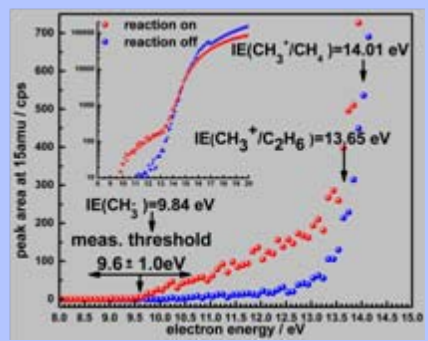
The transformation of natural gas components (e.g. methane) into chemicals like ethylene, methanol or formaldehyde is a challenge for catalysis research in the 21st century. High temperature catalytic alkane oxidations with reaction temperatures above 500 °C are a potential approach to accomplish these transformations but suffer from low yields in partial oxidation products. Whereas at low temperatures, catalytic reactions proceed by surface reaction steps only, high temperature catalytic reactions are characterized by a complex interplay between surface and gas phase chemistry. Surface and gas reactions are coupled by heat and mass transfer, whereby the exchange of reactive species such as free radicals is of particular interest. The partial oxidation products are intermediates in the surface and gas phase reaction network and the key to better yields in these products is a kinetically based optimization of catalyst, reaction conditions and reactor design.

To understand the gas phase chemistry in high temperature catalytic reactions we developed a Molecular Beam Mass Spectrometer to detect radicals over a working catalyst surface. By expanding the reacting gases from a catalytic reactor ($p_0 \geq 10^5$ Pa) into vacuum (Fig. 1), chemical reactions between gas molecules are quenched providing a snapshot of the gas composition over the catalyst surface including reactive intermediates. Radicals are detected by threshold ionization down to ppm concentrations.



catalytic wall reactor in the vacuum chamber of the MBMS

In first experiments we studied the methane oxidation on Pt. Below 1000°C only the thermodynamic products H_2, CO, H_2O and CO_2 are observed. At higher temperatures unsaturated C_2, C_3 and C_4 hydrocarbons are formed and hydrocarbon radicals (e.g. CH_3· (Fig. 2)) are detected over the catalyst. This result indicates that coupling products originate from free radical reactions in the gas phase.



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AC FHI Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Publications

2005

Max Planck Society
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Aszalos-Kiss, B., D. Zemlyanov, H. Gabasch, W. Unterberger, B. Klötzer, E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke and R. Schlögl: Oxygen dissolution: In situ XPS investigation of Pd(111) oxidation.
BESSY Annual Report 2004, 287-289 (2005).

Babu, S. M., A. Meeder, D. Fuertes Marron, T. Schedel-Niedrig, M. Hävecker, A. Knop-Gericke and M. C. Lux-Steiner: Thermal stability and environmental effects on CuGaSe2 thin film solar cells.
Journal of Crystal Growth **275**, 1-2, 1235-1240 (2005).

Blume, R., H. Niehus, H. Bluhm, M. Hävecker, A. Knop-Gericke, R. Schlögl and H. Conrad: High-Pressure oxidation of the Ru(0001) surface at elevated temperatures investigated by in situ X-ray photoelectron spectroscopy.
BESSY Annual Report 2004, 284-286 (2005).

Bron, M., D. Teschner, A. Knop-Gericke, A. Scheybal, B. Steinhauer, M. Hävecker, R. Födisch, R. Hönicke, R. Schlögl and P. Claus: In situ-XAS and catalytic study of acrolein hydrogenation over silver catalyst: Control of intramolecular selectivity by the pressure.
Catalysis Communications **6**, 5, 371-374 (2005).

Bron, M., D. Teschner, A. Knop-Gericke, B. Steinhauer, A. Scheybal, M. Hävecker, D. Wang, R. Födisch, R. Hönicke, A. Wootsch, R. Schlögl and P. Claus: Bridging the pressure and materials gap: in-depth characterisation and reaction studies of silver-catalysed acrolein hydrogenation.
Journal of Catalysis **234**, 37-47 (2005).

Brückner, A., U. Bentrup, M. Fait and B. Kubias: Structure-reactivity relationships in supported VOx catalysts for the oxyhydrative scission (OHS) of 1-butene and n-butane to acetic acid: A comprehensive catalytic and in situ study.
Catalysis Today **99**, 1-2, 123-129 (2005).

Bukhtiyarov, V. I., A. Nizovskii, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke and R. Schlögl: Combined high pressure XPS and PTRMS study of ethylene epoxidation over silver.
BESSY Annual Report 2004, 290-292 (2005).

Cai, Y., S. K. Chan, I. K. Sou, Y. F. Chan, D. S. Su and N. Wang: TEM investigation of nucleation and initial growth of ZnSe nanowires.
Symposium O: Scanning-Probe and Other Novel Microscopies of Local Phenomena in Nanostructured Materials. Eds.: S. V. Kalinin, B. Goldberg, L. M. Eng, B. D. Huey, Materials Research Society Symposium Proceedings **838E**. (2005) O14.11.1-O14.11.6.

Centi, G., S. Perathoner, P. Lanzafame, M. Gangeri, D. S. Su and R. Schlögl: Fe/Co SBA-15 materials for the dimensional control of carbon nanotubes.
Proceedings VII Convegno Nazionale Scienza e Tecnilogia delle Zeoliti Università della Calabria: Centro Editoriale e Librario (2005) 159-160.

de Groot, F. M. F., P. Glatzel, U. Bergmann, P. A. van Aken, R. A. Barrea, S. Klemme, M. Hävecker, A. Knop-Gericke, W. M. Heijboer and B. M. Weckhuysen: A multiplett analysis of 1s2p resonant inelastic scattering, 1s pre-edges and 2p X-ray absorption of iron oxides.
Journal of Physical Chemistry B **109**, 44, 20751-20762 (2005).

2005

Dennstedt, A., A. Deshpande, M. Niederberger, R. Schlögl and T. Ressler: Ternary Cu/ZrO_2CeO_2 catalysts for methanol steam reforming.
Hasylab Jahresbericht 2005, 1115-1116 (2005).

Dong, W.-S., J. K. Bartley, N. F. Dummer, F. Girgsdies, D. Su, R. Schlögl, J.-C. Volta and G. J. Hutchings: Reaction of vanadium phosphates with alcohols at elevated temperature and pressure.
Journal of Materials Chemistry **15**, 31, 3214-3220 (2005).

Dong, W.-S., J. K. Bartley, F. Girgsdies, R. Schlögl and G. J. Hutchings: The hydration and transformation of vanadyl pyrophosphate.
Journal of Materials Chemistry **15**, 38, 4147-4153 (2005).

Fuchs, M., B. Jenewein, S. Penner, K. Hayek, G. Rupprechter, D. Wang, R. Schlögl, J. J. Calvino and S. Bernal: Interaction of Pt and Rh nanoparticles with ceria supports: Ring opening of methylcyclobutane and CO hydrogenation after reduction at 373 – 723 K.
Applied Catalysis A: General **294**, 279-289 (2005).

Girgsdies, F., T. Ressler, U. Wild, T. Wübben, T. J. Balk, G. Dehm, L. Zhou, S. Günther, E. Arzt, R. Imbihl and R. Schlögl: Strained thin copper films as model catalysts in the materials gap.
Catalysis Letters **102**, 1-2, 91-97 (2005).

Grasset, F., G. Starukh, L. Spanhel, S. Ababou-Girard, D. S. Su and A. Klein-Hoffmann: From ZnO Colloids to Nanocrystalline Colored ZnxTiyOw-zNz-Spinel Films.
Advanced Materials **17**, 294-297 (2005).

Günther, S., L. Zhou, R. Imbihl, M. Hävecker, A. Knop-Gericke, E. Kleimenov and R. Schlögl: In situ X-ray photoelectron spectroscopy of the methanol oxidation over Cu(110).
BESSY Annual Report 2004, 299-301 (2005).

Győrffy, N., L. Tóth, M. Bartók, J. Ocskó, U. Wild, R. Schlögl, D. Teschner and Z. Paál: Palladium-platinum powder catalysts manufactured by colloid synthesis II. Characterization and catalytic tests after oxidizing and reducing treatment.
Journal of Molecular Catalysis A **238**, 1-2, 102-110 (2005).

Hävecker, M., B. Kniep, E. Kleimenov, P. Schnörch, D. Teschner, S. Zafeiratos, H. Bluhm, A. Knop-Gericke, T. Ressler and R. Schlögl: Combined in situ XPS and in situ soft XAS study of Cu/ZnO catalysts for methanol steam reforming.
BESSY Annual Report 2004, 281-283 (2005).

Hävecker, M., A. Knop-Gericke and R. Schlögl: X-Rays sight active sites: Dynamics of catalytic surfaces under reaction conditions.
BESSY Highlights 2004, 10-11 (2005).

Hävecker, M., N. Pinna, K. Weiß, H. Sack-Kongehl, R. E. Jentoft, D. Wang, M. Swoboda, U. Wild, M. Niederberger, J. Urban, D. S. Su and R. Schlögl: Synthesis and functional verification of the unsupported active phase of VxOy catalysts for partial oxidation of n-butane.
Journal of Catalysis **236**, 221-232 (2005).

Publications

2005

Max Planck Society
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Hahn, A. H. P., R. E. Jentoft, T. Ressler, G. Weinberg, R. Schlögl and F. C. Jentoft: Rapid Genesis of Active Phase during Calcination of Promoted Sulfated Zirconia Catalysts.
Journal of Catalysis **236**, 324-334 (2005).

Hess, C., I. J. Drake, J. D. Hoefelmeyer, T. D. Tilley and A. T. Bell: Partial Oxidation of Methanol over Highly Dispersed Vanadia Supported on Silica SBA-15.
Catalysis Letters **105**, 1-2, 1-8 (2005).

Huang, W., W. Ranke and R. Schlögl: Molecular Level Understanding the Catalytic Cycle of Dehydrogenation of Ethylbenzene to Styrene over Iron Oxide-based Catalyst.
Journal of Physical Chemistry B **109**, 19, 9202-9204 (2005).

Jentoft, F. C., J. Kröhnert and R. Schlögl: IR Spectroscopic Investigation of Heteropolymolybdate Catalysts: Acidic Properties and Reactivity towards Propene.
Zeitschrift für Physikalische Chemie **219**, 1019-1045 (2005).

Jentoft, R. E., A. H. P. Hahn, F. C. Jentoft and T. Ressler: XAS In Situ Cell for Measurements of Mn and Fe Promoted Sulfated Zirconia Catalysts.
Physica Scripta **T115**, 794-797 (2005).

Jentoft, R. E., A. H. P. Hahn, F. C. Jentoft and T. Ressler: In-situ XANES Study on Mn in Promoted Sulfated Zirconia Catalysts.
Physical Chemistry Chemical Physics **7**, 14, 2830-2838 (2005).

Karge, H. G.: Infrared Spectroscopic Investigation of Diffusion, Co-Diffusion and Counter-Diffusion of Hydrocarbon Molecules in Zeolites.
Comptes Rendus Chimie **8**, 303-319 (2005).

Ketteler, G. and W. Ranke: Epitaxial iron oxide growth on a stepped Pt(9 11 11) surface.
Journal of Vacuum Science and Technology A **23**, 4, 1055-1060 (2005).

Kirilenko, O., F. Girgsdies, R. E. Jentoft and T. Ressler: In situ XAS and XRD study on the structural evolution of ammonium paratungstate during thermal decomposition.
European Journal of Inorganic Chemistry **2005**, 11, 2124-2133 (2005).

Kleimenov, E., H. Bluhm, M. Hävecker, A. Knop-Gericke, A. N. Pestryakov, D. Teschner, J. A. Lopez-Sanchez, J. K. Bartley, G. J. Hutchings and R. Schlögl: XPS investigation of VPO catalysts under reaction conditions.
Surface Science **575**, 1-2, 181-188 (2005).

Klose, B. S., F. C. Jentoft and R. Schlögl: In Situ Diffuse Reflectance IR Spectroscopic Investigation of Promoted Sulfated Zirconia Catalysts during n-Butane Isomerization.
Journal of Catalysis **233**, 68-80 (2005).

Klose, B. S., F. C. Jentoft, R. Schlögl, I. R. Subbotina and V. B. Kazansky: Effect of Mn and Fe on the reactivity of sulfated zirconia toward H2 and n-butane: A diffuse reflectance IR spectroscopic investigation.
Langmuir **21**, 10465-10572 (2005).

2005

Kniep, B.-L., F. Girgsdies and T. Ressler: Effect of precipitate ageing on the microstructural characteristics of Cu/ZnO catalysts for methanol steam reforming.
Journal of Catalysis **236**, 1, 34-44 (2005).

Kondratenko, E.V., M. Cherian, M. Baerns, D.S. Su, R. Schlögl, X. Wang and I.E. Wachs: Oxidative dehydrogenation of propane over V/MCM-41 catalysts: Comparison of O2 and N2O as oxidant.
Journal of Catalysis **234**, 1, 131-142 (2005).

Li, D. F., D. S. Su, J. W. Song, X. Y. Guan, A. Klein-Hoffmann and F. S. Xiao: Highly Steam-Stable Mesoporous Silica Assembled from Preformed Zeolite Precursors at High-Temperatures.
Journal of Materials Chemistry **15**, 47, 5063-5069 (2005).

Li, X., K. Nagaoka, L. J. Simon, J. A. Lercher, S. Wrabetz, F. C. Jentoft, C. Breitkopf, S. Matysik and H. Papp: Interaction between Sulfated Zirconia and Alkanes: Prerequisites for Active Sites – Formation and Stability of Reaction Intermediates.
Journal of Catalysis **230**, 214-225 (2005).

Macia-Agullo, J. A., D. Cazorla-Amoros, A. Linares-Solano, U. Wild, D. S. Su and R. Schlögl: Oxygen functional groups involved in the styrene production reaction detected by quasi in-situ XPS.
Catalysis Today **102-103**, 248-253 (2005).

Macia-Agullo, J. A., D. Cazorla-Amoros, A. LInares-Solano, M. Hävecker, D. Teschner, E. Kleimenov, A. Knop-Gericke and R. Schlögl: Investigation of styrene production over carbon catalysts using high-pressure XPS.
BESSY Annual Report 2004, 278-280 (2005).

Mastalir, A., B. Frank, A. Szizybalski, H. Soerijanto, A. Deshpande, M. Niederberger, R. Schomäcker, R. Schlögl and T. Ressler: Steam reforming of methanol over Cu/ZrO2/CeO2 catalysts: a kinetic study.
Journal of Catalysis **230**, 2, 464-475 (2005).

Müller, J.-O., D. S. Su, R. E. Jentoft, J. Kröhnert, F. C. Jentoft and R. Schlögl: Morphology-controlled reactivity of carbonaceous materials towards oxidation.
Catalysis Today **102-103**, 259-265 (2005).

Ozensoy, E., C. Hess, D. Loffreda, P. Sautet and D. W. Goodman: Formation of a High Coverage (3×3) NO Phase on Pd(111) at Elevated Pressures: Interplay Between Kinetic and Thermodynamic Accessibility.
Journal of Physical Chemistry B **109**, 5414-5417 (2005).

Passalacqua, R., S. Perathoner, P. Lanzafame, G. Centi, G. Martra and D. S. Su: Preparation of nanostructured TiO2 photocatalysts based on the well-ordered hexagonal SBA-15 structure.
Proceedings VII Convegno Nazionale Scienza e Tecnologia delle Zeoliti Università della Calabria: Centro Editoriale e Librario (2005) 157-158.

Paál, Z., D. Teschner, N. Rodriguez, R. T. K. Baker, L. Tóth, U. Wild and R. Schlögl: Rh/GNF catalysts: Characterization and catalytic performance in methylcyclopentane reactions.
Catalysis Today **102–103**, 254-258 (2005).

Publications

2005

Max Planck Society
eDoc Server

Penner, S., D. Wang, R. Schlögl and K. Hayek: Rhodium particles supported by thin vanadia films as model systems for catalysis: An electron microscopy study.
Thin Solid Films **484**, 10-17 (2005).

Pestryakov, A., I. Tuzosvkaja, E. Smolentseva, N. Bogdanchikova, F. C. Jentoft and A. Knop-Gericke: Formation of Au Nanoparticles in Zeolites.
International Journal of Modern Physics B **19**, 15-17, 2321-2326 (2005).

Pinna, N., G. Garnweitner, P. Beato, M. Niederberger and M. Antonietti: Synthesis of Yttria-Based Crystalline and Lamellar Nanostructures and their Formation Mechanism.
Small **1**, 1, 112-121 (2005).

Pinna, N., S. Grancharov, P. Beato, P. Bonville, M. Antonietti and M. Niederberger: Magnetite nanocrystals: Nonaqueous synthesis, characterization, and solubility.
Chemistry of Materials **17**, 11, 3044-3049 (2005).

Polleux, J., N. Pinna, M. Antonietti, C. Hess, U. Wild, R. Schlögl and M. Niederberger: Ligand functionality as a versatile tool to control the assembly behavior of preformed titania nanocrystals.
Chemistry - A European Journal **11**, 12, 3541-3551 (2005).

Prescott, H. A., Z.-J. Li, E. Kemnitz, A. Trunschke, J. Deutsch, H. Lieske and A. Auroux: Application of Calcined Mg-Al Hydrotalcites for Michael Additions: An Investigation of Catalytic Activity and Acid-base Properties.
Journal of Catalysis **234**, 1, 119-130 (2005).

Radnik, J., A. Wahab, M. Schneider, M.-M. Pohl, R. Schlögl and B. Kubias: The influence of chemical transport via vapour phase on the properties of chloride and caesium doped V-Fe mixed oxide catalysts in the oxidation of butadiene to furan.
Applied Catalysis A: General **285**, 1-2, 139-150 (2005).

Ressler, T., B. L. Kniep, I. Kasatkin and R. Schlögl: The Microstructure of Copper Zinc Oxide Catalysts – Bridging the Materials Gap.
Angewandte Chemie International Edition **44**, 30, 4704-4707 (2005).

Ressler, T., O. Timpe and F. Girgsdies: In situ bulk structural study on solid-state dynamics and catalytic activity correlations of a H4[PNbMo11O40] partial oxidation catalyst.
Zeitschrift für Kristallographie **220**, 2/3, 295-305 (2005).

Ressler, T., O. Timpe, F. Girgsdies, J. Wienold and T. Neisius: In situ investigations of the bulk structural evolution of vanadium containing heteropolyoxomolybdate catalysts during thermal activation.
Journal of Catalysis **231**, 2, 279-291 (2005).

Ressler, T., J. Wienold and O. Timpe: Evolution of Catalyst Structure under Reaction Conditions From Time-resolved in situ XAS Investigations.
Physica Scripta **T115**, 66-71 (2005).

Rödel, E., R. Schlögl and T. Ressler: In situ XAS investigation of tungsten as structure directing agent during formation of Mo5O14 type partial oxidation catalysts.
Hasylab Jahresbericht 2005, 1105-1106 (2005).

2005

Schlögl, R.: Heterogeneous Catalysis for the C-H Transformation of Unfunctionalized Alkanes. Handbook of C-H Transformations: Applications in Organic Synthesis. Ed.: G. Dyker, Application in Organic Synthesis **2**. Wiley-VCH, Weinheim, (2005) 589-598.

Schlögl, R., S. Wrabetz (Eds.): Department of Inorganic Chemistry - Fritz-Haber-Institut der Max-Planck-Gesellschaft. 1. Edition Department of Inorganic Chemistry / FHI, Berlin (2005) 1-35.

Schüle, A., O. Shekhah, W. Ranke, R. Schlögl and G. Kolios: Microkinetic modelling of the dehydrogenation of ethylbenzene to styrene over unpromoted iron oxides.
Journal of Catalysis **231**, 1, 172-180 (2005).

Su, D. S., X. Chen, G. Weinberg, A. Klein-Hoffmann, O. Timpe, S. B. Abd Hamid and R. Schlögl: Hierarchically Structured Carbon: Synthesis of Carbon Nanofibers Nested inside or Immobilized onto Modified Activated Carbon.
Angewandte Chemie International Edition **44**, 34, 2-6 (2005).

Su, D. S., X. Chen, G. Weinberg, A. Klein-Hoffmann, O. Timpe, S. B. Abd Hamid and R. Schlögl: Hierarchisch strukturierter Kohlenstoff: Immobilisierung von Kohlenstoffnanofasern auf der Oberfläche und im Innern modifizierter Aktivkohle.
Angewandte Chemie **117**, 34, 5624-5628 (2005).

Su, D. S., N. I. Maksimova, J. J. Delgado, N. Keller, G. Mestl, M. J. Ledoux and R. Schlögl: Nanocarbons in Selective Oxidative Dehydrogenation Reaction.
Catalysis Today **102-103**, 110-114 (2005).

Su, D. S., Z. Zhu, X. Liu, G. Weinberg, N. Wang and R. Schlögl: Assembly of carbon tube-in-tube nanostructures.
Electronic Properties Of Novel Nanostructures. Eds.: H. Kuzmany, S. Roth, M. Mehring, J. Fink, AIP Conference Proceedings **786**. Springer, Secaucus, NJ (2005) 296-300.

Sun, J., H. Zhang, D. Ma, Y. Chen, X. Bao, A. Klein-Hoffmann, N. Pfänder and D. S. Su: Alkanes-assisted low temperature formation of highly ordered SBA-15 with large cylindrical mesopores.
Chemical Communcations **42**, 5343-5345 (2005).

Suprun, W. Y., D. P. Sabde, B. Kubias, H.-K. Schädlich and H. Papp: Transient isotopic studies on 1-butene oxidation over a VOx-TiO2 catalyst in presence of water vapour.
Applied Catalysis A: General **289**, 1, 66-73 (2005).

Szizybalski, A., F. Girgsdies, A. Rabis, Y. Wang, M. Niederberger and T. Ressler: In situ investigations of structure-activity relationships of a Cu/ZrO2 catalyst for the steam reforming of methanol.
Journal of Catalysis **233**, 2, 297-307 (2005).

Teschner, D., A. Knop-Gericke, E. Vass, S. Zafeiratos, A. N. Pestryakov, E. Kleimenov, M. Hävecker, H. Bluhm and R. Schlögl: Selective gas-phase hydrogenation of C-5 hydrocarbons using Palladium and Nickel based catalysts.
BESSY Annual Report 2004, 273-275 (2005).

Publications

2005

Max Planck Society eDoc Server

Teschner, D., A. Pestryakov, E. Kleimenov, M. Hävecker, H. Bluhm, H. Sauer, A. Knop-Gericke and R. Schlögl: High-pressure X-ray photoelectron spectroscopy of palladium model hydrogenation catalysts. Part 1: Effect of gas ambient and temperature.
Journal of Catalysis **230**, 1, 186-194 (2005).

Teschner, D., A. Pestryakov, E. Kleimenov, M. Hävecker, H. Bluhm, H. Sauer, A. Knop-Gericke and R. Schlögl: High-pressure X-ray photoelectron spectroscopy of palladium model hydrogenation catalysts. Part 2: Hydrogenation of trans-2-pentene on palladium.
Journal of Catalysis **230**, 1, 195-203 (2005).

Teschner, D., U. Wild, R. Schlögl and Z. Paál: Surface State and Composition of a Disperse Pd Catalyst after Its Exposure to Ethylene.
Journal of Physical Chemisty B **109**, 43, 20516-20521 (2005).

Tham, A. T., C. Rödel, M. Lerch, D. Wang, D. S. Su, A. Klein-Hoffmann and R. Schlögl: A TEM study on ZrO2-rich phases in the quasibinary system ZrO2-Zr3N4: Comparison between fast and slowly cooled samples.
Crystal Research and Technology **40**, 3, 193-198 (2005).

Veisz, B., L. Tóth, D. Teschner, Z. Paál, N. Győrffy, U. Wild and R. Schlögl: Palladium-platinum powder catalysts manufactured by colloid synthesis I. Preparation and characterization.
Journal of Molecular Catalysis A **238**, 1-2, 56-62 (2005).

Willinger, M.-G., D. S. Su and R. Schlögl: Electronic structure of β-VOPO4.
Physical Review B **71**, 155118-1-155118-8 (2005).

Würz, R., M. Rusu, T. Schedel-Niedrig, M. C. Lux-Steiner, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke and R. Schlögl: In situ X-ray photoelectron spectroscopy study of the oxidation of CuGaSe2.
Surface Science **580**, 1-3, 80-94 (2005).

Xia, W., D.S. Su, A. Birkner, L. Ruppel, Y. Wang, C. Wöll, J. Qian, C. Liang, G. Marginean, W. Brandl and M. Muhler: Chemical Vapor Deposition and Synthesis on Carbon Nanofibers: Sintering of Ferrocene-Derived Supported Iron Nanoparticles and the Catalytic Growth of Secondary Carbon Nanofibers.
Chemical Materials **17**, 5737-5742 (2005).

Xia, W., D. S. Su, R. Schlögl, A. Birkner and M. Muhler: Conical carbon filaments with axial cylindrical channels and open tips.
Advanced Materials **17**, 13, 1677-1679 (2005).

Zeitler, E.: Closed Form Integral.
The Mathematica Journal **9**, 4, (2005).

Zhu, Z. P., D. S. Su, G. Weinberg, R. E. Jentoft and R. Schlögl: Wet chemical assembly of carbon tube-in-tube nanostructures.
Small **1**, 1, 107-110 (2005).

2006

Bauer, F. and H. G. Karge: Characterization of Coke on Zeolites.
Molecular Sieves - Science and Technology. Eds.: H. G. Karge, J. Weitkamp, Springer-Verlag, Berlin (2006).

Beato, P., A. Blume, F. Girgsdies, R. E. Jentoft, R. Schlögl, O. Timpe, A. Trunschke, G. Weinberg, Q. Basher, F. A. Hamid, S. B. A. Hamid, E. Omar and L. Mohd Salim: Analysis of structural transformations during the synthesis of a MoVTeNb mixed oxide calalyst.
Applied Catalysis A: General **307**, 137-147 (2006).

Bentrup, U., A. Brückner, M. Fait, B. Kubias and J. B. Stelzer: Structure–reactivity relationships in VOx/TiO2 catalysts for the oxyhydrative scission of 1-butene and n-butane to acetic acid as examined by in situ-spectroscopic methods and catalytic tests.
Catalysis Today **112**, 1-4, 78-81 (2006).

Blume, R., M. Hävecker, S. Zafeiratos, D. Teschner, E. Kleimenov, A. Knop-Gericke, R. Schlögl, A. Barinov, P. Dudin and M. Kiskinova: Catalytically Active States of Ru(0001) Catalyst in CO Oxidation Reaction.
Journal of Catalysis **239**, 2, 354-361 (2006).

Blume, R., M. Hävecker, S. Zafeiratos, D. Teschner, E. Kleimenov, A. Knop-Gericke, R. Schlögl, A. Barinov, P. Dudin and M. Kiskinova: Catalytically active states of Ru(0001) catalysts in CO oxidation reaction.
BESSY Annual Report 2005, 270-272 (2006).

Bukhtiyarov, V. I., A. I. Nizovskii, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke and R. Schlögl: Combined in situ XPS and PTRMS study of ethylene epoxidation over silver.
Journal of Catalysis **238**, 2, 260-269 (2006).

Cai, Y., S.K. Chan, I.K. Sou, Y.F. Chan, D.S. Su and N. Wang: The Size-dependent growth direction of ZnSe nanowires.
Advanced Materials **18**, 1, 109-114 (2006).

Chen, W., X. Pan, M. Willinger, D. S. Su and X. Bao: Facile Autoreduction of Iron Oxide/Carbon Nanotube Encapsulates.
Journal of the American Chemical Society **128**, 10, 3136-3137 (2006).

Chen, X., D. S. Su and R. Schlögl: Immobilization of CNFs on the surface and inside of the modified activated carbon.
Physica Status Solidi B **243**, 13, 3533-3536 (2006).

Chen, X., M. Steinhart, C. Hess and U. Gösele: Ordered arrays of mesoporous microrods from recyclable macroporous silicon templates.
Advanced Materials **18**, 16, 2153-2156 (2006).

Conte, M., G. Budroni, J. K. Bartley, S. H. Taylor, A. F. Carley, A. Schmidt, D. M. Murphy, F. Girgsdies, T. Ressler, R. Schlögl and G. J. Hutchings: Chemically Induced Fast Solid-State Transitions of omega-VOPO4 in Vanadium Phosphate Catalysts.
Science **313**, 5791, 1270-1273 (2006).

Publications

2006

Max Planck Society
eDoc Server

Delgado, J. J., R. Vieira, G. Rehmann, D. S. Su, N. Keller, M. J. Ledoux and R. Schlögl: Supported Carbon Nanofibers for the Fixed-Bed Synthesis of Styrene.
Carbon **44**, 4, 809-812 (2006).

Delgado, J.J., D.S. Su, G. Rebmann, N. Keller, A. Gajovic and R. Schlögl: Immobilized carbon nanofibers as industrial catalyst for ODH reactions.
Journal of Catalysis **244**, 126-129 (2006).

Dennstedt, A., N. Frenzel, A. Trunschke, R. Schlögl, M. Lerch and T. Ressler: Zirconium oxynitride as new support for Cu in methanol steam reforming.
Hasylab Jahresbericht 2006, 817-818 (2006).

Dimitratos, N., A. Villa, D. Wang, F. Porta, D.S. Su and L. Prati: Pd and Pt catalysts modified by alloying with Au in the selective oxidation of alcohols.
Journal of Catalysis **244**, 113-121 (2006).

Gabasch, H., K. Hayek, B. Klötzer, A. Knop-Gericke and R. Schlögl: Carbon Incorporation in Pd(111) by Adsorption and Dehydrogenation of Ethene.
Journal of Physical Chemistry B **110**, 10, 4947-4952 (2006).

Gabasch, H., E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke, R. Schlögl, D. Zemlyanov, B. Aszalos-Kiss, K. Hayek and B. Klötzer: Carbon incorporation during ethene oxidation on Pd(111) studied by in situ X-ray photoelectron spectroscopy at 2 x 10(-3)mbar.
Journal of Catalysis **242**, 2, 340-348 (2006).

Gabasch, H., A. Knop-Gericke, R. Schlögl, S. Penner, B. Jenewein, K. Hayek and B. Klötzer: Zn Adsorption on Pd(111): ZnO and PdZn Alloy Formation.
Journal of Physical Chemistry B **110**, 23, 11391-11398 (2006).

Gabasch, H., W. Unterberger, K. Hayek, B. Klötzer, E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke, R. Schlögl, J. Han, F. H. Ribeiro, B. Aszalos-Kiss, T. Curtin and D. Zemlyanov: In situ XPS study of Pd(111) oxidation at elevated pressure, Part 2: Palladium oxidation in the 10-1 mbar range.
Surface Science **600**, 15, 2980-2989 (2006).

Gajović, A., I. Djerdj, K. Furić, R. Schlögl and D. S. Su: Preparation of nanostructured $ZrTiO_4$ by solid state reaction in equimolar mixture of TiO_2 and ZrO_2.
Crystal Research and Technology **41**, 11, 1076-1081 (2006).

Gajović, A., K. Furić, S. Musić, I. Djerdj, A. Tonejc, A. M. Tonejc, D.S. Su and R. Schlögl: Mechanism of ZrTiO4 synthesis by mechanochemical processing of TiO2 and ZrO2.
Journal of the American Ceramic Society **89**, 7, 2196-2205 (2006).

Gassenbauer, Y., R. Schafranek, A. Klein, S. Zafeiratos, M. Hävecker, A. Knop-Gericke and R. Schlögl: Surface states, surface potentials, and segregation at surfaces of tin-doped In2O3.
Physical Review B **73**, 24, 245312-1-245312-11 (2006).

2006

Gassenbauer, Y., R. Schafranek, A. Klein, S. Zafeiratos, M. Hävecker, A. Knop-Gericke and R. Schlögl: Surface potential changes of semiconducting oxides monitored by high-pressure photoelectron spectroscopy: Importance of electron concentration at the surface.
Solid State Ionics **177**, 35-36, 3123-3127 (2006).

Gassenbauer, Y., R. Schafranek, A. Klein, S. Zafeiratos, M. Hävecker, A. Knop-Gericke and R. Schlögl: High-Pressure XPS of transparent conducting oxides: Fermi level position and composition at ITO surface.
BESSY Annual Report 2005, 386-387 (2006).

Girgsdies, F., W.-S. Dong, J. K. Bartley, G. J. Hutchings, R. Schlögl and T. Ressler: The crystal structure of ε-VOPO4.
Solid State Sciences **8**, 7, 807-812 (2006).

Günther, S., L. Zhou, M. Hävecker, A. Knop-Gericke, E. Kleimenov, R. Schlögl and R. Imbihl: Adsorbate coverages and surface reactivity in methanol oxidation over Cu(110): An in situ photoelectron spectroscopy study.
The Journal of Chemical Physics **125**, 11, 114709-1-114709-10 (2006).

Habel, D., J. B. Stelzer, E. Feike, C. Schröder, A. Hösch, C. Hess, A. Knop-Gericke, J. Caro and H. Schubert: Phase development in the catalytic system V2O5/TiO2 under oxidising conditions.
Journal of the European Ceramic Society **26**, 15, 3287-3294 (2006).

Hao, Y.-J., J. B. Wagner, D. S. Su, G.-Q. Jin and X.-Y. Guo: Beaded Silicon Carbide Nanochains via the Carbothermal Reduction of Carbonaceous Silica Xerogel.
Nanotechnology **17**, 2870-2874 (2006).

Herbert, R., U. Wild, C. Hess and R. Schlögl: Nanostrukturierte Vanadiumoxid-Modell-Katalysatoren auf Basis von mesoporösem SBA-15.
Chemie Ingenieur Technik **78**, 9 (2006) 1263-1263.

Hess, C.: Characterization of the Synthesis and Reactivity Behavior of Nanostructured Vanadia Model Catalysts using XPS and Vibrational Spectroscopy.
Surface Science **600**, 3695-3701 (2006).

Hess, C., M. H. Looi, S. B. Abd Hamid and R. Schlögl: Importance of nanostructured vanadia for selective oxidation of propane to acrylic acid.
Chemical Communications, 4, 451-453 (2006).

Hess, C., E. Ozensoy, C.-W. Yi and D. W. Goodman: NO dimer and dinitrosyl formation on Pd(111): From ultra-high vacuum to elevated pressure conditions.
Journal of the American Chemical Society **128**, 9, 2988-2994 (2006).

Hess, C. and R. Schlögl: The influence of water on the dispersion of vanadia supported on silica SBA-15.
Chemical Physics Letters **432**, 1-3, 139-145 (2006).

Hess, C., U. Wild and R. Schlögl: The Mechanism for the Controlled Synthesis of Highly Dispersed Vanadia Supported on Silica SBA-15.
Microporous and Mesoporous Materials **95**, 339-349 (2006).

Publications

2006

Max Planck Society
eDoc Server

Hoang, D. L., S. Farage, A. Dittmar, A. Trunschke, H. Lieske and A. Mart
Studies on CrOx/La2O3/ZrO2 catalysts modified by Mg.
Catalysis Letters **112**, 3-4, 173-180 (2006).

Horn, R., K. Ihmann, J. Ihmann, F. C. Jentoft, M. Geske, A. Taha, K. Pelzer and R. Schlögl: Molecular Beam Mass Spectrometer Equipped with a Catalytic Wall Reactor for In Situ Studies in High Temperature Catalysis Research.
Review of Scientific Instruments **77**, 054102-1-054102-9 (2006).

Huang, W. and W. Ranke: Autocatalytic partial reduction of FeO(111) and Fe3O4(111) films by atomic hydrogen.
Surface Science **600**, 4, 793-802 (2006).

Hébert, C., W.-D. Schöne and D. S. Su: Experimental and theoretical Determination of Low electron Energy Loss spectra of Ag and Ru.
Ultramicroscopy **106**, 11-12, 1115-1119 (2006).

Jenewein, B., S. Penner, H. Gabasch, B. Klötzer, D. Wang, A. Knop-Gericke, R. Schlögl and K. Hayek: Hydride formation and stability on a Pd-SiO2 thin-film model catalyst studied by TEM and SAED.
Journal of Catalysis **241**, 1, 155-161 (2006).

Kaichev, V. V., V. I. Bukhtiyarov, D. Y. Zemlyanov, S. Belochapkine, B. K. Hodnett, E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke and R. Schlögl: Combined application of XPS, XANES and mass spectrometry to in situ study of methanol oxidation over vanadium based catalysts.
BESSY Annual Report 2005, 277-279 (2006).

Kazansky, V. B., I. R. Subbotina and F. C. Jentoft: Intensities of Combination IR Bands as an Indication of the Concerted Mechanism of Proton Transfer from Acidic Hydroxyl Groups in Zeolites to Ethylene Hydrogen-Bonded by Protons.
Journal of Catalysis **240**, 1, 66-72 (2006).

Kazansky, V. B., I. R. Subbotina, F. C. Jentoft and R. Schlögl: Intensities of C-H IR Stretching Bands of Ethane and Propane Adsorbed by Zeolites as a New Spectral Criterion of Their Chemical Activation via Polarization Resulting from Stretching of Chemical Bonds.
Journal of Physical Chemistry B **110**, 17468-17477 (2006).

Kazansky, V. B., I. R. Subbotina, A. A. Pronin, R. Schlögl and F. C. Jentoft: Unusual Infrared Spectrum of Ethane Adsorbed by Gallium Oxide.
Journal of Physical Chemistry B **110**, 15, 7975-7978 (2006).

Kharrazi, S., D.C. Kundaliya, G.-Q. Gosavi, S.K. Kulkarni, T. Venkatesan, S.B. Ogale, J. Urban, S. Park and S.-W. Cheong: Multiferroic TbMnO3 nanoparticles.
Solid State Communications **138**, 395-398 (2006).

Klose, B. S., F. C. Jentoft, P. Joshi, A. Trunschke, R. Schlögl, I. R. Subbotina and V. B. Kazansky: In Situ Spectroscopic Investigation of Activation, Start-Up and Deactivation of Promoted Sulfated Zirconia Catalysts.
Catalysis Today **116**, 121-131 (2006).

2006

Kovnir, K., M. Armbrüster, D. Teschner, T. Venkov, F. C. Jentoft, A. Knop-Gericke, Y. Grin and R. Schlögl: A New Approach to Well-Defined, Stable and Site-Isolated Catalysts.
Science and Technology of Advanced Materials, accepted (2006).

Kurr, P., A. Furche, A. Trunschke, R. Schlögl and T. Ressler: In situ investigations of Cu/ZnO catalysts during calcination in different gas atmospheres.
HASYLAB Annual Report 2006, 1347-1348 (2006).

Kustov, A. L., K. Egeblad, M. Kustova, T. W. Hansen and C. H. Christensen: Mesoporous Fe-Containing ZSM-5 Zeolite Single Crystal Catalysts for Selective Catalytic Reduction of Nitric Oxide by Ammonia.
Topics in Catalysis **45**, 1-4, 159-163 (2006).

Lu, Y., D. S. Su, Z. P. Zhu, G. Weinberg, R. Schlögl and L. Zhenyu: Blowing Behavior of Carbon Nanotube.
Nano Letters, submitted (2006).

Ma, H.-L., D. S. Su, A. Klein-Hoffmann, G.-Q. Jin and X.-Y. Guo: Morphologies and microstructures of tree-like carbon produced at different reaction conditions in a CVD process.
Carbon **44**, 11, 2254-2260 (2006).

Müller, J.-O., D. S. Su, R. E. Jentoft, U. Wild and R. Schlögl: Diesel Engine Exhaust Emission: Oxidative Behavior and Microstructure of Black Smoke Soot Particulate.
Environmental Science and Technology **40**, 4, 1231-1236 (2006).

Paál, Z., A. Wootsch, I. Bakos, S. Szabo, H. Sauer, U. Wild and R. Schlögl: Effect of hydrogen pressure on intentional deactivation of unsupported Pt catalyst: Catalytic properties and physical characterization.
Applied Catalysis A **309**, 1-9 (2006).

Penner, S., B. Jenewein, H. Gabasch, B. Klötzer, D. Wang, A. Knop-Gericke, R. Schlögl and K. Hayek: Growth and structural stability of well-ordered PdZn alloy nanoparticles.
Journal of Catalysis **241**, 1, 14-19 (2006).

Penner, S., B. Jenewein, D. Wang, R. Schlögl and K. Hayek: Structure–activity correlations in thin film model catalysts: CO hydrogenation on Rh/VOx Part I. The morphology, composition and structure of vanadia-supported and -promoted Rh particles upon oxidation and reduction.
Applied Catalysis A: General **308**, 31-42 (2006).

Penner, S., B. Jenewein, D. Wang, R. Schlögl and K. Hayek: Rh-V alloy formation in Rh-VOx thin films after high-temperature reduction studied by electron microscopy.
Physical Chemistry Chemical Physics **8**, 10, 1223-1229 (2006).

Penner, S., D. Wang, B. Jenewein, H. Gabasch, B. Klötzer, A. Knop-Gericke, R. Schlögl and K. Hayek: Growth and decomposition of aligned and ordered PdO nanoparticles.
Journal of Chemical Physics **125**, 9, 094703-1-094703-8 (2006).

Perathoner, S., P. Lanzafame, R. Passalacqua, G. Centi, R. Schlögl and D. S. Su: Use of mesoporous SBA-15 for nanostructuring titania for photocatalytic applications.
Microporous and Mesoporous Materials **90**, 347-361 (2006).

Publications

2006

Max Planck Society
eDoc Server

Pozdnyakova, O., D. Teschner, A. Wootsch, J. Kröhnert, B. Steinhauer, H. Sauer, L. Tóth, F. C. Jentoft, A. Knop-Gericke, Z. Paál and R. Schlögl: Preferential CO oxidation in hydrogen (PROX) on ceria-supported catalysts PART I. Oxidation state and surface species on Pt/CeO2 under reaction conditions.
Journal of Catalysis **237**, 1, 1-16 (2006).

Pozdnyakova, O., D. Teschner, A. Wootsch, J. Kröhnert, B. Steinhauer, H. Sauer, L. Tóth, F. C. Jentoft, A. Knop-Gericke, Z. Paál and R. Schlögl: Preferential CO oxidation in hydrogen (PROX) on ceria-supported catalysts PART II. Oxidation states and surface species on Pd/CeO2 under reaction conditions, suggested reaction mechanism.
Journal of Catalysis **237**, 1, 17-28 (2006).

Pozdnyakova, O., D. Teschner, A. Wootsch, H. Sauer, A. Knop-Gericke and R. Schlögl: Surface and structural properties of Pt/CeO2 catalyst under preferential CO oxidation in hydrogen (PROX).
Reaction Kinetics and Catalysis Letters **87**, 2, 235-247 (2006).

Prati, L., A. Villa, D. S. Su, D. Wang, Z. Krpetic and F. Porta: Single-phase bimetallic system for the selective oxidation of glycerol to glycerate.
SCIENTIFIC BASES FOR THE PREPARATION OF HETEROGENEOUS CATALYSTS Studies in Surface Science and Catalysis **162**. Elsevier, Amsterdam (2006) 553-560.

Ranke, W., A. Schüle, O. Shekhah, G. Kolios, U. Nieken and R. Schlögl: Deactivation of styrene catalysts: A microkinetic modelling approach to technical catalysts.
10th International Symposium on Catalyst Deactivation, Book of Extended Abstracts DECHEMA e.V., Frankfurt am Main (2006) 234-238.

Riebau, R.-B. and U. Siebeky: Open Access und Copyright. Ein Leitfaden für Autoren wissenschaftlicher Publikationen. Nützliche Hinweise für Wissenschaftlerinnen und Wissenschaftler des Fritz-Haber-Instituts der Max-Planck-Gesellschaft. 1. Version (2006) 1-47.

Rödel, T. C., D. Wang, D. S. Su, M. Lerch, A. Prokofiev, K. D. Luther and W. Assmus: Nitrogen-doped zirconia single crystals.
Crystal Research and Technology **41**, 10, 950-954 (2006).

Schlögl, R.: High-Resolution Aberration-Corrected TEM of Oxidation Catalysis.
Microscopy and Analysis / European Edition / Supplement **20**, 7-7 (2006).

Schlögl, R., S. Wrabetz (Eds.): Department of Inorganic Chemistry - Fritz-Haber-Institut der Max-Planck-Gesellschaft. 2. Edition Department of Inorganic Chemistry / FHI, Berlin (2006) 1-43.

Schnörch, P., E. Vass, S. Zafeiratos, D. Teschner, M. Hävecker, A. Knop-Gericke and R. Schlögl: In situ XPS study on (MoV)5O14 selective oxidation catalysts.
BESSY Annual Report 2005, 286-288 (2006).

Su, D. S., J.-O. Müller, D. Rothe, E. Jacob and R. Schlögl: Carbon Nanoparticles in Soot from Low Emission Diesel Engine.
Nature, submitted (2006).

2006

Sun, J., D. Ma, H. Zhang, C. L. Wang, X. Bao, D. S. Su, A. Klein-Hoffmann, G. Weinberg and S. Mann: Phase evolution in the alkane-P123-water-TEOS quadru-component system: a feasible route to different complex mesostructured materials.
Journal of Materials Chemistry **16**, 16, 1507-1510 (2006).

Sun, J.M., D. Ma, H. Zhang, X.M. Liu, X.W Han, X.H. Bao, G. Weinberg, N. Pfänder and D.S. Su: Toward Monodispersed Silver Nanoparticles with Unusual Thermal Stability.
Journal of the American Chemical Society **128**, 49, 15756-15764 (2006).

Sun, J., H. Zhang, R. Tian, M. Ding, X. Bao, D. S. Su and H. Zou: Ultrafast enzyme immobilization over large-pore nanoscale mesoporous silica particles.
Chemical Communications, 12, 1322-1324 (2006).

Teschner, D., E. Vass, M. Hävecker, S. Zafeiratos, P. Schnörch, H. Sauer, A. Knop-Gericke, R. Schlögl, M. Chamam, A. Wootsch, A. S. Canning, J. J. Gamman, S. D. Jackson, J. McGregor and L. F. Gladden: Alkyne Hydrogenation over Pd Catalysts: A New Paradigm.
Journal of Catalysis **242**, 26-37 (2006).

Teschner, D., E. Vass, S. Zafeiratos, P. Schnörch, M. Hävecker, A. Knop-Gericke, H. Sauer, J. Kröhnert, F. C. Jentoft, R. Schlögl, O. Pozdnyakova and A. Wootsch: Preferential CO oxidation in H2 (PROX) on Pt/CeO2 catalyst, high-pressure XPS and in-situ DRIFTS study.
BESSY Annual Report 2005, 254-256 (2006).

Teschner, D., E. Vass, S. Zafeiratos, P. Schnörch, E. Kleimenov, M. Hävecker, A. Knop-Gericke and R. Schlögl: Selective gas-phase hydrogenation of aliphatic triple and double bond using palladium based catalysts.
BESSY Annual Report 2005, 257-259 (2006).

Tomašić, N., A. Gajović, V. Bermanec, D. S. Su, M. Rajić-Linarić, T. Ntaflos and R. Schlögl: Recrystallization mechanisms of fergusonite from metamict mineral precursors.
Physics and Chemistry of Minerals **33**, 2, 145-159 (2006).

Trunschke, A., R. Schlögl, V. V. Guliants, A. Knoester and H. Brongersma: Surface analysis of the ab-plane of MoVTeNbOx catalysts for propane (amm) oxidation by low energy ion scattering (LEIS).
Proceedings of the 232nd ACS National Meeting, San Francisco. American Chemical Society, Washington, D. C, San Francisco, CA, United States (2006).

Unterberger, W., B. Jenewein, B. Klötzer, S. Penner, W. Reichl, G. Rupprechter, D. Wang, R. Schlögl and K. Hayek: HYDROGEN-INDUCED METAL-OXIDE INTERACTION STUDIED ON NOBLE METAL MODEL CATALYSTS.
Reaction Kinetics and Catalysis Letters **87**, 2, 215-234 (2006).

Vass, E., D. Teschner, A. Knop-Gericke, M. Hävecker, S. Zafeiratos, P. Schnörch, E. Kleimenov and R. Schlögl: Dehydrogenation of C4 hydrocarbons using vanadium based catalysts.
BESSY Annual Report 2005, 267-269 (2006).

von Dahl, C. C., M. Hävecker, R. Schlögl and I. T. Baldw
Caterpillar-elicited methanol emission: a new signal in plant-herbivore interactions?.
The Plant Journal **46**, 6, 948-960 (2006).

Publications

2006

Max Planck Society
eDoc Server

Wagner, J. B., N. D. Othman, D. S. Su, S. B. Abd Hamid and R. Schlögl: Characterization of Nanostructured Binary Molybdenum Oxide Catalyst Precursors for Propene Oxidation.
Journal of Microscopy **223**, 3, 216-219 (2006).

Wagner, J. B., O. Timpe, F. A. Hamid, A. Trunschke, U. Wild, D. S. Su, R. K. Widi, S. B. Abd Hamid and R. Schlögl: Surface Texturing of Mo-V-Te-Nb-Ox Selective Oxidation Catalysts.
Topics in Catalysis **38**, 1-3, 51-58 (2006).

Wagner, J. B., M.-G. Willinger, J.-O. Müller, D. S. Su and R. Schlögl: Surface-Charge-Induced Reversible Phase Transitions of Bi Nanoparticles.
Small **2**, 2, 230-234 (2006).

Wang, D., A. Villa, F. Porta, D. S. Su and L. Prati: Single-phase bimetallic system for the selective oxidation of glycerol to glycerate.
Chemical Communications, 18, 1956-1958 (2006).

Willneff, E. A., S. Braun, D. Rosenthal, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke, R. Schlögl and S. L. M. Schroeder: Dynamic Electronic Structure of a Au/TiO_2 Catalyst under Reaction Conditions.
Journal of the American Chemical Society **128**, 37, 12052-12053 (2006).

Xiao, F.-S., L. Wang, C. Yin, K. Lin, Y. Di, J. Li, R. Xu, D. S. Su, R. Schlögl, T. Yokoi and T. Tatsumi: Catalytic Properties of Hierarchical Mesoporous Zeolites Templated with a Mixture of Small Organic Ammonium Salts and Mesoscale Cationic Polymers.
Angewandte Chemie - International Edition **45**, 19, 3090-3093 (2006).

Yang, X., Z. Li, B. Liu, A. Klein-Hoffmann, G. Tian, Y. Feng, Y. Ding, D. S. Su and F.-S. Xiao: "Fish-in-Net" Encapsulation of Enzymes in Macroporous Cages for Stable, Reusable, and Active Heterogeneous Biocatalysts.
Advanced Materials **18**, 4, 410-414 (2006).

Yang, X., R. E. Jentoft and F. C. Jentoft: n-Butane Isomerization Catalyzed by Sulfated Zirconia Nanocrystals Supported on Silica or γ-Alumina.
Catalysis Letters **106**, 3-4, 195-203 (2006).

Zafeiratos, S., G. Papakonstantinou, F. Paloukis, A. Knop-Gericke, S. G. Neophytides and R. Schlögl: A comparative in situ XPS study of PtRuCo catalyst for CH_3OH and CO oxidation using water.
BESSY Annual Report 2005, 283-285 (2006).

Zemlyanov, D., B. Aszalos-Kiss, E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke, R. Schlögl, H. Gabasch, W. Unterberger, K. Hayek and B. Klötzer: In-situ XPS study of Pd(111) oxidation, Part 1: 2D oxide formation in 10-3 mbar O2.
Surface Science **600**, 5, 983-994 (2006).

Zhang, H., J.M. Sun, D. Ma, G. Weinberg, D. S. Su and X.H. Bao: Engineered Complex Emulsion System: Toward Modulating the Pore Length and Morphological Architecture of Mesoporous Silicas.
Journal of Physical Chemistry B **110**, 51, 25908-25915 (2006).

2006 / 2007

Zimowska, M., J. B. Wagner, J. Dziedzic, J. Camra, B. Borzecka-Prokop and M. Najbar: Some aspects of metal-support strong interactions in Rh/Al2O3 catalyst under oxidising and reducing conditions.
Chemical Physics Letters **417**, 1-3, 137-142 (2006).

Blume, R., M. Hävecker, S. Zafeiratos, D. Teschner, E. Vass, P. Schnörch, A. Knop-Gericke, R. Schlögl, S. Lizzit, P. Dudin, A. Barinov and M. Kiskinova: Monitoring in-situ catalytically active states of Ru catalysts for different methanol oxidation pathways.
Physical Chemistry Chemical Physics **9**, 27, 3648-3657 (2007).

Bron, M., D. Teschner, A. Knop-Gericke, F. C. Jentoft, J. Kröhnert, J. Hohmeyer, C. Volckmar, B. Steinhauer, R. Schlögl and P. Claus: Silver as acrolein hydrogenation catalyst: intricate effects of catalyst nature and reactant partial pressures.
Physical Chemistry Chemical Physics **9**, 27, 3559-3569 (2007).

Cai, Y., S. K. Chan, I. K. Sou, Y. F. Chan, D. S. Su and N. Wang: Temperature-Dependent Growth Direction of Ultrathin ZnSe Nanowires.
Small **3**, 1, 111-115 (2007).

Centi, G., R. Passalacqua, S. Perathoner, D. S. Su, G. Weinberg and R. Schlögl: Oxide thin films based on ordered arrays of 1D nanostructure. A possible approach toward bridging material gap in catalysis.
Physical Chemistry Chemical Physics **9**, 35, 4930-4938 (2007).

Chen, X., D. S. Su, S. B. Abd Hamid and R. Schlögl: The morphology, porosity and productivity control of carbon nanofibers or nanotubes on modified activated carbon.
Carbon **45**, 4, 895-898 (2007).

Chen, X., Z. P. Zhu, M. Hävecker, D. S. Su and R. Schlögl: Carbon nanotube-induced preparation of vanadium oxide nanorods: application as a catalyst for the partial oxidation of n-butane.
Materials Research Bulletin **42**, 354-361 (2007).

Delgado, J. J., X. Chen, D. S. Su and R. Schlögl: A Novel Catalyst for Synthesis of Styrene: Carbon Nanofibers Immobilized on Activated Carbon.
Journal of Nanoscience and Nanotechnology **7**, 3495--3501 (2007).

Denkwity, Y, S. Kielbassa, B. Schumacher, J. Bansmann, P. Schnörch, E. M. Vass, M. Hävecker, A. Knop-Gericke, R. Schlögl and R. J. Behm: In situ X-ray photoelectron spectroscopy on supported powder and model Au/TiO2 catalysts - influence of the material gap.
BESSY Annual Report 2006, 110-112 (2007).

Djerdj, I., G. Garnweimer, D. S. Su and M. Niederberger: Morphology-Controlled Nonaqueous Synthesis of Anisotropic Lanthanum Hydroxide Nanoparticles.
Journal of Solid State Chemistry **180**, 7, 2154-2165 (2007).

Frank, B., F. C. Jentoft, H. Soerijanto, J. Kröhnert, R. Schlögl and R. Schomäcker: Steam reforming of methanol over copper-containing catalysts: influence of support material on microkinetics.
Journal of Catalysis **246**, 177-192 (2007).

Fu, Q., G. Weinberg and D. S. Su: Selective filling of carbon nanotubes with metals via selective washing. Carbon, submitted (2007).

Publications

2007

Max Planck Society
eDoc Server

Gabasch, H., A. Knop-Gericke, R. Schlögl, M. Borasio, C. Weilach, G. Rupprechter, S. Penner, B. Jenewein, K. Hayek and B. Klötzer: Comparison of the reactivity of different Pd-O species in CO oxidation.
Physical Chemistry Chemical Physics **9**, 4, 533-540 (2007).

Gajović, A., D. Gracin, I. Djerdj, N. Tomašić, K. Juraić and D. S. Su: Nanostructure and Optical Properties of the Thin Silicon Films.
Journal of Applied Crystallography, submitted (2007).

Gajović, A., N. Tomašić, I. Djerdj, D. S. Su and K. Furić: Influence of mechanochemical processing to luminescence properties in Y2O3.
Journal of Alloys and Compounds, accepted (2007).

Gajović, A., A. Šantić, I. Djerdj, N. Tomašić, A. Moguš-Milanković and D. S. Su: Zirconium Titanate Ceramics for Humidity Sensors Synthesized by Mechanochemical Treatment and Sintering.
Journal of European Ceramics Society, submitted (2007).

Gutel, T., J. Garcia-Antõn, K. Pelzer, K. Philippot, C. C. Santini, Y. Chauvin, B. Chaudret and J.-M. Basset: Influence of the self-organization of ionic liquids on the size of ruthenium nanoparticles: Effect of the temperature and stirring.
Journal of Materials Chemistry, accepted (2007).

Hess, C.: Direct correlation of the dispersion and structure in vanadium oxide supported on silica SBA-15.
Journal of Catalysis **248**, 120-123 (2007).

Hébert, C., D. S. Su and P. Pongratz: Mechanism for the reduction of V2O5 to VO by electron irradiation.
Philosophical Magazine, submitted (2007).

Huang, W., W. Ranke and R. Schlögl: Reduction of an α-Fe2O3(0001) Film Using Atomic Hydrogen.
Journal of Physical Chemistry B **111**, 5, 2198-2204 (2007).

Kaneko, K., K. Inoke, B. Freitag, A.B. Hungria, P.A. Midgley, T.W. Hansen, J. Zhang, S. Ohara and T. Adschiri: Structural and morphological characterization of cerium oxide nanocrystals prepared by hydrothermal synthesis.
Nano Letters **7**, 2, 421-425 (2007).

Kasatkin, I., B.-L. Kniep and T. Ressler: Cu/ZnO and Cu/ZrO2 interactions studied by contact angle measurement with TEM.
Physical Chemistry Chemical Physics **9**, 7, 878-883 (2007).

Kornelak, P., B. Borzęcka-Prokop, L. Lityńska-Dobrzyńska, J. B. Wagner, D. S. Su, J. Camra and A. Wesełucha-Birczyńska: The physicochemical properties of rutile-supported V-O-Mo catalyst.
Catalysis Today **119**, 204-208 (2007).

Kubias, B., M.J.G. Fait and R. Schlögl: Mechanochemical Methods.
2nd Handbook of Heterogeneous Catalysis., accepted (2007).

2007

Li, H., G. Sun, N. Li, S. Sun, D. S. Su and Q. X
Design and Preparation of Highly Active Pt-Pd/C Catalyst for the Oxygen Reduction Reaction.
The Journal of Physical Chemistry C **111**, 5605-5617 (2007).

Liu, X., D.S. Su and R. Schlögl: ODH of 1-butene to Butadien over Carbon nanotubes catalyst.
Chemical Communications, submitted (2007).

Ma, H.-L., D.S. Su, G.-Q. Jin and X.-Y. Guo: The influence of formation conditions on the growth and structure of carbon trees.
Carbon **45**, 8, 1622-1627 (2007).

Müller, J.-O., D. S. Su, U. Wild and R. Schlögl: Bulk and Surface Structural Investigations of Diesel Engine Soot and Carbon Black.
Physical Chemistry Chemical Physics **9**, 30, 4018-4025 (2007).

Pelzer, K., J.-P. Candy, G. Bergeret and J.-M. Basset: Ru nanoparticles stabilized by organosilane fragments: Influence of the initial Si/Ru ratio and thermal stability.
European Physical Journal D **43**, 197-200 (2007).

Pelzer, K., J.-P. Candy, G. Godard and J.-M. Basset: Surface Organometallic Chemistry on Metal: Synthesis, Characterization and Application in Catalysis. Ed.: D. Astruc, Wiley VCH Verlag, Weinheim, in press (2007).

Pietraszek, A., P. Da Costa, R. Marques, P. Kornelak, T.W. Hansen, J. Camra and M. Najbar: The effect of the Rh-Al, Pt-Al and Pt-Rh-Al surface alloys on NO conversion to N2 on alumina supported Rh, Pt and Pt-Rh catalysts.
Catalysis Today **119**, 187-193 (2007).

Pozdnyakova-Tellinger, O., D. Teschner, J. Kröhnert, F. C. Jentoft, A. Knop-Gericke, R. Schlögl and A. Wootsch: Surface water assisted preferential CO oxidation on Pt/CeO2 catalyst.
The Journal of Physical Chemistry C **111**, 14, 5426-5431 (2007).

Prati, L., A. Villa, F. Porta, D. Wang and D.S. Su: Single-phase gold/palladium catalyst: the nature of synergistic effect.
Catalysis Today **122**, 386-390 (2007).

Reichelt, R., S. Günther, M. W. Rößler, J. Wintterlin, B. Kubias, B. Jacobi and R. Schlögl: High-pressure STM of the interaction of oxygen with Ag(111).
Physical Chemistry Chemical Physics **9**, 27, 3590-3599 (2007).

Ressler, T. and O. Timpe: Time-resolved studies on correlations between dynamic electronic structure and selectivity of a H5[PV2Mo10O40] partial oxidation catalyst.
Journal of Catalysis **247**, 231-237 (2007).

Rödel, E., O. Timpe, A. Trunschke, G. A. Zenkovets, G. N. Kryukova, R. Schlögl and T. Ressler: Structure stabilizing effect of tungsten in mixed molybdenum oxides with Mo5O14-type structure.
Catalysis Today **126**, 1-2, 112-118 (2007).

Publications

2007

Max Planck Society
eDoc Server

Sakthivel, A., A. Trunschke, T. W. Hansen, A. Celaya Sanfiz, F. Girgsdies, R. E. Jentoft and R. Schlögl: A novel synthetic route to mesostructured MoVTeNb mixed oxide.
Chemical Communications, submitted (2007).

Schlögl, R.: Ammonia Synthesis.
Handbook of Heterogeneous Catalysis: 2nd Edition in 8 Volumes. Eds.: G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Wiley-VCH Verlag, Weinheim, accepted (2007).

Schlögl, R.: Carbons.
Handbook of Heterogeneous Catalysis: 2nd Edition in 8 Volumes. Eds.: G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Wiley-VCH Verlag, Weinheim, accepted (2007).

Schlögl, R.: Fused Catalysts.
Handbook of Heterogeneous Catalysis: 2nd Edition in 8 Volumes. Eds.: G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Wiley-VCH Verlag, Weinheim, accepted (2007).

Schnörch, P., E. Vass, S. Zafeiratos, D. Teschner, M. Hävecker, A. Knop-Gericke and R. Schlögl: In situ XPS study on (MoV)5O14 selective oxidation catalysts.
BESSY Annual Report 2006, 83-85 (2007).

Schüle, A., U. Nieken, O. Shekhah, W. Ranke, R. Schlögl and G. Kolios: Styrene synthesis over iron oxide catalysts: from single crystal model system to real catalyst.
Physical Chemistry Chemical Physics **9**, 27, 3619-3634 (2007).

Su, D. S. and X. Chen: Natural Lavas as Catalysts for Efficient Production of Carbon Nanotubes and Nanofibers.
Angewandte Chemie International Editon **46**, 11, 1823-1824 (2007).

Su, D. S., N. I. Maksimova, G. Mestl, V. L. Kuznetsov, V. Keller, R. Schlögl and N. Keller: Oxidative dehydrogenation of ethylbenzene to styrene over ultra-dispersed diamond and onion-like carbon.
Carbon **45**, 11, 2145-2151 (2007).

Su, D.S., A. Rinaldi, W. Frandsen and G. Weinberg: Nanocarbons: Efficient synthesis using natural lava as catalyst and support.
physica status solidi b, submitted (2007).

Sun, J. M., D. Ma, H. Zhang, X. H. Bao, G. Weinberg and D. S. Su: Macro–mesoporous silicas complex and the carbon replica.
Microporous and Mesoporous Materials **100**, 1-3, 356-360 (2007).

Teschner, D., E. Vass, S. Zafeiratos, P. Schnörch, M. Hävecker, A. Knop-Gericke, H. Sauer, J. Kröhnert, F. C. Jentoft, R. Schlögl, G. Hutchings, O. Pozdnyakova-Tellinger, K. Lazar and A. Wootsch: Preferential oxidation of CO over supported and alloy catalysts in H2-rich gas for fuel cell application.
BESSY Annual Report 2006, 89-91 (2007).

Teschner, D., A. Wootsch, O. Pozdnyakova-Tellinger, J. Kröhnert, E. Vass, M. Hävecker, S. Zafeiratos, P. Schnörch, F. C. Jentoft, A. Knop-Gericke and R. Schlögl: Partial pressure dependent in-situ spectroscopic study on the preferential CO oxidation in hydrogen (PROX) over Pt/ceria catalysts.
Journal of Catalysis **249**, 318-327 (2007).

2007

Tessonnier, J.-P., T.W. Hansen, C. Hess, D.S. Su and R. Schlögl: Nanostructured catalysts: unusual activity of MoxOy thin films supported on carbon nanotubes.
Journal of the American Chemical Society, submitted (2007).

Vass, E. M., D. Teschner, M. Hävecker, S. Zafeiratos, P. Schnörch, A. Knop-Gericke and R. Schlögl: Dehydrogenation and Oxidative Dehydrogenation of n-Butane using Vanadium Based Catalysts: an in situ XPS study.
BESSY Annual Report 2006, 94-96 (2007).

Venkov, T. V., C. Hess and F. C. Jentoft: Redox Properties of Vanadium Ions in SBA-15 Supported Vanadium Oxide: an FTIR Spectroscopic Study.
Langmuir **23**, 4, 1768-1777 (2007).

Virnovskaia, A., S. Jørgensen, J. Hafizovic, Ø. Prytz, E. Kleimenov, M. Hävecker, H. Bluhm, A. Knop-Gericke, R. Schlögl and U. Olsbye: In situ XPS investigation of Pt(Sn)/Mg(Al)O catalyst during ethane dehydrogenation experiments.
Surface Science **601**, 1, 30-43 (2007).

Wagner, J. B., N. D. Othman, S. Knobl, D. Niemeyer, A. Trunschke, D. S. Su, S. B. Abd Hamid and R. Schlögl: Electron Microscopy Studies of Nanostructured Binary Molybdenum Oxide Catalysts for Propene Oxidation.
Journal of Catalysis, submitted (2007).

Wang, D., F. Ammari, R. Touroude, D. S. Su and R. Schlögl: TEM Characterisation of Pt-ZnO catalysts for selective hydrogenation of crotonaldehyde to crotyl alcohol.
Journal of Catalysis, submitted (2007).

Wang, L., J.J. Delgado, Z. Zhang, Z.L. Shan, D.S. Su and F.-S. Xiao: A simple and efficient anion-exchange route to hierarchical porous carbon materials.
Journal of Catalysis, submitted (2007).

Wang, L., J. Zhang, D.S. Su, Y. Ji, X. Cao and F.-S. Xiao: Simple Preparation of Honeycomb-like Macrostructured and Microporous Carbons with High Performance in Oxidative Dehydrogenation of Ethylbenzene.
Chemistry of Materials **19**, 11, 2894-2897 (2007).

Wu, Y., H.-M. Liu, B.-Q. Xu, Z.-L. Zhang and D. S. Su: Single-Phase Titania Nanocrystallites and Nanofibers from Titanium Tetrachloride in Acetone and Other Ketones.
Inorganic Chemistry **46**, 12, 5093-5099 (2007).

Zafeiratos, S., V. I. Bukhtiyarov, M. Hävecker, D. Teschner, E. Vass, P. Schnörch, G. Weinberg, A. Knop-Gericke and R. Schlögl: Ethylene epoxidation over copper-silver bimetallic catalyst: surface characterisation under reaction conditions.
BESSY Annual Report 2006, 71-73 (2007).

Zemlyanov, D., H. Gabasch, B. Klötzer, A. Knop-Gericke and R. Schlögl: Kinetics of palladium oxidation and methane oxidation on Pd(111) and (110).
BESSY Annual Report 2006,121-123 (2007).

Publications

2007

Max Planck Society
eDoc Server

Zenkovets, G. A., G. N. Kryukova, V. Y. Gavrilov, S. V. Tsybulya, V. A. Anufrienko, T. A. Larina, D. F. Khabibulin, O. B. Lapina, E. Rödel, A. Trunschke, T. Ressler and R. Schlögl: The structural genesis of a complex (MoVW)5O14 oxide during thermal treatments and its redox behavior at elevated temperatures. Materials Chemistry and Physics **103**, 2-3, 295-304 (2007).

Zhang, J., M. Comotti, F. Schüth, R. Schlögl and D. S. Su: Commercial Fe- or Co-Containing Carbon Nanotubes as Catalysts for NH3 Decomposition.
Chemical Communications, 19, 1916-1918 (2007).

Zhang, J., Y. Hu, J.-P. Tessonnier, G. Weinberg, J. Maier, R. Schlögl and D. S. Su: CNFs@CNTs: Superior Carbon for Electrochemical Energy Storage.
Science, submitted (2007).

Zhang, J., D.S. Su, A. Zhang, D. Wang, R. Schlögl and C. Hébert: Nanocarbon as Robust Catalyst: Mechanistic Insight into Carbon-Mediated Catalysis.
Angewandte Chemie International Edition **46**, 38, 7319-7323 (2007).

Zhang, Z. and D.S. Su: Behaviour of TEM metal-grids during in-situ heating experiments.
Ultramicroscopy, submitted (2007).

Patents

1993 - 2007

EP635515/PN, July 23, 1993
"Metallfullerene intercalation compounds, process for their preparation and use as catalysts"
Inventors: R. Schloegl, H. Werner, M. Wohlers

DE4404329/PN February 11, 1994, EP0667180
"Process for the disposal of halogenated hydrocarbons"
Inventors: C. Scholz, W. Holzinger, R. Schloegl

DE19637205/PN, September, 12, 1996
„Ion molecule reaction mass spectroscopy method for gas analysis"
Inventors: H. Hertl, D. Bassi, I. Povo, R. Schloegl

Patents

1993 - 2007

EP925111/PN September 5, 1997
„Catalyst of process for its manufacture"
Inventors: R. Schloegl, M. Wohlers, Th. Belz, Th. Braun

DE 19843329/PN, April 08, 1999
„Preparation of methacrylic acid"
Inventors: F. Rosowski, H. Hibst, R. Schloegl, D. Herein, S. Berndt

DE 198 10 539, October 7, 1999/US No.6, 212,253 B1 April 3, 2001
„Apparatus and method for X-ray absorption spectroscopy"
Inventors, Th. Schedel-Niedrig, A. Knop-Gericke, M. Haevecker

PCT/EP2004/002765 March 17, 2004 based on EP03 005 953.9,
"Cu-Cu0/ZrO2 catalyst in Steam reforming of Methanol"
Inventors: R. Schloegl, Th. Ressler, F. Giergsdies, H. Purnama, R. Schomaecker, M. Antonietti, J.H. Schattka, Y. Wang, R. Caruso

EP04009874, April 26, 2004
"Assembly of carbon tube-in-tube nanostructures"
Inventors: Z. Zhu, D. Su, R. Schloegl

EP2005/008022, July 22, 2005
"Metal oxide catalyst and method for the preparation"
Inventors: R. Schlögl, O.Timpe, S.B. Abd Hamid

WO06008049A1, January 26,2006
"Catalyst comprising nanocarbon structures for the production of unsaturated hydrocarbons"
Inventors: R. Schlögl, G. Mestl

EP06005209.9, March 14, 2006
"Zirconium oxynitride catalysts for ammonia decomposition"
Inventors: R. Schlögl, T. Ressler, R. Jentoft

EP 06005310.5, March 15, 2006
"Palladium-Gallium intermetallic compounds as catalysts for the selective hydrogenation of acetylene"
Inventors: J. Grin, R. Schlögl, J. Osswald

EP2006/00346, April 13, 2006
"Nanocarbon-activated carbon composites"
Inventors: R. Schlögl, S.B. Abd Hamid

Guest - lectures
2003 - 2007

Date	Guest - Lucturer	Titel
08.01.2003	**Dr. Johan Carlsson** Fritz-Haber-Institut, Abt. Theorie	First-principles study of oxygen activation of carbon materials for styrene catalysis
15.01.2003	**Dipl.-Phys. Gerrit Herbst** Fimea, Berlin	"Athermischer Lasermaterialabtrag" ein neuer Ansatz zur schädigungsfreien Mikromaterialbearbeitung und zur Oberflächenstrukturierung bis in den nm-Bereich
22.01.2003	**Dr. D. Herein** Institut für Angewandte Chemie, Berlin	The use of hard X-rays for XAS at BESSY II: Status and future perspectives
05.03.2003	**Dr. Elizabeth Duplock** School of Physical Sciences, University of Kent at Canterbury, England	Insights into the Absorption of Hydrogen on Carbon Nanotubes from First Principles
07.03.2003	**Prof. Dr. Lynn Gladden** Department of Chemical Engineering, University of Cambridge, U.K.	New Directions in Applied Catalysis Research
12.03.2003	**Dr. Luis M. Liz-Marzan** Department of Physical Chemistry, University of Vigo, Spain	Optical Properties of Metal Nanoparticles and Assemblies
10.04.2003	**Prof. Dr. Kenneth C Waugh** Universty of Manchester, UMIST, Manchester, England	Reconstruction Leading to Unstable Behaviour in Methanol Synthesis and Methanol Oxidation on $Cu/ZnO/Al_2O_3$ Catalysts
16.04.2003	**Prof. Dr. V. Kazansky** N. D. Zelinsky Institute of the Russian Academy of Sciences, Moscow, Russia	Intensities of IR stretching bands as a criterion of activation of adsorbed molecules in heterogeneous acid and acid-base catalysis
23.04.2003	**Dr. B. Klötzer** Institut für Physikalische Chemie der Universität Innsbruck	V in different oxidation states on Rh- and Pd-surfaces: structural and catalytic aspects

Date	Guest - Lecturer	Titel
14.05.2003	**Prof. Dr. François Garin** Universität Strasburg	Nanosciences in catalysis and automotive pollution control
18.06.2003	**Dr. John Titantah** University of Antwerp, Belgium	DFT calculation of the carbon K-edges of carbon structures: sp2/sp3 characterisation
6.08.2003	**Prof. Dr. Meisel** Humboldt Universität, Berlin	Von molekularen Aggregaten zu Koordinationspolymeren - Neues zur Bildung und Strukturchemie von Organophosphonaten des Vanadiums
20.08.2003	**Dr. Fabrice Dassenoy** Ecole Centrale de Lyon, France	Mo-S-I nanotubes as new lubricant additives : tribological properties
27.08.2003	**Dr. Simon R. Bare** UOP LLC, Des Plaines, IL, USA	Recent in situ and operando XAFS catalyst characterization at UOP
24. 09.2003	**Priv.-Doz. Dr. Thomas Schedel-Niedrig** Hahn-Meitner-Institut Berlin GmbH	Dünnschichten für die Anwendung in der Photovoltaik: Strukturelle und elektronische Eigenschaften von CVD-Chalkopyrit
01.10.2003	**Prof. Dr. Hasinger und Prof. Dr. Strüder** Max-Planck-Institut für extraterrestrische Physik, Garching	Roentgendiagnose im Kosmos & Ortsaufgeloeste Hoechstraten-spektroskopie mit Roentgenstrahlen

Date	Guest - Lecturer	Titel
14. 01.2004	**Prof. Dr. Piotr Dluzewski** University of Warschau, Poland	Structure of Pd nanocrystals in carboaceous thin film studied by TEM
15. 01.2004	**Prof. Dr. Alfred Frennet** Université Libre de Bruxelles, Belgique	Mechanistic informations from chemical transient kinetic studies on the catalytic syngas reaction
11. 02.2004	**Prof. Dr. Valery A. Zazhigalov** Institute for Sorption and Problems of Endoecology, National Academy of Sciences of Ukraine	The process of n-pentane partial oxidation and the catalysts for its realization

AC FHI Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Guest - lectures

2003 - 2007

Date	Guest - Lecturer	Titel
12. 02.2004	**Dr. Frank Ogletree** Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA	Oxygen on Pd(111) investigated with variable temperature STM and in-situ photoemission
31. 03.2004	**Dr. Cécile Hébert** Institut für Festkörperphysik , TU Wien, Austria	New aspects of the reduction of V_2O_5 in the TEM
18.05.2004	**Prof. Dr. Lanny Schmidt** Dept. of Chemical Engineering and Material Sciences, Univ. Minneapolis, USA	Hydrogen from Fossil and Renewable Fuels by Autothermal Reforming
09.06.2004	**Dr. Martin Steinhart** Max Planck Institute of Microstructure Physics, Halle	Template wetting - a modular assembly for 1D nanostructures
03.11.2004	**Prof. Dr. Joachim Mayer** Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen und Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen am Forschungszentrum Jülich	Hochauflösende analytische TEM und ihre Anwendungen in der Nanowissenschaft
15.11.2004	**Prof. Dr. Freek Kapteijn** Reactor and Catalysis Engineering, DCT-TU Delft, The Netherlands	Catalysis Engineering - putting Science into Practice
01.12.2004	**Prof Dr. H. Kuzmany** Institut für Materialphysik, Universität Wien	Physics and Chemistry Inside Carbon Nanocages

Date	Guest - Lecturer	Titel
05.01.2005	**Dr. Harry Bitter** Department of Inorganic Chemistry, Debye Istitute, Universiteit Utrecht	Tunable carbon nanofibers based catalysts - synthesis, characterization and catalysis

Date	Speaking Guest	Titel
24.01.2005	**Dr. A. Barinov** Sincrotrone Trieste	Electron Confinement Effect on the Reactivity of Thin Mg Films
23.03.2005	**Prof. Dr. M. Rühle** MPI für Metallforschung, Stuttgart	Nanoanalysis of materials by TEM techniques
06.04.2005	**Prof. Dr. J. W. Niemantsverdriet** Schuit Institute of Catalysis, Eindhoven University of Technology	Planar Models of Supported Catalysts for Polymerization
15.06.2005	**Prof. Dr. Pérez Omil, José A.** Solid chemistry and Catalysis group; Inorganic Department; University of Cadiz	Contributions of Electron Microscopy to Understanding the Redox Behaviour of Ce-based catalysts
13.07.2005	**Prof. Francesca Porta** Dip. Chimica Inorganica Metallorganica ed Analitica Via Venezian 21, 20133 Milano, Italia	Preparation of metallic sols dedicated to catalysis and biology: Properties and applications
27.07.2005	**Prof. Michael Giersig** Forschungszentrum Cesaer, Bonn	Fabrication of Nanoscale Rings, Dots, and Rods by Combining Shadow Nanosphere Lithography and Annealed Polystyrene Nanosphere Masks
07.09.2005	**Prof. Dr. Bo-Qing Xu** Department of Chemistry, Tsinghua University, Beijing, China	New approach for the preparation of advanced heterogeneous metal catalysts
21.09.2005	**Prof. Norbert Kruse** Université Libre de Bruxelles Chimie-Physique des Matériaux,	Catalytic and Non-catalytic Surface Reaction at the Atomic Scale
12.10.2005	**Dr. Gang Hu** Inorganic Chemistry Laboratory, South Parks Road, Oxford OX1 3QR, U.K.	Some Progresses in LDHs Chemistry: From a Synthetic Point of View

Guest - lectures

2003 - 2007

Date	Speaking Guest	Titel
02.11.2005	**Prof. Archie Howie** Cavendish Laboratory, University of Cambridge, U.K.	Magnifying the Contribution of Electron Microscopy to Catalyst Characterization
09.11.2005	**Dr. Karoly Lázár** Institute of Isotope and Surface Chemistry, Chemical Research Centre of the Hungarian Academy of Sciences	In situ Mossbauer spectroscopy in catalysts studies
23.11.2005	**Prof. Dr. K.-P. Dinse** Phys. Chem. III, Darmstadt University of Technology	Multifrequenz EPR in Chemie und Materialwissenschaften
07.12.2005	**Dr. Frederic Goettmann** Max Planck Institute for Colloids and Interfaces	Zirconium rich mesoporous powders in catalysis, more than just a support
21.12.2005	**Prof. Julie L. d'Itri** Department of Chemical Engineering, University of Pittsburgh	Controlling the Rate of more than One Elementary Reaction Step with One Surface

Date	Speaking Guest	Titel
04.01.2006	**Dr. Maja Mrak** National Institute of Chemistry and University of Ljubljana	New mesoporous catalysts
11.01.2006	**Dr. Thierry Visart de Bocarmé** Université Libre de Bruselles	Catalytic Surface Reactions on the Atomic Scale
18.01.2006	**Prof. Dr. Guido Busca** Department of Chemical and Process Engineering, University of Genova,	On the use of CO and nitriles as probe molecules in the IR characterization of different catalysts (oxides, supported metals, zeolites)
25.01.2006	**Dr. Polona Umek** Institute "Jožef Stefan",Ljubljana, Slovenia	Impact of Structure and Morphology of Titanate-Based Nanotubes and Nanoribbons Effect on Gas Adsorption of NO_2
29.03.2006	**Prof. Dr. Silvana Fiorito** LCVN-CNRS, Universite Montpellier	Toxicity of Carbon nanoparticles towards human cells
30.03.2006	**Dr. Cécile Hébert** Inst. f. Festkörperphysik, TU Wien	Low Loss EELS and the measurment of optical properties

Date	Speaking Guest	Titel
06.04.2006	**Dr. Jean-Pierre Candy** CPE-Lyon, CNRS, France	Surface Organo-Metallic Chemistry on Metals: Genesis, Characterization and Application
12.04.2006	**Prof. Dr. Arne Andersson** Department of Chemical Engineering, University, Lund, Sweden	The V-Sb-W-Al- and Mo-V-Nb-Te-oxide systems for propane ammoxidation
09.05.2006	**Prof. Hengyong Xu,** Dalian Institute for Chemical Physics, Chinese Academy of Science	Novel Technologies for Palladium Membrane Preparation and Hydrogen Production
14.06.2006	**Prof. Dr. Daniel Resasco** University of Oklahoma School of Chemical, Biological and Materials Engineering	Controlled Growth of SWNT on Solid Catalysts with Narrow (n,m) Distribution
21.06.2006	**Prof. Panagiotis Smirniotis** Chemical & Materials Engineering Department, University of Cincinnati	Molecular Sieve-based Photocatalysts for Photodegradation Reactions of Organics
23.08.2006	**Prof. Dr. Serafin Bernal** University of Cadiz, Spain	Nano-structural properties and redox behaviour of ceria-zirconia mixed oxides"
13.09.2006	**Prof. Dr. Helmut Knözinger** Ludwig-Maximilians-Universität München , Department of Chemie, Physikalische Chemie	n-Pentan-Isomerisierung an promotierten WZr-Katalysatoren
15.09.2006	**Dr. Michel Daage** ExxonMobil Research and Engineering, USA	Modeling Catalysts: An Experimentalist Point of View
29.09.2006	**Dr. Konstantinos Fostiropoulos** Hahn-Meitner-Institut Berlin GmbH	Organic nano-structures for photovoltaic applications
02.10.2006	**Prof. Dr. Hui Gu** Chinese Academy of Sciences , Shanghai Institute of Ceramics	Quantitative EELS analysis of grain boundary and Interface
18.10.2006	**Prof. Dr. Florian Banhart** Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany	Carbon Onions and Nanotubes as Nanolaboratories in the Electron Microscope

Guest - lectures

2003 - 2007

Date	Speaking Guest	Titel
22.11.2006	**Prof. Feng-shou Xiao** Jilin University, Changchun, China	Hydrothermally Stable Mesoporous Materials and Functionality of Catalytically Active Species in Mesoporous Materials
29.11.2006	**Prof. Krijn P. de Jong** Inorganic Chemistry and Catalysis, Department of Chemistry, Utrecht University, The Netherlands	Fundamental Studies on the Preparation of Supported Catalysts

Date	Speaking Guest	Titel
10.01.2007	**Dr. Xiaoming Ren** Acta S.p.A., Crespina (PI) - Italy	Non-Pt catalysts for advanced direct alcohol fuel cells
17.01.2007	**Prof. Claus Hviid Christensen** Technical University of Denmark, Center for Sustainable and Green Chemistry, Department of Chemistry	Rational Approaches to Catalyst Design and Discovery
23.01.2007	**Prof. Zhenping Zhu** Institute for Coal Research, Chinese Academy of Science, Taiyuan, China	Construction, mechanism and properties of nanostructures
24.01.2007	**Dr. Vincent Huc** Université Paris – ORSAY	Beyond the C60: from Calixarenes to metallic nanoparticules
07.02.2007	**Prof. Jürgen Behm** Abt. Oberflächenchemie und Katalyse, Universität Ulm	Electrocatalysis in Polymerelectrolyte Fuel Cell: Problems, Challenges and New Developments
15.02.2007	**Dr. Frank de Groot** Department of Chemistry, Utrecht University , Netherlands	New X-ray spectro-microscopic techniques for the in-situ study of heterogeneous catalysts
28.02.2007	**Dr. Susana Valencia** Instituto de Tecnología Química (UPV-CSIC), Valencia	New trends in the synthesis of zeolites
25.04.2007	**Dr. Xinyu Xia** Industrial Chemistry, Ruhr-University Bochum, Germany	Temperature-Programmed Desorption from Porous Materials in a Flow Set-up: Experiments and Simulation
08.05.2007	**Prof. Tao Zhang** Dalian Institute of Chemical Physics, Dalian, China	Catalysis for aerospace applications

Date	Speaking Guest	Titel
09.05.2007	**Prof. Dmitry Yu. Murzin** Laboratory of Industrial Chemistry, Abo Akademi University, Turku, Finland	Challenges in developing catalysts for cleaning exhaust gases from diesel engines: HC-SCR of NOX
13.06.2007	**Dr. Bruno Chaudret** Toulouse, CNRS, France	Organometallic Nanoparticles: Synthesis and Surface Chemistry
11.07.2007	**Dr. Christophe Coperet** CNRS, France	Design and understanding of heterogeneous olefin metathesis catalysts
18.07.2007	**Prof. Michael Köhler** TU Ilmenau, Germany	Micro fluid segment technique for miniaturized synthesis and screening
12.09.2007	**Prof. Valerii I. Bukhtiyarov,** Boreskov Institute of Catalysis, Novosibirsk, Russia	Size effects of supported nanoparticles in catalysis

External Funds

Project Name	Akronym	Referenz No.	Funds´ Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
"Upgrading of natural gas and palm oil to higher added value speciality chemicals using combinatorial technologies and catalysis"	COMBICAT	PS 681	University of Malaya	2002 - 2007	Prof. Dr. R. Schlögl Dr. A. Trunschke	Prof. Dr. S. B. Abd Hamid	Prof. Dr. S. B. Abd Hamid
Integrated Design of Nanostructured Catalytic Materials for a Sustainable Development	IDECAT	PSFHI 805	European Union	2005 - 2010	Prof. Dr. R. Schlögl	Prof. H.J. Freund Prof. M. Scheffler Prof. M. Reetz Prof. F. Schüth and other (17 European partners) http://.idecat.org	Prof. Dr. G. Centi
In situ Characterization of Propene Oxidation Catalysts and Catalysis	Sumitomo	PS 251	Sumitomo Chemical Co., Ltd	1.10..2004 - 2007	Prof. Dr. R. Schlögl Dr. A. Knop-Gericke	Prof. Dr. Hiroshi Yamachika (Japan)	Prof. Dr. R. Schlögl Prof. Dr. Hiroshi Yamachika
ENERCHEM Nanochemical Concepts for a Sustainable Energy Supply Projects of Max Planck Institutes	ENERCHEM		MPG	2005 - 2010	Prof. R. Schlögl Dr. D. S. Su	Prof. F. Schüth (MPI für Kohleforschung), Prof. J. Maier (MPI für Festkörper-forschung), Prof. K. Müllen (MPI für Polymerforschung)	Verbundprojekt
Entwicklung von Methanolsynthesekatalysatoren als Basis für nachhaltige Ressourcennutzung – TP3	BMBF	PSFHI 102	BMBF	1.7.2005 – 30.6.2008	Prof. R. Schlögl Dr. A. Trunschke	Südchemie, Prof. M. Muhler (Ruhr-Uni. Bochum), Lurgi AG, Prof. S.B. Abd Hamid (Uni. of Malaya / NanoC, Kuala Lumpur)	Südchemie
Oxidnitride des Zirconiums als Materialien und Modellverbindungen für die katalytische Aktivierung von Ammoniak	DFG	SCHL 332/9-2	Deutsche Forschungs-gemeinschaft	23.10.2006 continuing	Prof. R. Schlögl	Prof. M. Lerch Prof. R. Schomäcker	Prof. T. Ressler
Mischoxide		PSFHI 253	Südchemie	2007 - 2008	Prof. Dr. R. Schlögl Dr. A. Trunschke		Dr. A. Trunschke

External Funds

Project Name	Akronym	Referenz No.	Funds´ Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Joint project with Bayer AG “Carbo Scale”			Bayer AG	2007 - 2009	Prof. Dr. R. Schlögl	TU Berlin Ruhr-Uni. Bochum Univ. Erlangen Univ. Clausthal	Dr. D.S. Su
“Unifying Concepts in Catalysis”, application to become Cluster of Excellence	CoE		German Federal and State Governments to Promote Science and Research at German Univ.	decision end 2007		Prof. R. Schlögl Prof. H.J. Freund Prof. G. Meijer Prof. M. Scheffler	Prof. M. Driess (TU Berlin)
International Partnership for Research and Education: “Molecular Engineering for Conversion of Biomass derived Reactants to Fuels, Chemicals and Materials”	PIRE			2012	Prof. R. Schlögl (host German site)	Prof. M. Antonietti Prof. M. Scheffler Prof. R. J. Davis Prof. J. A. Dumesic Prof. M. Neurock Prof. B. Shanks Prof. C. Christensen Prof. I. Chorkendorff Prof. J. K. Nørskov Prof. S. Hellweg	Prof. A.K.Datye (Univ.of New Mexico)
Identification of local environment of transition metal promoter cations in zirconia-based heterogeneous catalysts.	DFG	436 MOL	Deutsche Forschungs-gemeinschaft	2004 – 2006 continuing	Dr. F. C. Jentoft	Prof. Dr. S. Klokishner (Kishinev, Acad. Sci. Moldova)	
Intensities of IR stretching bands as a criterion of polarization and activation of adsorbed molecules in heterogeneous acid-base catalysis	DFG	Je 267/2-1 und 436 RUS 113/788/0-1	Deutsche Forschungs-gemeinschaft	2004 – 2007	Dr. F. C. Jentoft	Prof. V. Kazansky (RAS Moskow, Russian)	
Bridging the gap between ideal and real systems in heterogeneous catalysis: Project " From single crystals to real catalysts using selective hydrogenation over silver as case study"	DFG Schwerpunkt-programm 1091	Je 267/3-1	Deutsche Forschungs-gemeinschaft	2004 – 2006 continuing	Dr. F. C. Jentoft	Prof. P. Claus (TU Darmstadt)	
PROX catalysts	PROX		MPG	2004 – 2006 continuing	Dr. F. C. Jentoft	Dr. A. Knop-Gericke Dr. A. Wootsch (Budapest, Hungarian)	Dr. F. C. Jentoft

External Funds

Project Name	Akronym	Referenz No.	Funds´ Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Mechanismus of alkane activation by sulfated zirconia materials	IDECAT ELCASS	PSFHI 805 MAPAFHI 00001	European Union MPG and CNRS (Centre nationale de la recherche scientifique)	2005 - 2010 2004 - 2010	Prof. Dr. R. Schlögl Dr. F. C. Jentoft	http://idecat.org Prof. Dr. F. Garin	Prof. Dr. G. Centi Dr. D. S. Su
Heterogeneous - Homogeneous Catalytic Oxidations			Alexander von Humboldt-Stiftung	2005-2007	Dr. F. C. Jentoft Dr. K. Pelzer	Prof. L. D, Schmidt Dr. R. Horn (Uni. of Minnesota)	
Struktur, Dynamik und Reaktivität von Übergangsmetalloxid- Aggregaten	Sfb	Sfb 546	Sonder-forschungs-bereich	2000 - 2007	Dr. D.S. Su Dr. C. Hess	Prof. Dr. R. Schlögl	Prof. Dr. J. Sauer
Carbon Nanotubes for Applications in Electronics, Catalysis, Composites and Nano-Biology	CANAPE	PSFHI 809	European Union	2.6.2004 – 1.6.2008	Dr. D. S. Su	http://www.canapeweb.com	Prof. Dr. J. Robertson
Electrocatalytic Gas-Phase Convertion of CO_2 in Confined Catalysts	ELCAT	PSFHI 807	European Union	1.9.2004 – 31.8.2011	Dr. D. S. Su	http://www.elcat.org	Prof. Dr. G. Centi
Nanocarbon – Nanocarbon related materials in heterogeneous catalysis	ELCASS	MAPAFHI 00001	MPG and CNRS (Centre nationale de la recherche scientifique)	2004 - 2010	Dr. D. S. Su	Prof. G. Centi Dr. Cuong Pham-Huu Prof. M. Ledoux Prof. F. Garin	Dr. D. S. Su
1)Electron microscopy study of one-dimensional II-VI semiconductor nanostructures grown by molecualr-beam epitaxy 2) Nanostructured transition metal oxides as new humidity sensors materials 3) Synthesis, characterization and catalytic properties of mesoporous materials	DAAD	PS 963	Deutscher Akademischer Austauschdienst DAAD	1) 2004 - 2005 2) 2006 - 2007 3) 2006 - 2007	Dr. D. S. Su	2) Dr. A. Gajovic 3) Prof. Feng-Shou Xiao (Changchun, China)	DAAD
Partner group Dalian, Chinese Academy of Sciences. "Carbon-based challenging nanostructured materials for catalytic application"	Bao	MCHAFHI 00001	MPG	1.10.2000 – 30.9.2005 1.7.2006 – 1.1.2007 – 2009 (2011)	Dr. D. S. Su		Prof. Dr. Xinhe Bao
Nonstructural catalysts for environment protection and green chemistry	Krakow		MPG	2002 – 2007	Dr. D. S. Su	Prof. Dr. M. Najbar	Dr. D. S. Su

External Funds

Project Name	Akronym	Referenz No.	Funds´ Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Cooperation Zagreb "TEM and Raman spectroscopy of nanostructured transition metal oxides"	Zagreb	K 500Z	MPG	2004 – 2005 continuing	Dr. D. S. Su	Dr. K. Furic (Zagreb, Kroatien)	Dr. D. S. Su
Raman-Spektroskopie als diagnostisches Tool zur Bestimmung der Struktur-Reaktivitäts-Korrelation von Ruß unterschiedlicher Mikrostruktur	DFG	SCHL 332/10-1	Deutsche Forschungs-gemeinschaft	15.10.2007 – 14.10.2009	Dr. D. S. Su	Prof. R. Nießner Dr. N. Ivleva	Prof. R. Schlögl
In situ studies of oxygen species in the ethylene epoxidation over silver			MPG	1999 – 2006 continuing	Dr. A. Knop-Gericke	Prof. V. L. Bukhtiyarov (Novosibirsk, Russian)	Dr. A. Knop-Gericke
Development of a high pressure photoelectron spectrometer			MPG and Lawrence Berkeley National Laboratories, USA	2001 – 2006 continuing	Dr. A. Knop-Gericke	Prof. Dr. M. Salmeron	Prof. Dr. M. Salmeron
Advanced Technology in Catalytic Chemistry and Engineering for Novel Applications	ATHENA	PS 960	Uni of Glasgow, EPSRC (Engineering and Physical Sciences Reseach Council, UK)	2003 - 2007	Prof. Dr. R. Schlögl Prof. H.-J. Freund Dr. A. Knop-Gericke Dr. D. S. Su	Prof. Dr. G. Hutchings Prof. Dr. D. Jackson Prof. P. C. Stair	Prof. Dr. D. Jackson
Pd model catalysts in oxidation reactions			MPG	2004 - 2007	Dr. A. Knop-Gericke	Dr. B. Klötzer (Innsbruck, Austria) Dr. D. Zemlyanov (Limerick, Irland)	Dr. A. Knop-Gericke
Entwicklung, Charakterisierung und in situ-Katalyseverhalten neuartiger, nanostrukturierter Übergangsmetalloxid-Modell-Katalysatoren für Partialoxidationen	Emmy-Noether-Nachwuchs-gruppe	HE 4515/1-1 HE 4515/1-2	Deutsche Forschungs-gemeinschaft	2004-2008	Dr. C. Hess		
Functional analysis of noble metal catalysts in selective hydrogenation	Partner Group	M.PG.A.FHI00 002	MPG and Inst. of Isotopes (Budapest, Hungary)	2006 – 2009 (2011)	Prof, Dr. R. Schlögl Dr. A. Knop-Gericke	Prof. Dr. Z. Paál	Prof, Dr. R. Schlögl Prof. Dr. Zoltán Paál
In situ XPS collaboration			UOP LLC, a Honeywell company	2006 continuing	Dr. A. Knop-Gericke	Ally S. Chan Simon Bare	

Cluster of Excellence CoE

Excellence Initiative by the German Federal and State Governments to Promote Science and Research at German Universities

application to become CoE, decision end 2007

unicat
Unifying Concepts in Catalysis

What is UniCat ?

UniCat is the acronym for a new initiative on the area of catalysis research in the Berlin-Brandenburg area (Germany). This initiative is being developed within the bounds of the Excellence Initiative started by the German Federal and State Governments, under the supervision of the German Research Foundation (Deutsche Forschungsgemeinschaft: DFG). UniCat aims to become a Cluster of Excellence, which should open, if successful, at the end of 2007.

Overview

Current challenges in catalysis range from the efficient exploitation of energy resources to the creative use of natural and artificial enzymes.
Our strategic goal is to unify concepts in catalysis by bridging the gaps between homogeneous and heterogeneous catalysis, between elementary gas-phase reactions and complex processes in highly organised biological systems, as well as between fundamental and applied catalysis research.
Our initiative focuses on analysing catalytic mechanisms, designing novel catalytic materials and strategies, and developing new catalytic processes on laboratory and miniplant scales. We want to integrate the expertise in chemistry, biology, physics, and engineering in the Berlin area into an innovative research program. We aim at creating a centre of catalytic research and generating new synergisms in this central field of science and technology.

UniCat is currently being developed by the

Coordinator

Prof. Dr. Matthias Driess
(Technische Uni. Berlin)

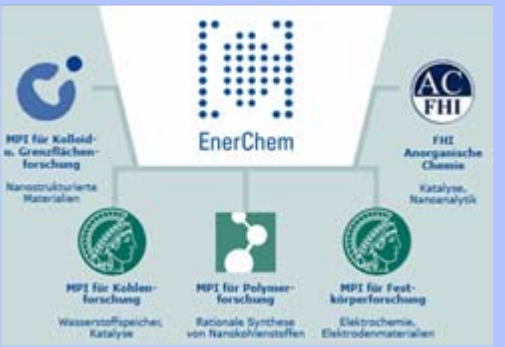
http://www.unicat.tu-berlin.de

EnerChem

Projects of Max Planck Institutes
Nanochemical Concepts for a Sustainable Energy Supply

What is EnerChem ?

EnerChem is a research association, initiated by five Max Planck institutes. The aim is to combine the chemical expertise and capacities of these institutes to generate solutions to the emerging problems of energy supply, storage and saving with the focus on nanostructured carbon materials. The Department of Inorganic Chemistry is member of the Project House EnerChem of the Max-Planck Society.



The world energy consumption is at present based nearly to 90% on fossil sources of energy (coal, oil, natural gas). Three quarters of the world‘s energy production are used only by one quarter of the world‘s population, the industrial nations. Bearing the energy needs of emerging markets in mind, the fossil resources will be exhausted before long. A simple improvement of current know-how is no longer adequate for future-oriented power supplies. With the establishment of the research initiative „nano-chemical concepts of lasting power supplies – EnerChem“, a scientific basis for new mobile energy storage and more effective methods of energy production was founded.

The projects of AC in the EnerChem are:

1. Ammonia as energy carrier
2: Carbon-based metal-free catalysis
3. Novel carbon nanostructure as electrode materials for Li-ion batteries
4. Structural characterization of novel carbon materials

http://www.enerchem.de

European Union - Network of Excellence / NoE

What is the SIXTH FRAMEWORK PROGRAMME (FP6) ?

At the Lisbon summit in March 2000, EU governments called for a better use of European research efforts through the creation of an internal market for science and technology - a 'European Research Area' (ERA). FP6 is the financial instrument to help make ERA a reality.

http://cordis.europa.eu

SIXTH FRAMEWORK PROGRAMME

ERIC

CANAPE

Integrated Design of Catalytic Nanomaterials for a Sustainable Production (IDECAT)

The development of high-performance and conceptually innovative catalytic nanomaterials is crucial for industry and for Europe's sustainable future. In Europe, several excellent research teams exist in catalysis, but there is a significant fragmentation in the area due to separate scientific communities (heterogeneous, homogeneous, and bio-catalysis) and a lack of thematic identity. IDECAT Network of Excellence will address this fragmentation, creating a coherent framework of research, know-how and training between the various catalysis communities (heterogeneous, homogeneous, bio-catalysis) with the objective of achieving a lasting integration between the main European Institutions in the area.

37 laboratories from 17 Institutions, gathering over 500 researchers
The work is divided in 13 work packages.

Final objective of IDECAT is the creation of an European Research Institute of Catalysis (**ERIC**) to realize top level projects in the field of catalysis and to develop catalytic functional materials.

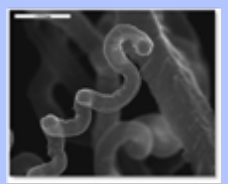
http://idecat.org

Carbon Nanotubes for Applications in Electronics, Catalysis, Composites and Nano-Biology (CANAPE)

The consortium gathers 15 research and industrial partners to improve the fundamental knowledge of carbon nanotubes as well as their applications.
http://www.pa.msu.edu/cmp/csc/nanotube.html

To improve efficiency, the consortium work is divided in 7 work packages.

WP1: Growth and process optimization.
WP2: Applications in chemistry.
WP3: Applications in electronics.
WP4: Applications in composites.
WP5: Nano-bio.
WP6: Health.
WP7: Electrolyte Fuel Cell.



SEM image of Carbon Nano Tubes, HV 25kV, el-opt magn. 35000x

http://www.canapeweb.com

Contact: Dr. Sabine Wrabetz or Dorothea Damm
wrabetz@fhi-berlin.mpg.de, damm@fhi-berlin.mpg.de

Electrocatalytic Gas-Phase Conversion of CO_2 in Confined Catalysts (ELCAT)

NEST Adventure

NEST is a new activity in the Sixth Framework Programme (FP6). It aims at support unconventional and visionary research with the potential to open new fields for European science and technology, as well as research on potential problems uncovered by science.

New and emerging science and technology (NEST)

The project is focussed on the electrocatalytic gas-phase conversion of CO_2 to Fischer- Tropsch (FT)-like products (C1-C10 hydrocarbons and alcohols).

This project will address three relevant challenges of catalysis:
- Use of a selective source of energy in catalytic reactions as an alternative to the unselective thermal energy.
- Find a feasible way to convert CO_2 to chemicals.
- Use the confinement effect in nanomaterials to promote unconventional catalytic reactions.

http://www.elcat.org

Teaching Activities

Staff scientists are regularly involved in the course programme of the Technische Universität and Humboldt Universität in Berlin.

The AC Department covers teaching aspects within the IMPRS (International Max Planck Research School; http://www.imprs-cs.mpg.de) of the FHI on the chemistry of heterogeneous catalysts and on the aspects of preparation of inorganic solids.

Modern Methods in Heterogeneous Catalysis Research
Robert Schlögl, Friederike Jentoft et al.
http://w3.rz-berlin.mpg.de/cat
"Modern Methods in Heterogeneous Catalysis Research" is a class aimed at giving advanced students, who are interested or involved in catalysis research, insight into the methods of catalyst preparation, catalyst testing, and catalyst characterization. The class consists of a series of individual and largely independent lectures given by different instructors.

Physical Chemistry Laboratory Class (WS only)
Instructors: F. Jentoft & S. Wrabetz
http://w3.rz-berlin.mpg.de/ac/teaching/teaching.html
"Adsorption Calorimetry" is an experiment in the Physical Chemistry laboratory class for 7th semester students at the Humboldt Universität in Berlin.

Humboldt Universität in Berlin, Institute of chemistry, Department of Anorganic Chemistry
Instructor: A. Trunschke
"Reaction Mechnisms in Heterogeneous Catalysis"

Humboldt Universität Berlin, Department of Chemistry, Advanced Physical Chemistry Laboratory Class (WS only)
Instructor: C. Hess
http://w3.rz-berlin.mpg.de/ac/teaching/teaching.html
"Raman Spectroscopy" is an experiment in the Physical Chemistry laboratory class for 7th semester students at the Humboldt Universität in Berlin.

Humboldt Universität Berlin, Department of Chemistry
Instructor: C. Hess
Lecture for Chemistry majors (Dipl. Chem.)
"Kinetics"
http://w3.rz-berlin.mpg.de/ac/teaching/teaching.html

Dept. of Industrial Chemistry and Engineering of Materials Univ. Messina, Sicily, Italy
Instructor: D. S. Su
"Basics of Transmission Electron Microscopy"

Dalian Institute for Chemical Physics, Chinese Academy of Science, Dalian, China
Instructor: D. S. Su
"Electron Microscopy and Its Application in Heterogeneous Catalysis: A basic lecture to understanding electron microscopy"

Dipartimento di Chimica Inorganica Metallorganica e Analitica, Milano, Italy
Instructor: D. S. Su
"Basics Course on Electron Microscopy and Its Applications"

Practical Courses

jugend forscht

This is the competition in natural sciences, mathematics and technique for young people up to the age of 21. They can do research on their on own or in groups of two or three. „Jugend forscht“ fields of research are: working world, biology, chemistry, geo and space sciences, mathematics/computer science, physics, engineering. It goes without saying that the **participants can win awards or incentives, such as a 2-weeks research training at the Fritz-Haber-Institut of the MPG**. This research training is especially looked for and popular. The young participants appreciate to be included into the daily working routine of highly-qualified scientists. Under professional guidance they may tackle their own research tasks.

H. Münkler, A. Rudolph *(March 2006)*
Während unseres Praktikums am Fritz-Haber-Institut der MPG war es uns möglich, einen Einblick in die Forschung an Katalysatoren zu gewinnen, wobei wir uns hauptsächlich mit der Analyse von Graphitkristallen mithilfe der Photoelektronenspektroskopie beschäftigten. Hier konnten wir selbst Versuchsreihen aufnehmen und erhielten nebenbei auch eine Einführung in die theoretischen Aspekte der angewendeten Verfahren, die sich von der Probenpositionierung bis zu Auger-Linien erstreckten. Die Zeit am FHI war für uns sehr interessant und lehrreich.


H. Münkler, A. Rudolph „Bionische Solarzell - Energie der Zukunft“

Occupation practical course

LetteVerein

Today the Lette Foundation incorporates five more or less independent educational institutions. Courses are currently offered for the following diplomas in the following departments: Technical Assistant in Metallography and Physical Material Analysis Chemistry and Biology Electronics and Data Processing Pharmacy Laboratory Medicine and Radiology.

Nadine Schechner *(3.-18.1.2005)*
Das 4-wöchige Berufspraktikum am FHI verging viel zu schnell. Es waren eindrucksvolle 4 Wochen. Ich lernte viele neue Labor-Geräte und Labor-Apparaturen kennen sowie neue Messtechniken, konnte aber auch gelerntes anwenden. Alles war sehr spannend für mich. Die Mitarbeiter waren alle hilfsbereit und freundlich. Das Labor war unglaublich gut organisiert.

Förderverein Chemie-Olympiade e.V.

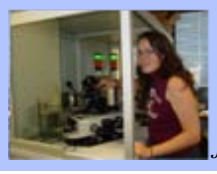
Olympic games in Chemistry are an international competition for pupils of comprehensive schools. About 60 groups of pupils from different countries annually meet to compete and to put their knowledge in Chemistry to the test. Each nation is self-responsible for the selection of participants. In Germany candidates have to pass a 4-round test procedure. Some pupils from the 3rd round are given the chance to take part in a **2-weeks taster course at Fritz-Haber-Institut der Max-Planck-Gesellschaft.**


M. Martineau, A. Altman, F. Kühne June 2003

Pupil practical course

Oliver Höckendorf Juli 2007:
Mein Name ist Oliver Höckendorf und ich besuche das Heinitz-Gymnasium in Rüdersdorf. Am Ende der 12. Klasse steht bei uns ein einwöchiges Praktikum an. Auf Grund meines naturwissenschaftlichen Interesses bewarb ich mich beim FHI, wo ich in die Abteilung Anorganische Chemie kam.
Das Hauptaugenmerk in dieser Woche lag auf dem Verständnis und Umgang mit XPS, einem Verfahren, bei dem mit Hilfe von Röntgenstrahlen u. a. Oberflächen analysiert werden können. Am Anfang der Woche erarbeitete ich mir die Grundkenntnisse über dieses Verfahren mit kräftiger Unterstützung der Institutmitarbeiter. In der zweiten Wochenhälfte war ich an Messungen beteiligt und hatte diese in Form eines Protokolls auszuwerten.
Es war faszinierend, einmal das mitzuerleben, was man normalerweise nur aus dem Fernsehen oder den Medien kennt, und das in entspannter Arbeitsatmosphäre. Vor allem die Zusammenarbeit unter den Mitarbeitern war beeindruckend, weil es trotz der vielen verschiedenen Nationalitäten doch keine Kommunikationsprobleme gab.
Deshalb bedaure ich, dass ich am FHI lediglich eine Woche arbeiten durfte und hoffe in der Zukunft noch einmal ein längeres Praktikum an diesem Institut absolvieren zu können, um mich eingehender mit der wissenschaftlichen Arbeitsweise vertraut zu machen.


Nina K. Januar 2005


Anne T. July 2006


Swantje P. Sept. 2006

Lange Nacht der Wissenschaften

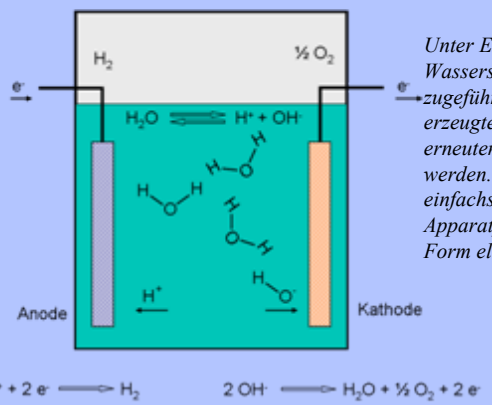
LANGE NACHT DER WISSENSCHAFTEN 2007

Wasserstofftechnologie

Anhaltende Diskussionen um die Gestaltung der zukünftigen Energieversorgung haben auch das allgemeine öffentliche Interesse erreicht. Innovative Ansätze umfassen dabei die unter dem Begriff *Wasserstofftechnologie* zusammengefassten Prozesse, dabei kommt der Brennstoffzellentechnologie eine zentrale Bedeutung zu.

Die Abteilung Anorganische Chemie (AC) am Fritz-Haber-Institut der MPG ist in ihrer Forschungstätigkeit mit fundamentalen Prozessen der heterogen katalysierten Stoffumwandlung befasst. Untersucht werden beispielsweise Eigenschaften von Katalysatormaterialien. Dabei kommen Methoden zur Anwendung, die Einblicke in Mechanismen des katalytischen Prozesses selbst auf atomarer Ebene gewähren. So sind Mitarbeiter der Abteilung seit längerem mit der Aufklärung der Wirkungsweise von Katalysatoren für die Methanol-Reformierung wie auch der Wassergas-Shift-Reaktion befasst. Beides Prozesse, die im Rahmen der Wasserstofftechnologie eine Rolle spielen.

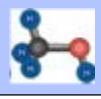
Anlässlich der Langen Nacht der Wissenschaften am 12.06.2004 und 11.06.2005 hat die Abteilung Anorg. Chemie einen generellen Überblick der physikalischen und chemischen Grundlagen zur Nutzung von Wasserstoff als Energieträger dargeboten. Mit einigen Exponaten und Versuchen wurden dem Besucher Entwicklungen und Techniken der Wasserstoffwirtschaft veranschaulicht. Mit einem Stirlingmotor wurden prinzipielle Gesetzmäßigkeiten der Energieumwandlung demonstriert. Mit einer Brennstoffzelle wurde der aktuelle Stand der Technik vorgestellt. (http://w3.rz-berlin.mpg.de/ac/news)

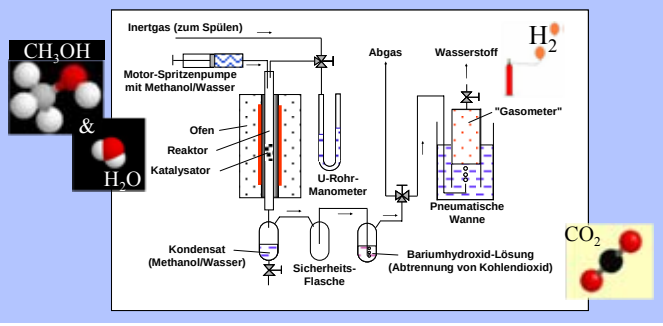


Unter Energiezufuhr kann Wasser in seine Bestandteile Wasserstoff und Sauerstoff gespalten werden. Die zugeführte Energie ist dann quasi in der Form des erzeugten Wasserstoffes gespeichert und kann bei erneuter Bildung von Wasser wieder freigesetzt werden. Die Spaltung des Wassers lässt sich am einfachsten in einer Elektrolysezelle (Hofmannscher Apparat) bewerkstelligen. Die Energie wird hier in Form elektrischer Energie zugeführt.

Woher kommt der Wasserstoff / Where does hydrogen come from?

z.B. aus Methanol CH_3OH





DMFC – Direct Methanol Fuel Cell

The DMFC converts methanol and oxygen electrochemically into electrical power, heat, carbon dioxide and water. At the anode (negative electrode), the methanol is first split into hydrogen and carbon dioxide before the same catalyst splits the hydrogen into protons and electrons. These reactions require a special platinum/ruthenium catalyst. The protons then diffuse across the polymer membrane to the cathode (positive electrode), while the electrons pass as current through the external circuit. At the cathode, the electrons then recombine with the protons that have passed across the membrane and with oxygen to form water. The cathode reaction is catalyzed by e.g. platinum particle. The voltage generated by a single DMFC cell is 0.3-0.9 V.

Reformer/ Katalysator :	$CH_3OH + H_2O$	$\rightarrow CO_2 + 3H_2$
Anodenreaktion:	H_2	$\rightarrow 2H^+ + 2e^-$
Kathodenreaktion:	$½\,O_2$ (Luft) $+ 2H^+ + 2e^-$	$\rightarrow H_2O$

AC FHI
Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Long Night of Science

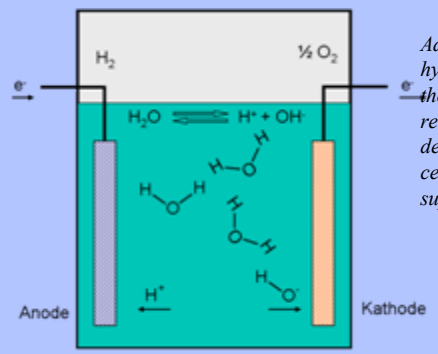
LANGE NACHT DER WISSENSCHAFTEN 2007

Hydrogen Technology

Ongoing discussions about power supply in future resulted in a general Public interest. Innovative approaches comprise the processes well-known as hydrogen technology. Among these fuel cells are of special importance.

The Department of Inorganic Chemistry (IC) at the Fritz-Haber-Institut of the MPG is doing research related to basic processes of heterogeneously catalysed transformation of materials. We are studying for example properties of catalyst materials applying methods to allow insights into the mechanism of the catalytic process itself even on atomic level. Members of the department have been working for some time to explain the mode of action of catalysts for methanol reforming as well as the watergas-shift-reaction. Both are processes important for hydrogen technology.

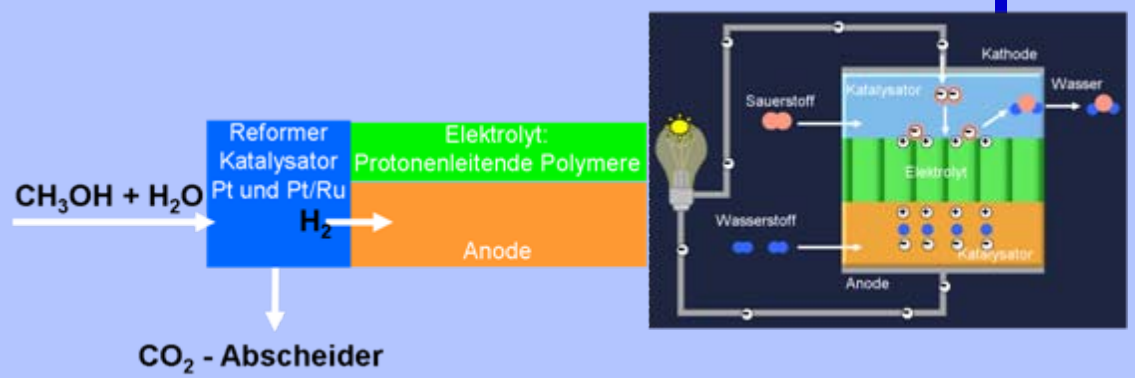
On occasion of the Long Night of Sciences on June 12th, 2004 and June 11th, 2005, the IC department gave a general overview of the physical and chemical basis for the use of hydrogen as a source of energy. Various experiments and exhibits were illustrating to the visitors the development and techniques of hydrogen economy. By means of a sterling motor basic principles of energy transformation were shown. A fuel cell demonstrated the state-of-the-art. (http://w3.rz-berlin.mpg.de/ac/news)



Additional energy makes water decompose into hydrogen and oxygen. Energy is saved in form of the generated hydrogen molecule and may be released again when water reforms.. Water decomposition is done best within an electrolysis cell (Hofmannscher Apparat). Here energy is supplied in form of electric energy.

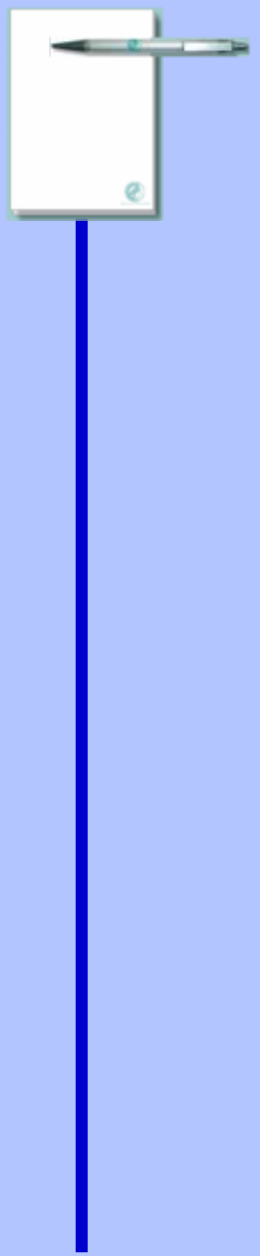
$2\,H^+ + 2\,e^- \longrightarrow H_2$ $\qquad$ $2\,OH^- \longrightarrow H_2O + ½\,O_2 + 2\,e^-$

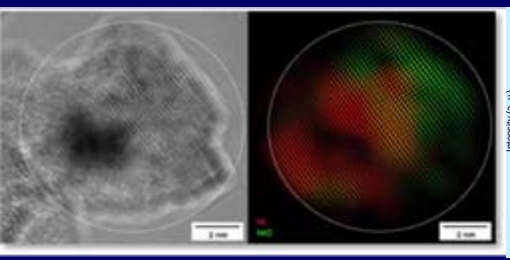
Funktionsweise einer BZ / Function principle of a fuel cell

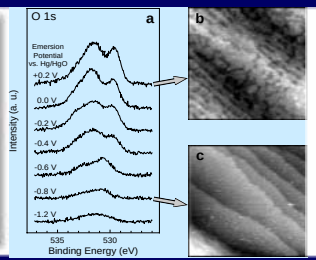


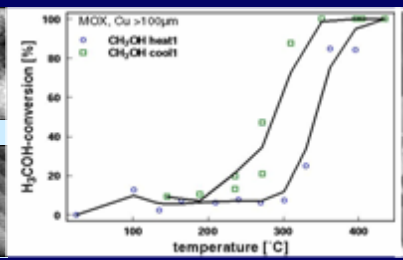
Anwendung / Application

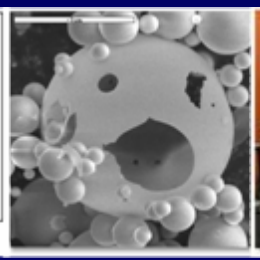
Notes

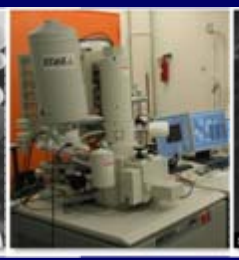


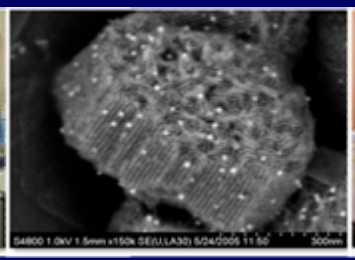




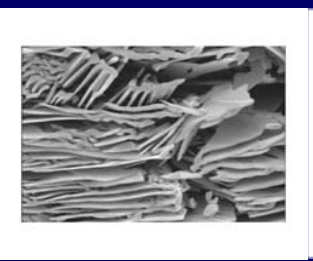


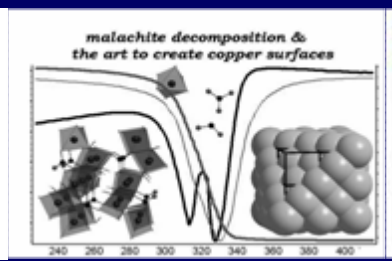


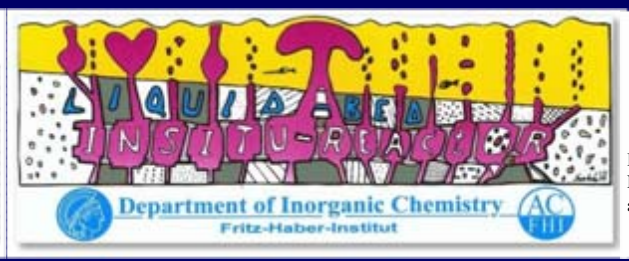


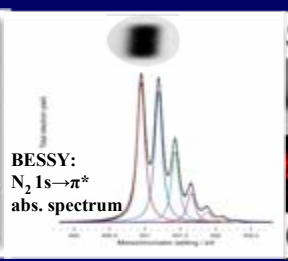


http://www.fhi-berlin.mpg.de

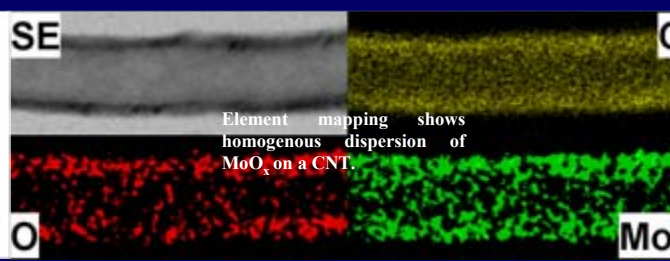








BESSY:
N_2 1s→π*
abs. spectrum



Element mapping shows homogenous dispersion of MoO_x on a CNT.

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