



DEPARTMENT OF

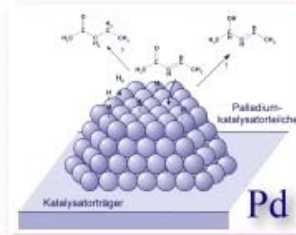
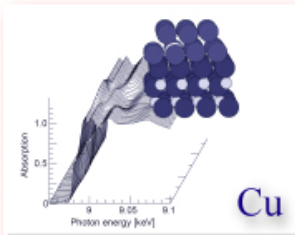
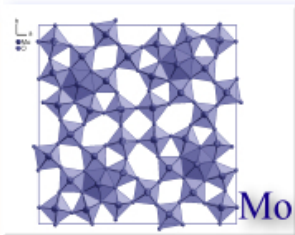
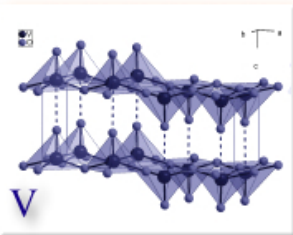
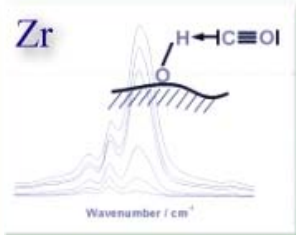
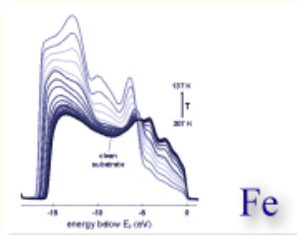


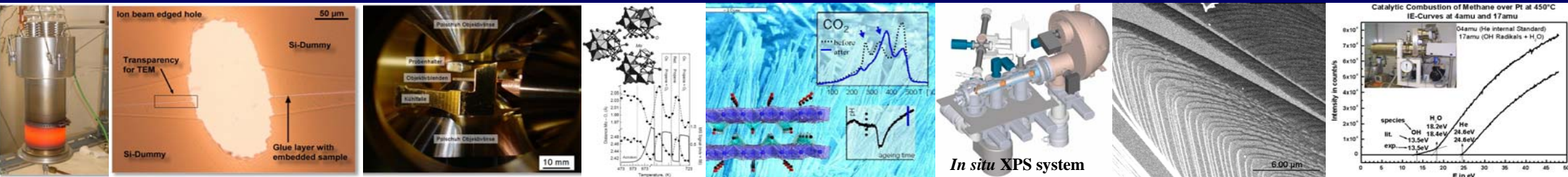
MAX-PLANCK-GESELLSCHAFT

INORGANIC CHEMISTRY



FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT





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

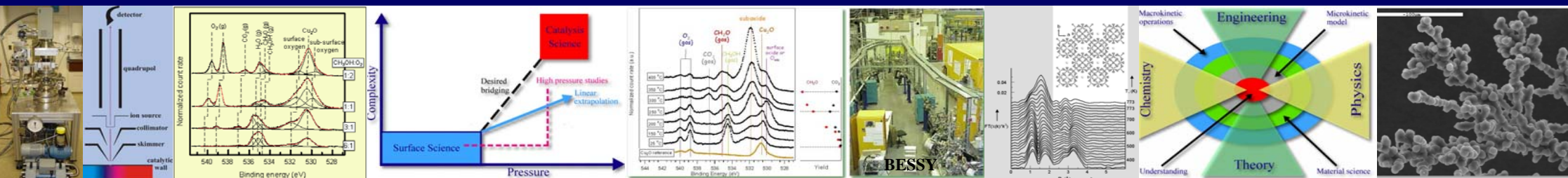


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History of the Fritz-Haber-Institut



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



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

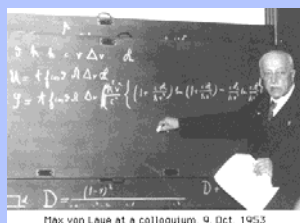
What is now called the Fritz-Haber-Institut of the Max-Planck-Gesellschaft was founded in 1911 as the Kaiser-Wilhelm-Institut for Physical Chemistry and Electrochemistry, together with the Kaiser-Wilhelm-Institut for Chemistry. These were in fact the first two institutes of the Kaiser-Wilhelm Society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

How to reach the Institute



MAX-PLANCK-GESellschaft

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:

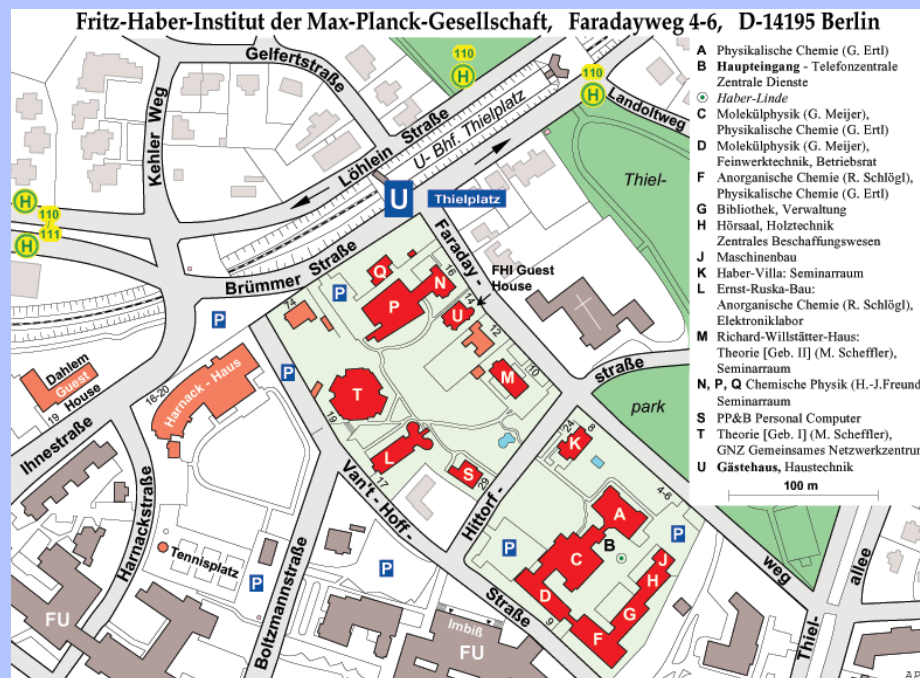
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs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



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The main field of activity in the Department of Inorganic Chemistry at the Fritz-Haber-Institut is to link scientific understanding and technical feasibility in the field of heterogeneous catalysis. Catalysis is the science and technique to control the speed of chemical reactions. This is of decisive importance for the manufacture of about 90 % of all the products in chemical and petrochemical industry. There is an urgent requirement to develop new materials as the overall efficiency in manufacturing most of the products is 50% only. Today all the new materials are developed on an empirical basis, i.e. by trial and error although the basic processes of reaction control are well understood here as well as in the other departments of this institute.

To overcome the gaps between theoretical knowledge and practice is our general concern. Thus, we are studying technically relevant reactions in different fields such as partial oxidation, dehydrogenation and isomerization of hydrocarbons. Within the framework of publicly-relevant mobility technologies we are actively contributing to the protection of environment by studies on Diesel emission particles and to the field of new energies by studies on the generation of hydrogen by means of steam reforming for fuel cells.

We are applying and developing analytical methods allowing an insight into the dynamic behavior of catalysts at work and use the results to develop new processes for the synthesis of catalysts based on the knowledge of how to control reactions. Among these methods experiments with synchrotron radiation in different energy ranges play an important role. We are aiming at generic approaches but always in relation to practical problems. Numerous scientific as well as technical cooperation agreements ensure that we are competent to tackle the inter-disciplinary challenges of physics, nanotechnology and chemistry. We are now about to understand that analysis and control of the dynamic character of function materials „catalysts“ form the missing link between surface sciences and catalysis. We see the chance for a principal breakthrough in this field by developing chemically simple but structurally complex systems..

Prof. Dr. Robert Schlögl

Vorwort



DIREKTOR:
PROF. DR. ROBERT SCHLÖGL

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RS

Die Abteilung Anorganische Chemie des FHI befasst sich mit der Verknüpfung von wissenschaftlichem Verständnis und technischer Anwendbarkeit im Bereich der heterogenen Katalyse. Katalyse ist die Wissenschaft und Technologie der Steuerung der Geschwindigkeit chemischer Reaktionen. Dies wird zur Herstellung von etwa 90% aller Produkte der chemischen und petrochemischen Industrie ausgenutzt. Alle Materialentwicklungen, deren Notwendigkeit sich auch heute noch drastisch stellt, da wir nur etwa 50% Gesamteffizienz bei der Herstellung der meisten Wertstoffe erzielen, laufen rein empirisch (trial and error) obwohl man, wie auch in den übrigen Abteilungen unseres Institutes, die grundsätzlichen Prozesse der Reaktionssteuerung gut versteht.



Die Überwindung der Lücken zwischen Wissen und Praxis ist unser Anliegen, das wir in verschiedenen Feldern technisch relevanter Reaktionen wie der Partialoxidation, der Dehydrogenierung und der Iso-merisierung von Kohlenwasserstoffen studieren. Im Bereich der öffentlich relevanten Mobilitätstechnologien sind wir beim Umweltschutz mit Arbeiten zum Dieselpartikelemissionsproblem und bei den neuen Energien mit Arbeiten zur Wasserstoffherzeugung durch Dampfreformierung für die Brennstoffzelle aktiv. Wir verwenden und entwickeln analytische Methoden, die uns Einblick in das dynamische Verhalten von Katalysatormaterialien während der Arbeit geben und setzen die Ergebnisse um, indem wir neuartige Verfahren zur Synthese von Katalysatoren entwerfen, die wiederum auf einer Kontrolle des Reaktionsgeschehens während ihrer Bildung beruhen. Unter diesen Methoden spielen Experimente mit Synchrotronstrahlung in verschiedenen Energiebereichen eine wesentliche Rolle. Wir streben dabei nach generischen Ansätzen, die jedoch immer mit praktischen Problemen verbunden werden. Zahlreiche wissenschaftliche aber auch technische Kooperationen stellen sicher, dass wir den interdisziplinären Herausforderungen zwischen Physik, Nanotechnologie und Chemie kompetent begegnen.

Wir beginnen zu verstehen, dass die Analyse und Kontrolle des dynamischen Charakters der Funktionsmaterialien "Katalysatoren" das fehlende Glied zwischen Oberflächenwissenschaften und Katalysertechnologie darstellt. Wir sehen die Chance, einen breiten Durchbruch in diesem Gebiet mit der Entwicklung von chemisch einfachen aber strukturell komplexen Systemen zu erzielen.

Prof. Dr. 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 main methodical activities.



PREPARATION

Synthesis, Raman, UV-vis, Reactor design,
Elemental analysis, BET,
XRD, TG, DSC
Dr. A. Trunschke



FUNCTIONAL CHARACTERIZATION

IR, UV-vis-NIR, Calorimetry,
Gas phase reactions, Sorption methods,
Elemental analysis
Dr. F. C. Jentoft
(Habilitation)

In situ
Catalysis



SURFACE ANALYSIS

Photoelectron spectroscopy,
TP desorption, TP reaction, BESSY II
Dr. A. Knop-Gericke



MICROSTRUCTURE

TEM, SEM, ELNES, Nanoreaction
Dr. D. S. Su



Prof. Dr. Robert Schlögl

Prof. Schlögl's Office

Damm, Röper

Functional Characterization	Surface Analysis	Preparation	Microstructure	Central Services
Jentoft	Knop-Gericke	Trunschke	Su	Wrabetz
N.N.	Ranke	Kubias	Hansen	
Kröhnert	Armbrüster	Blume	Chen, X	Lehmann
Klokishner	Hävecker	Busser	Delgado Jaen	
Pelzer	Hess	Engelschalt	Frandsen	
Reu	Kleimenov	Girgsdies	Fu	
Taha	Swoboda	Jentoft, R.	Klein-Hoffmann	
Tzolova-Müller	Teschner	Klaeden	Kruse	
Venkov	Vass	Kovnir	Pfänder	
++Chan Thaw	Wild	Lorenz	Müller	
++Geske	Zafeiratos	Makwana	Sack-Kongehl	
++Hohmeyer	++Aburous	Timpe	Sauer	
++Klose	++Gabasch	++Celaya Sanfiz	Tessonnier	
++Lloyd	++Herbert	++Dennstedt	Wang	
	++Schnörch	++Kurr	Weinberg	
	++Steinhauer	++Maamor	Willinger	
	++Vimovskaia	++Osswald	Zhang	
		++Rödel	++Echegoyen Sanz	
		++Soertjanto	++Liu	
		++Zakaria	++Said	
++ doctoral student			++Sun	

September 2005

Mission

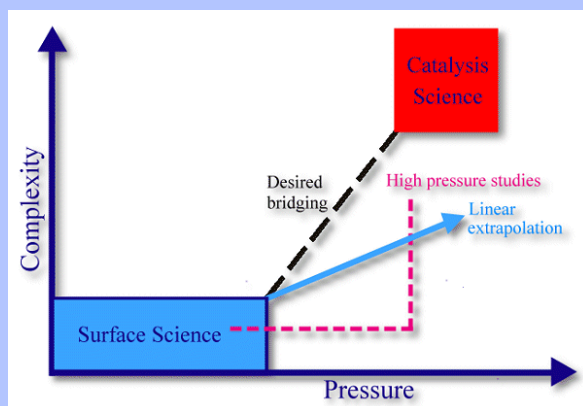
„Catalysis is too difficult."
„We see the exorcism of the
mysticism of catalysis."

R. v. Veen, Dronten, 1999

These words from a representative of the International Chemical Industry signalise the still unsatisfactory development of catalysis science, in particular of heterogeneous catalysis. This contrasts strongly with the expectations raised by academic researchers about the understanding of catalytic processes achieved by surface science, physical chemistry and theory.

The extrapolation of surface science results under „academic" conditions into the regime of practical catalysis science is still problematic and limited to very few cases. Methodical problems limit the interdisciplinary activity to creating a more efficient way of developing heterogeneous catalysis. The activities of the Department aim at finding generic procedures to reduce these methodical problems.

Link Surface Science and Catalysis Science



Conventional approaches to link surface science and catalysis science. The desired bridge is often not reached by linear extrapolation of microkinetic data (blue) from surface science nor by applying "high pressure" experiments with single crystal samples (red) which tend to lose their model system qualities upon high pressure exposition to reactants.

The results of catalysis science which uses the tools of surface chemistry and chemical kinetics are also internally consistent but refer to a different set of basic assumptions than those of surface science even when they are targeted on the nominally same chemical reaction. The relation of the two data sets is not clear. The apparent disagreement has led to the terminology of "gaps" between these two sciences, with the most prominent terms being the pressure gap and the material gap.

In the endeavour to correlate the two sets of results on a quantitative basis one often finds no satisfactory agreement. In recent years the surface science has adopted the development of numerous high-pressure studies with model systems in order to experimentally bridge the apparent gap between the two fields. These experiments are very demanding and still do often not reproduce the functionality of the genuine technical system.

The Department of Inorganic Chemistry concentrates on finding methods and procedures to bridge the gaps between catalysis and surface science for heterogeneous gas-solid interface reactions. In view of the other research fields pursued in the institute the Department concentrates on the chemical aspects of catalysts under technical working conditions. Besides typically chemical methods it uses and adopts also physical methods from surface science to deal with the analytical problems. The study of related surface science problems is left to or conducted with the other departments in the institute leading to a close and for the AC Department essential co-operation within the institute.

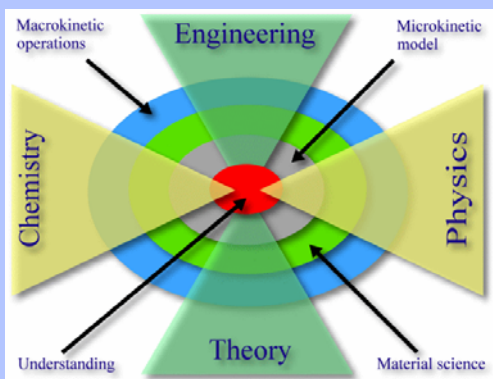
Vision

„Heterogeneous Catalysis is an interesting mixture of engineering and art.“

F. M. Hoffmann; D. J. Dwyer
ACS, 1992

Heterogeneous catalysis is neither a mature science nor a mature technology despite the long time it is worked with. Although the principles of its operation seem to be understood, the exact mode of operation of a selection of generic examples of reactions is still far from understood. The industrial and political needs require massive improvements in the technology of chemical manufacturing, environmental clean-up and energy management. These improvements are in principle possible but require on the side of catalysis technology major efforts in view of the results achieved so far. These efforts will benefit greatly when the empirical search for optimised solutions is supported or eventually replaced by a knowledge-driven development procedure. **The Department seeks to contribute to this transformation process.**

Heterogeneous catalysis is a complex science and technology with several disciplines and levels of knowledge contributing.



Heterogeneous catalysis is a complex science and technology with several disciplines and levels of knowledge contributing. Some key factors are mentioned in the Figure.

The situation is still much as depicted here with the participating scientific disciplines having insufficient overlap. The Department of inorganic chemistry thus tries to bring together activities from some of the disciplines in one organisation. The Department can fulfil its mission in this complex situation only with multiple and intensive co-operations with academic institutions and with industry.

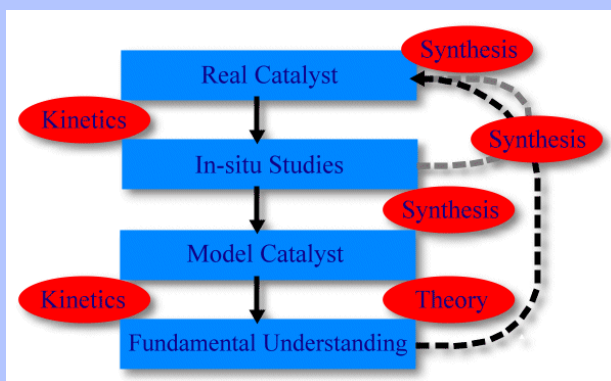
With the core competence in functional and structural in-situ analysis and controlled inorganic synthesis of heterogeneous catalysts the Department develops a specific profile.

The long term goal is to collect for a set of generic reactions the experimentally founded relations between structural, electronic and chemisorption properties of relevant catalysts and the respective catalytic functions. Such an understanding can only be achieved by analysing at least several related processes such as in selective oxidation. A benefit from it would be deep understanding of operating processes, the prediction of optimised reaction conditions and ultimately the evolution of new catalytic chemistry both for catalysts and for new processes. Such a vision is fundamentally different from the current attempt to replace the difficult analysis of existing systems by a high throughput testing strategy allowing to find directly the new catalysts and reactions looked for.

Strategy of Research

Basis of all investigations is the assumption that the knowledge of the structure of the reacting solid at and below its surface must be known in order to perform meaningful functional studies (kinetic experiments). In addition, the reactivity and dynamics of the system must be known in order to understand the influence on the system of changing reaction conditions. To obtain this information, an integrated approach is taken of complementary analytical techniques and dedicated material synthesis. The resulting **strategy is outlined in the Figure**. The term "real catalyst" describes the technical catalyst with all its complexities (support, promoters, additives) resulting from empirical optimisation

Research strategy to achieve a fundamental understanding of heterogeneous catalytic processes



The red areas designate vital influx from not immediately catalysis-connected research efforts into the strategy which are often not sufficiently co-ordinated with catalysis science. Of particular relevance are advanced synthetic efforts which aim not at the discovery of new materials but which need to produce a well-defined material with already known functional properties. Kinetics with in-situ studies relates to macrokinetics, whereas the microkinetic method is meant in relation to the model system studies. Theory designates the application of quantum chemical methods and molecular dynamics for the exploration of reaction mechanisms and reaction energy profiles



The synthesis of such a real catalyst is an area of research in its own, as usually difficult-to control procedures are required to achieve the desired functional (catalytic) properties which are best obtained from the performance data of technical plants. Reactor experiments are thus required as well as the conduct of a collection of inorganic preparative methods.

A key feature in this strategy is the existence of a suite of complementary in-situ analytical techniques probing the geometric and electronic structure of working catalysts. Each in-situ experiment requires the simultaneous detection of catalytic performance and spectroscopic structural property in a way allowing a quantitative correlation to be established.

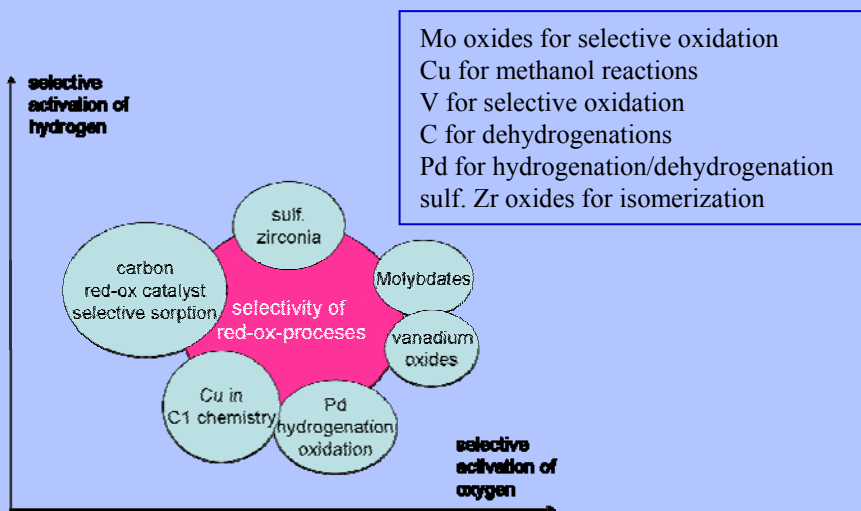
The creation of suitable model systems is an indispensable step in the overall strategy for understanding catalysis. Realistic model systems are constructed which are based upon the knowledge of the properties of the real system. Several steps of reducing the complexity are taken, as outlined in the Figure. These model systems of intermediate complexity are studied with in-situ techniques at intermediate pressures. The model systems are indispensable to disentangle the complex interplay of surface processes and bulk chemical reactions contributing to the performance of a catalyst.

The final target of such a strategy is the fundamental understanding resulting in a quantitatively correct microkinetic model of the system. The fundamental knowledge can be used and put to the test in attempts to synthesize new and alternative catalyst systems.

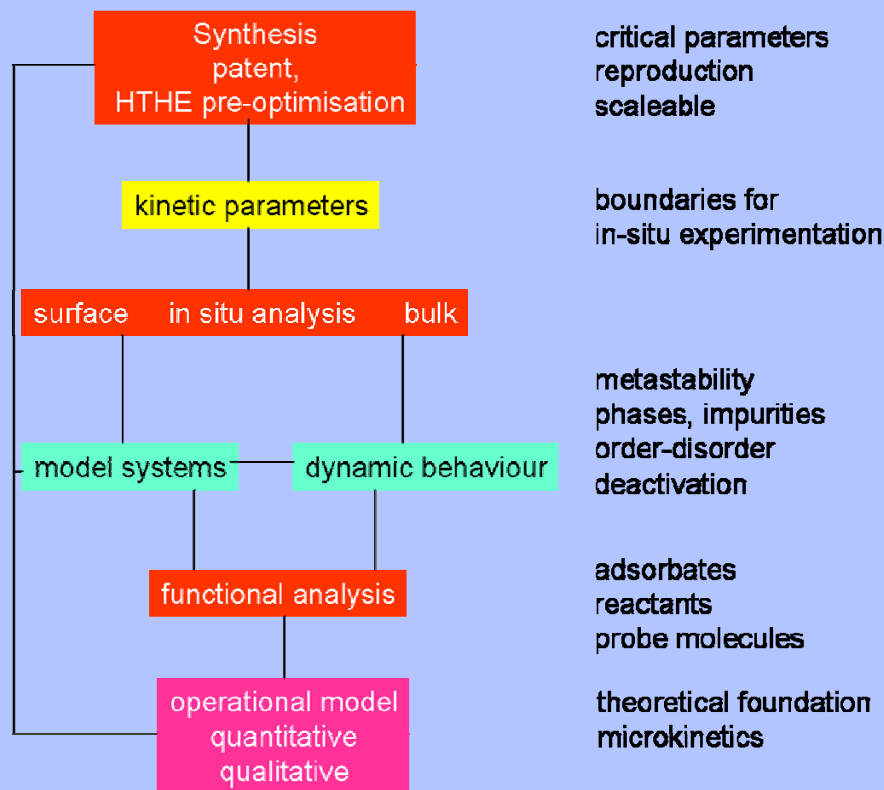
Scientific Progress

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:

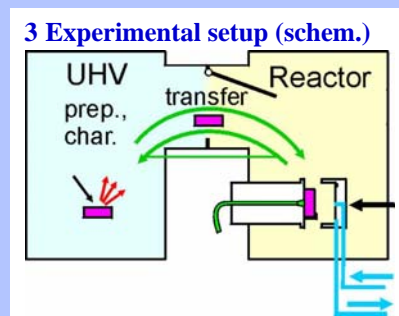
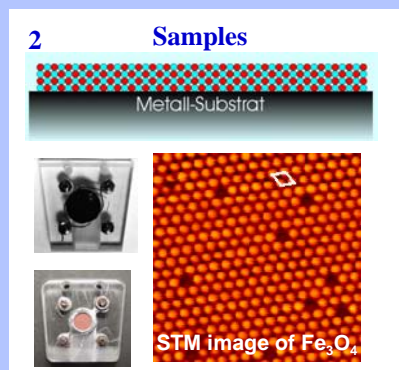
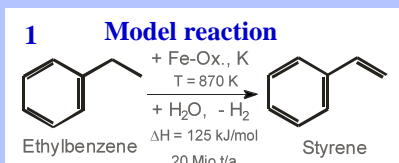


The target of the Department is the rational development of complex model systems. The current profile of the Department allows defining the choices of systems to be synthesized on the basis of in-situ observations of technical systems rather than on pragmatic arguments of nominal catalyst composition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



Scientific Progress

Iron oxide based model catalysts

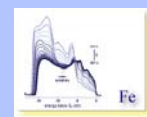


The project represents an in-depth model catalysis study on a complex system, the dehydrogenation of ethylbenzene (EB) to styrene (St) (fig. 1). Technically this reaction is run at $\sim 870 \text{ K}$ over potassium-promoted iron oxide catalysts with water vapor added in excess.

The model catalysts consist of unpromoted or potassium-promoted iron oxide films of single crystalline quality (fig. 2) which are prepared and characterized in ultrahigh vacuum (UHV) using surface science methods. In order to bridge the pressure and material gap, the reaction is studied at reactive gas pressures between 10^{-6} and 36 mbar. For the high-pressure studies, the samples are transferred under vacuum into a stagnation point micro-flow reactor (fig. 3). For post-reaction characterization they are transferred back into UHV. For comparison, pressed powder samples are investigated in the same setup.

Results

Surface defects turn out to be a prerequisite for catalytic activity. Clean hematite Fe_2O_3 is an excellent catalyst but deactivates quickly by reduction and by coking (fig. 4, lower curve). Addition of H_2O limits reduction to the oxidation state of magnetite Fe_3O_4 and counteracts coking.

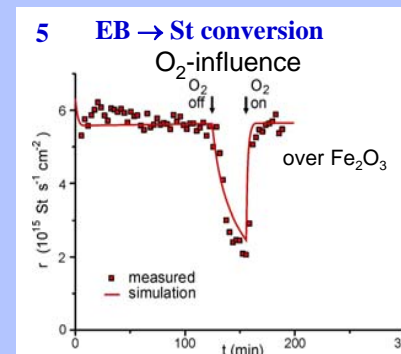
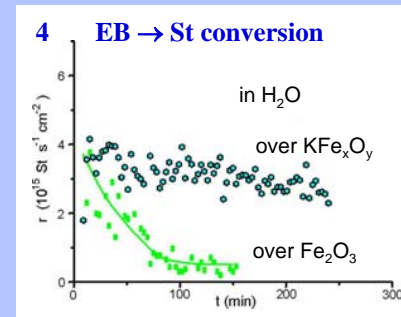


Both deactivation mechanisms can be avoided by addition of some O_2 to the feed (fig. 5).

Potassium has basically the same functions as O_2 in preventing of deactivation. It does not seem to be involved in the catalytic dehydrogenation step but rather to block active sites if its concentration is high. Long-term deactivation occurs mainly by potassium removal in form of volatile KOH. Regeneration by “steaming” in pure H_2O accelerates this process while ethylbenzene in the feed stabilizes potassium. This is ascribed to the formation of non-volatile K_2CO_3 which is an intermediate in potassium catalysed coke removal. The addition of O_2 instead of K-promotion may be an alternative reaction route.

In cooperation with A. Schüle and G. Kolios (Univ. of Stuttgart), microkinetic modeling was performed, using energetic and kinetic adsorption-desorption data for EB, St, H_2O on different iron oxide phases and carbon from UHV experiments and adjusting unknown parameters using the conversion data. Excellent fitting is achieved (example: O_2 on-off experiments fig. 5).

Present activities concentrate on the surface chemistry of H_2O , H_2 and atomic H on the iron oxide model catalyst films for which details are lacking so far.



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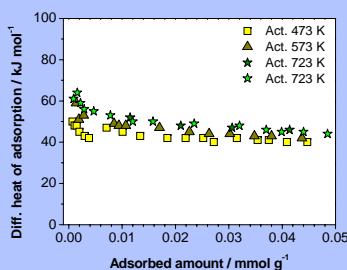
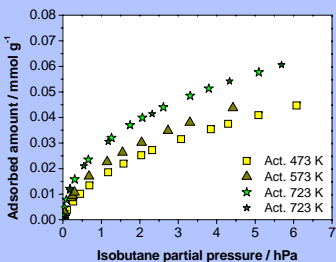
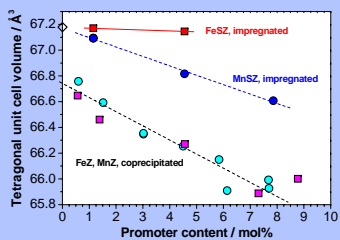
External collaborations:
 Univ. Stuttgart, Inst. f. Chem. Verfahrenstechnik (Dr. G. Kolios, A. Schüle)
 ACCELRYs, Unterhaching (Dr. M. Grillo)
 Univ. Sci. Technol. of China, Dept. of Chem. Phys., Hefei, China (Prof. W. Huang)

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 A. v. Humboldt Foundation
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Scientific Progress

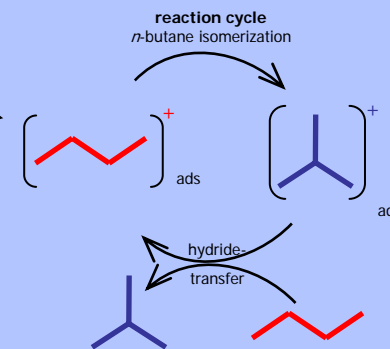
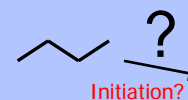
Zirconia and heteropoly acids in hydrocarbon activation

Sulfated zirconia materials are attractive catalysts for the low temperature skeletal isomerization of alkanes. Our efforts are devoted to: (i) the solid state chemistry of the catalysts, (ii) the characterization of surface functionalities by interaction with probe molecules using IR spectroscopy and calorimetry as analytical methods, and (iii) in situ studies.



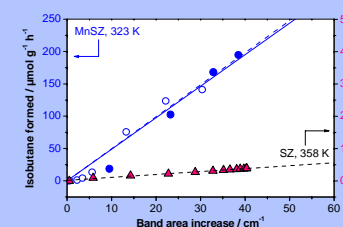
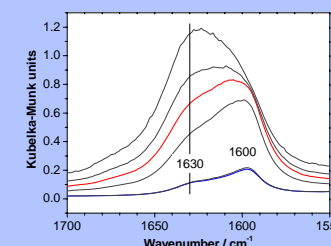
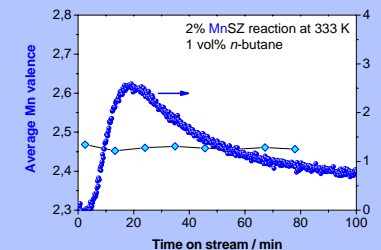
Sulfated zirconia can be promoted through the addition of small amounts of manganese or iron. Shrinkage of the unit cell of the tetragonal zirconia phase with increasing promoter content (analyzed by XRD, Fig.1) indicates these promoters are incorporated into the zirconia lattice, to an extent that depends on the catalyst preparation. Hence, we are now investigating whether promoter surface species or the modification of the zirconia bulk are responsible for the increased activity.

Small alkanes are used to probe the catalytically relevant sites. Interaction becomes stronger with advancing dehydration of the catalyst as the adsorption isotherms and differential heats demonstrate (example sulfated zirconia, Figs. 2 & 3). However, adsorption of alkanes occurs on active and inactive samples, and differently active catalysts cannot be distinguished. The number of sites interacting at typical reactant pressures (1-5 kPa) is small and corresponds to only a fraction of the sulfate groups.



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 and 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 are checking for ODH products, namely water, alkenes, and reduced catalyst species. In situ X-ray absorption and UV-vis spectroscopic data reveal that the Mn valence can be altered through treatments despite the incorporation of Mn into the zirconia lattice; however, Mn is not reduced during catalysis (Fig. 4). In situ diffuse reflectance IR spectra (Fig. 5) document the growth of several bands at 1600-1700 cm^{-1} , maybe indicating water accumulation on the surface. During the period of increasing conversion the isomerization rate is proportional to the area of these bands (Fig. 6). Future in situ studies will address the reaction initiation and events at longer times on stream.



In situ

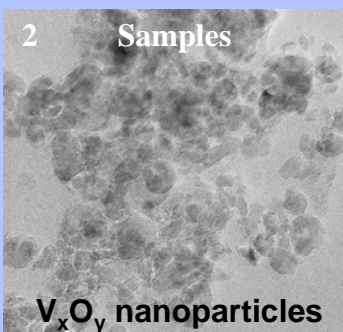
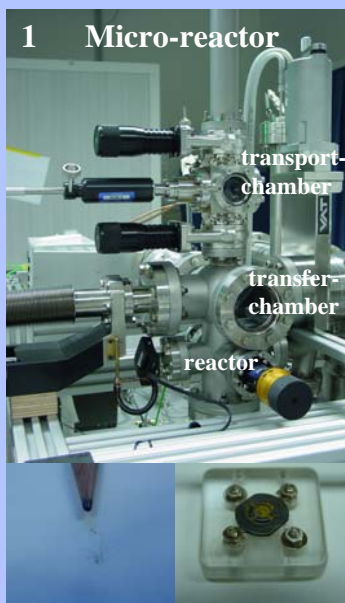
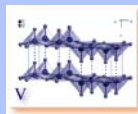
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Financial support:
DFG
Priority Program 1091

Scientific Progress

Vanadia in C4 selective oxidation



A micro-reactor for catalyst testing in the micrometer regime (fig. 1) was successfully implemented within the framework of the SFB 546 of the Deutsche Forschungsgemeinschaft. V_xO_y nanoparticles were studied in the selective oxidation of *n*-butane towards maleic anhydride. Changes in the electronic and geometric structure of the material were monitored by transmission electron microscopy (TEM), electron diffraction, electron energy-loss spectroscopy (EELS) and X-ray photoelectron spectroscopy (XPS) before and after the reaction at different temperatures within 200 - 400°C. In the course of the temperature treatment the particles did undergo a radical modification of the geometric and electronic structure that finally resulted in V_2O_5 crystals.

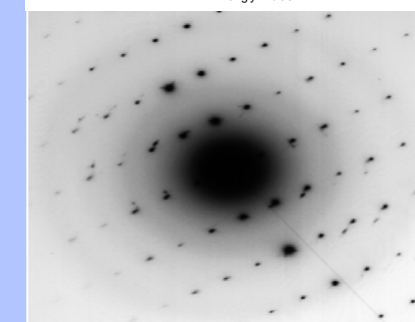
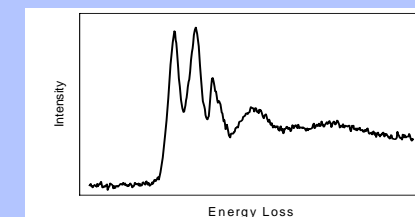
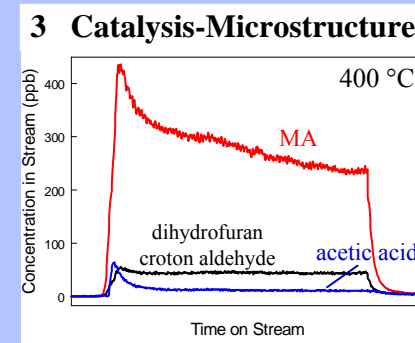
V_xO_y nanocrystals (fig. 2) were synthesised by an alkoxide/benzyl alcohol route in a steel autoclave at 200°C using vanadium (V) triisopropoxide as starting material.

Results

During the equithermal experiments at 200°C and 400°C temporal changes in the catalytic activity are observed, which point to an evolution of the catalyst structure (fig. 3). At 300°C, the steady state behavior indicates a stable structure of the catalyst.

It is evident from XPS and the relative intensity changes in the V and O edge of the EEL spectra that in the course of the temperature treatment the electronic structure of the nanoparticles changes from a variety of vanadium species with different oxidation states in the range of V^{3+} to V^{5+} to a material that contains only V^{5+} species (fig. 3). Electron diffraction shows that the material consists nearly exclusively of V_2O_5 crystals after treatment at 400°C (fig. 3). The formation of solely V_2O_5 seems to be detrimental for the reactivity of the material. This conclusion is supported by the fact, that material that has been heated to 400°C for a prolonged time showed a lower MA yield when it was cooled down to 200°C than a material that was heated from room temperature to 200°C.

Using the above approach it was possible to follow the structural transformations from a supramolecular system into the highly active selective oxidation phase and into its deactivated stable form of V_2O_5 . Morphological, geometric structural and electronic structural details of the metastable state of V_xO_y were collected, which can be used for developing experimentally supported structural models of the active sites.



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Financial support:

Athena

Deutsche Forschungsgemeinschaft



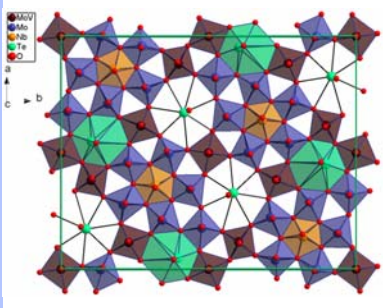
Scientific Progress

Molybdenum oxide based catalysts in C3 selective oxidation

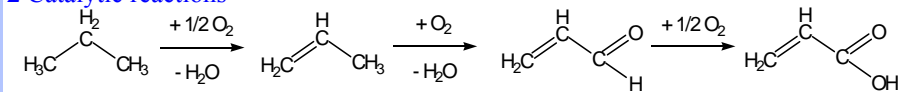
Background and objective

Molybdenum oxide is an essential constituent of catalysts applied in the selective oxidation of hydrocarbons. Mo-V-W oxides are used for oxidation of propene to acrylic acid. The direct conversion of propane to acrylic acid has been achieved with mixed Mo-V-Te-Nb oxides (Fig.1). Different from Mo-based multi metal oxides, structurally well-defined bulk orthorhombic MoO₃ is fully inactive in these complex reactions (2) that require the simultaneous activation of di-oxygen and carbon-hydrogen bonds and the availability of weakly bound surface oxygen as reactant.

1 Structural model of an orthorhombic Mo-V-Te-Nb-O_x phase



2 Catalytic reactions

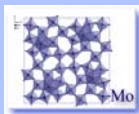


3 a) Rotating furnace/Xerion, FHI

b) Autoclave/Parr



Within the project, catalytic properties of modified molybdenum oxides are systematically studied as a function of structural characteristics and chemical composition. Reproducible methods for the preparation of reference materials and model catalysts ranging from pure MoO₃ over binary Mo-V and Mo-Nb oxides to complex Mo-M mixed oxides (M=V, Nb, Te) are developed with the aim to control phase composition and nanostructure of the product.

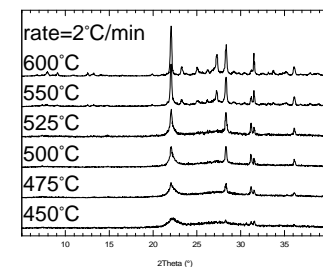


Results

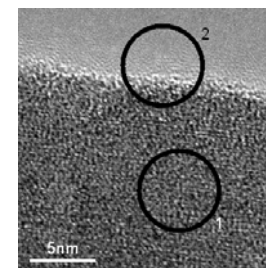
The mixed oxides are currently prepared by hydrothermal synthesis (Fig.3b) or spray drying of aqueous polyoxometalate solutions. Self-assembling processes of oxoanions involved in the latter preparation procedure have been studied by Raman spectroscopy. Heteropolyanions of the Anderson-type represent the dominating structural unit in mixed MoVTe solutions. These Anderson-type species are preserved after spray drying. Crystalline phases are formed by rearrangement of the molybdotellurate building blocks during thermal activation of the catalyst (Fig.3a and 4). A complex precursor phase (Spot 1 in Fig.5) carries nanoparticles made from a network of oxoclusters (Spot 2 in Fig.5) active as catalyst for the conversion of propane to acrylic acid.

Thin films of metal oxides on Si have been prepared by spin-coating of metal ion containing solutions to access surface science techniques like *in-situ* XPS. Sol-gel procedures employing alcoholic media are used for wet chemical thin film deposition. A new micro-reactor concept suitable for thin film *in-situ* optical spectroscopy has been developed (Fig.6). The catalytic properties of complex thin oxide films have been studied during selective oxidation of propene.

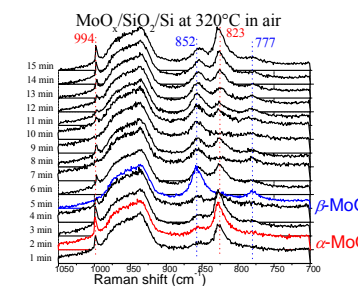
4 XRD during thermal activation



5 TEM image of Mo-V-Te-Nb-O_x



6 Raman spectra of a thin film



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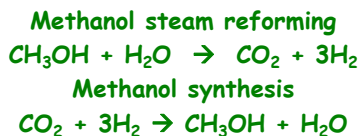
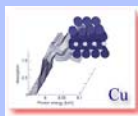
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Financial support:

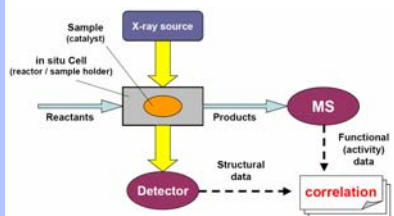
Degussa AG

Scientific Progress

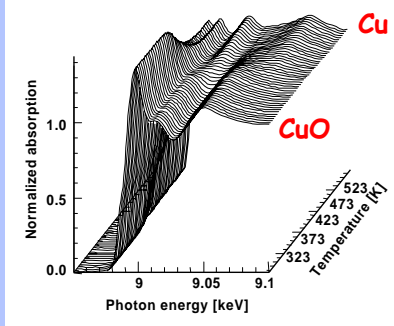
Copper catalysts in methanol chemistry



1 Instrumentation



2 Time-resolved studies



Introduction

The progressing shift in resources used in the petrochemical industry from crude oil to natural gas increases the importance of methanol as a basic chemical. Copper zinc oxide catalysts are industrially used for methanol synthesis and the water gas shift reaction and are also active for the steam reforming of methanol for the production of hydrogen. Because methanol is a potential candidate for hydrogen production in fuel cell applications, Cu/ZnO catalysts offer a high potential for future applications (e.g. in automobiles). Therefore, a detailed knowledge of the relationships between catalytic activity and surface structure and bulk structure is desirable in order to prepare new and improved catalysts according to a knowledge-based (rational) catalyst design.

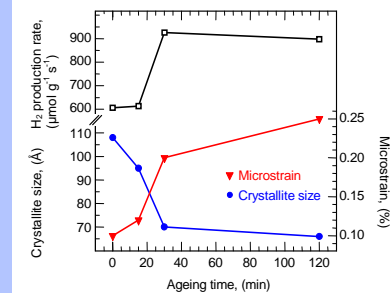
Results

From structural studies under dynamic reaction conditions (1+2) we could show that copper nanoparticles exhibit surfaces with different catalytic activities. In addition to the surface area, bulk structural parameters like microstrain in the copper particles were identified to correlate with the catalytic activity of Cu/ZnO catalysts in methanol synthesis and methanol steam reforming (3).

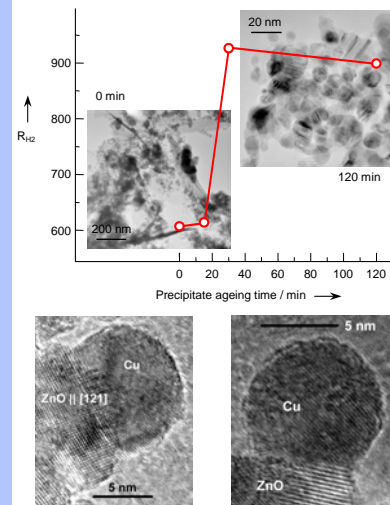
The “real” structure of copper catalysts deviates considerably from that of ideal bulk copper metal and emphasizes that structural complexity is a prerequisite for an active heterogeneous catalyst (3+4).

With respect to designing new improved copper catalysts, our investigations have shown that the microstructural characteristics of Cu/ZnO catalysts can be tailored directly during the preparation, for instance, by an appropriate ageing procedure (4). The structure-activity relationship of Cu/ZnO catalysts revealed and the possibility to tailor the “real structure” of a catalyst during the preparation, are a step forward to a rational design of improved catalysts. Accordingly, it emerges, that microstructure design of superior heterogeneous catalysts has to start at the very first stages of catalyst preparation. A lack of understanding of the performance-governing character of the early stages will render a successful design of new catalysts impossible. Hence, in addition to studying structure-activity relationships of solid catalysts, the “memory” of the material on proper and improper treatment of its precursor needs to be elucidated and considered in a rational catalyst design.

3 Structure & activity



4 Microstructure of Cu/ZnO



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Financial support:
ZEIT-Stiftung
Deutsche Forschungsgemeinschaft



Scientific Progress

Palladium based catalyst
(Athena Project)

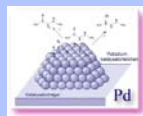


Fig.1 1-Pentyne hydrogenation on Pd foil

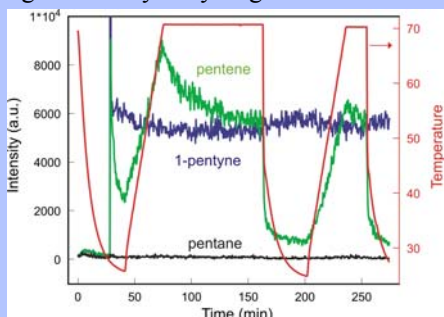
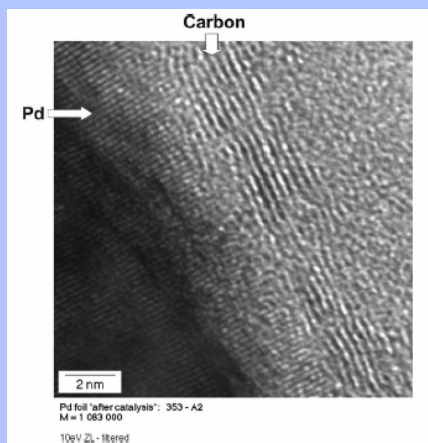


Fig.2



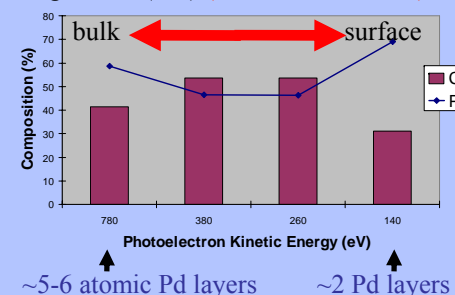
Pd based catalysts are applied for many hydrogenation and oxidation reactions. The hydrogenation of C5 compounds like trans-2-pentene or 1-pentyne over model and real catalysts, the oxidation of carbon monoxide and ethylene and methane combustion over Pd(111) were studied. The correlation between the 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.

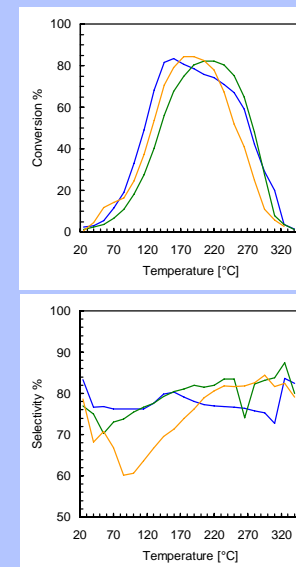
A further aspect of the project is the improvement of the selectivity of Pd based hydrogenation catalyst. The project follows the approach of the site isolation concept. Intermetallic compounds like PdGa and Pd₃Ga₇ have been prepared by mixing the two molten metals followed by milling of the intermetallic compound. The surface of the obtained powder is rather low (1m²/g), but the selectivity was enhanced compared to Pd catalyst supported on Al₂O₃ showing the same conversion rate (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 Pd (foil) (reaction mix; 85°C)



Acetylene Hydrogenation
PdGa – Pd₃Ga₇ – Pd/Al₂O₃

Fig.4



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Univ. Limerick, Materials and Surface Science Institute (Dr. D. Zemlianov)

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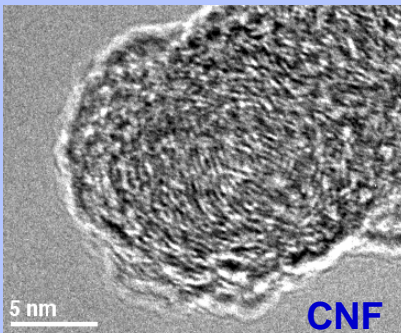
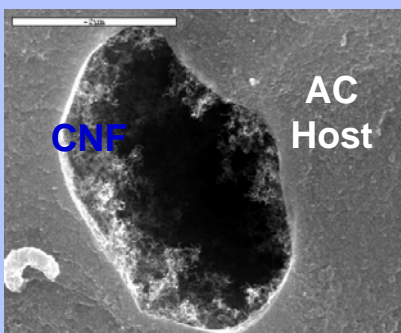
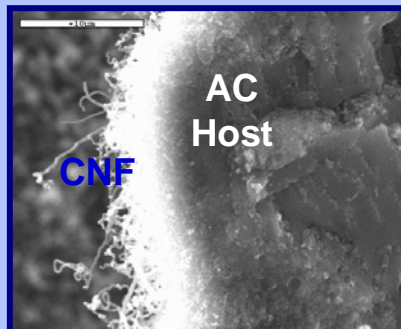
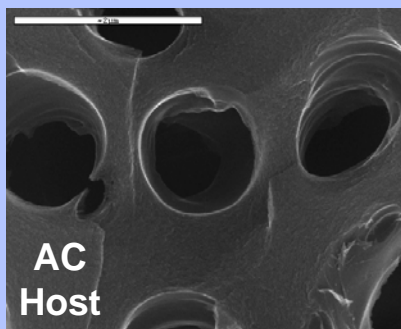
EPRSC
Johnson & Mathew

Scientific Progress

Carbon in catalysis

Synthesis of Nano Architected Carbon

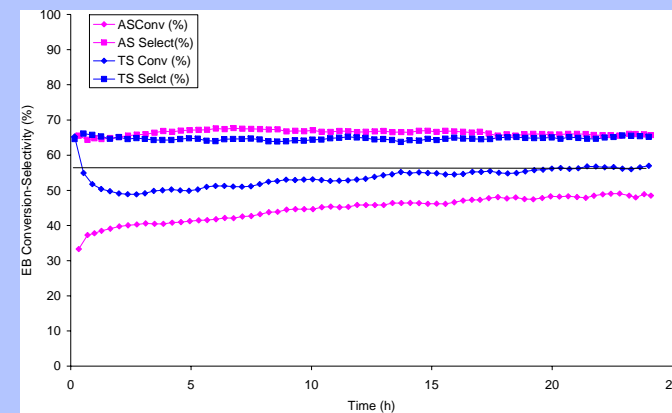
Hierarchically structured carbon systems with CNFs nested inside or immobilized onto modified activated carbon has been successfully synthesized by means of chemical vapour decomposition of ethylene. The activated carbon is obtained from bio-waste of palm oil production, followed by a mild oxidation as pre-treatment and the impregnation of catalyst. The nano-architected carbon system has great potential in the environmental application: abundance of the adsorbed heteropolymolybdate $[PMo_{12}O_{40}]^{3-}$ increases a factor of 27 after the growing of CNFs on and inside the activated carbon.



Nanocarbon in Oxidative Dehydrogenation Reaction (EU Sixth Framework Programme)

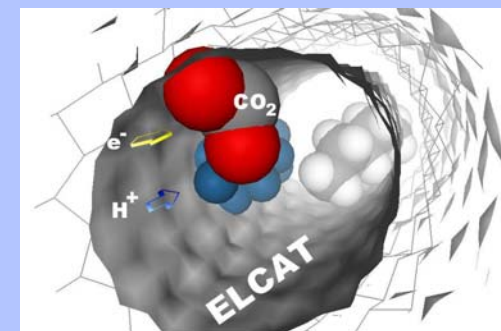
Single-walled (blue) and multi-walled (pink) CNTs were tested for oxidative dehydrogenation of ethyl benzene to styrene.

The promising performance at 400°C opens the horizon for an industrial application of CNTs in polymer synthesis.



Electrocatalytic Gas-Phase Conversion of CO₂ in Confined Catalysts (EU Sixth Framework Programme)

Novel functionalized CNTs are developed for the use as novel electro-catalyst materials for gas-phase conversion of CO₂ to Fischer-Tropsch like products (C1-C10 hydrocarbons and alcohols).



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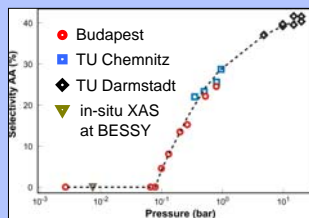
External collaborations:
European Laboratory for Catalysis and Surface Science
(ELCASS)

Financial support:
European Union
Deutsche Forschungsgemeinschaft

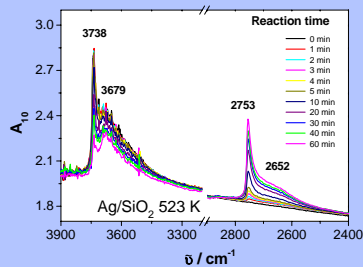


Scientific Progress

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, and the app. activation energy for H_2 cleavage is similar to that of acrolein hydrogenation. Next, acrolein adsorption and reaction will be studied by in situ IR spectroscopy.



Silver catalysts are also well-known to be active and selective in the ethylene oxidation to ethylene oxide. To reveal correlations between evolving microscopic structural changes at the silver surfaces and the resulting catalytic properties, STM¹ investigations and catalytic experiments in model reactors are in progress. Long-term batch experiments using $^{13}\text{C}_2\text{H}_4$ and O_2 containing feeds and polycrystalline Ag or Ag single crystals as catalysts were performed under low (100 mbar > p > 0.02 mbar) and enhanced (1.8 bar) pressures. In these experiments, a significant formation of ethylene oxide was observed at 120°C (the maximum working temperature of STM). Due to an unexpected formation of ethylene oxide on the inner surfaces of the model reactor future studies will be aimed at the reduction or quantification of the undesired blank reaction. In situ XPS measurements show two different types of oxygen on the surface of the active catalyst in the ethylene epoxidation reaction. The peaks at binding energies of 530.1 eV and 529.4 eV are assigned to electrophilic and nucleophilic oxygen respectively. The yield of CO_2 has a maximum when the abundance of nucleophilic and electrophilic on the Ag surface is the same. This finding supports the hypothesis that ionic Ag acts as adsorption site for ethylene and electrophilic oxygen is required for the oxidation.

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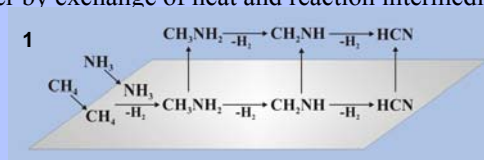
External collaborations:

Prof. Dr. P. Claus, Dr. M. Bron (TU Darmstadt),
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Scientific Progress

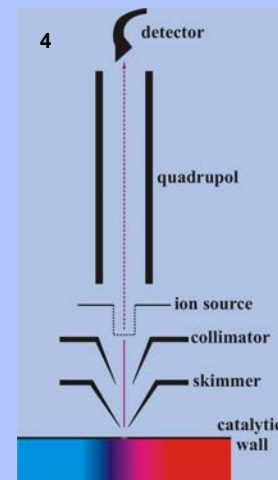
In situ molecular beam mass spectrometry for high temperature catalysis research

Heterogeneous catalytic reactions at high temperatures are of enormous industrial importance. Many reactions like partial oxidations of hydrocarbons, the HCN synthesis or the ammonia oxidation are performed at reaction temperatures of several hundred up to more than thousand degrees Centigrade. A fundamental question arising from such severe conditions is whether these reactions proceed exclusively on the catalyst surface or to some extent also homogeneously in the gas phase (Fig 1). There are strong indications that the latter is true and goal of our research is to understand how surface and gas phase reactions interact with each other by exchange of heat and reaction intermediates.



Horn R.; Mestl G.; Thiede M.; et al.
Phys. Chem. Chem. Phys. 2004, 6,
4514-4521

A high temperature catalytic wall reactor (Fig. 2) mounted in a molecular beam mass spectrometer (Fig. 3) allows us to study high temperature reactions *in situ*.



By free jet expansion of the reacting gases from the catalyst – gas phase boundary layer (Fig. 4) reaction intermediates are quenched and can be identified by their mass spectrometric pattern or their ionization potential (threshold ionization).



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Max Planck Society
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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)

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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)

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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)

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2005

Willinger, M.G., D. S. Su, R. Schlögl: Electronic Structure of β -VOPO₄. Physical Review B **71**, 155118-1 – 151518-8, 2005-07-28

Wurz, R; M. Rusu, T. Schedel-Niedrig, M. C. Lux-Steiner, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke, 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, R. Schlögl, A. Birkner, M. Muhler: Conical Carbon Filaments with Axial Cylindrical Channels and open Tips. Advanced Materials **17**, 1677-1679, (2005)

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 in press (2005)

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Patents

1993 - 2004

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

PCT/EP2004/002765 March 17, 2004 based on EP03 005 953.9,
"Cu-CuO/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

DE 198 10 539, October 7, 1999/US 6, 212,253 B1 April 3, 2001
"Apparatus and method for X-ray absorption spectroscopy"
Inventors, Th. Schedel-Niedrig, A. Knop-Gericke, M. Haevecker

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

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

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

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

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

Guest - Lectures

2003 - 2005

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 University of Manchester, UMIST, Manchester, England	Reconstruction Leading to Unstable Behaviour in Methanol Synthesis and Methanol Oxidation on Cu/ZnO/Al ₂ O 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 Strassburg	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: sp ² /sp ³ 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 Hochstratenspektroskopie mit Roentgenstrahlen

Date	Guest - Lecturer	Titel
14. 01.2004	Prof. Dr. Piotr Dluzewski University of Warsaw, 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

Guest - Lectures












2003 - 2005

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 Institute, Universiteit Utrecht	Tunable carbon nanofibers based catalysts - synthesis, characterization and catalysis

Date	Guest - Lecturer	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

External Funds

Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Photocatalytic Activity of Transparent Conducting Oxide Films	UNAXIS	PSFHI 250	UNAXIS - Balzers AG – Display Division 	01.01.2004 -	Prof. Dr. R. Schlögl	Dr. F. Atamny	Prof. Dr. R. Schlögl, Dr. R. Horn
New tailored Carbon Nanofilaments for Catalytic Applications	DFG 	SCHL 332/7-2	Deutsche Forschungsgemeinschaft	03.11.2004	Prof. Dr. R. Schlögl		
Mikroskopische Strukturbildung von Katalysatoroberflächen unter Realbedingungen	DFG	SCHL 332/8-1 SCHL 332/8-2	Deutsche Forschungsgemeinschaft	11.11.2004	Prof. Dr. R. Schlögl	Prof. Dr. J. Winterlin	
Optimized Acrolein Catalysts	Degussa	PS 252	Degussa AG	1.10.2004 – 30.09.2005	Prof. Dr. R. Schlögl		Prof. Dr. R. Schlögl
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	Prof. Dr. S. B. Abd Hamid	Prof. Dr. S. B. Abd Hamid
Integrated Design of Nanostructured Catalytic Materials for a Sustainable Development	IDECAT		European Union	2005 - 2010	Prof. Dr. R. Schlögl		Prof. Dr. G. Centi
Forschungsprogramm Cu-ZnO II			Südchemie	2003 - 2005	Prof. Dr. R. Schlögl	Prof. Dr. M. Muhler	Prof. Dr. M. Muhler
In situ Characterization of Propene Oxidation Catalysts and Catalysis	Sumitomo 	PS 251	Sumitomo Chemical Co., Ltd	1.1.2005 -	Prof. Dr. R. Schlögl Dr. A. Knop-Gericke	Prof. Dr. Hiroshi Yamachika	Prof. Dr. R. Schlögl Prof. Dr. Hiroshi Yamachika
Projekthaus „ENERCHEM“ Energie und Chemie	ENERCHEM		MPG	2005 - 2010	Prof. R. Schlögl Dr. D. S. Su		Prof. Dr. H. Möhwald
Entwicklung von Methanolsynthesekatalysatoren als Basis für nachhaltige Ressourcennutzung – TP3		PSFHI 102 	BMBF	1.7.2005 – 30.6.2008	Prof. R. Schlögl	Südchemie, Ruhr-Uni. Bochum (Prof. M. Muhler) Lurgi AG	Südchemie 

External Funds




Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Brückenschläge zwischen idealen und realen Systemen in der Heterogenen Katalyse Projekt "Säure-Base-katalysierte Alkanaktivierung"	DFG-Schwerpunktprogramm 1091	DFG-SPP 1091 Je 267/1-1 Je 267/1-2 Je 267/1-3	Deutsche Forschungsgemeinschaft	Nov. 2002 - Dez. 2006	Dr. F. C. Jentoft	Prof. Dr. J. Lercher, Prof. Dr. H. Papp, Prof. Dr. J. Sauer, Prof. Dr. W. Widdra	Prof. Dr. R. Imbihl
Identification of local environment of transition metal promoter cations in zirconia-based heterogeneous catalysts.	DFG	436 MOL	Deutsche Forschungsgemeinschaft	17/1/04 - 2005	Dr. F. C. Jentoft	Prof. Dr. S. Klokishner	
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 113788/0-1	Deutsche Forschungsgemeinschaft	2004 - 2006	Dr. F. C. Jentoft	Prof. V. Kazansky	
Brückenschläge zwischen idealen und realen Systemen in der Heterogenen Katalyse Projekt "Vom Einkristall zu realen Katalysatoren am Beispiel der Hydrierung an Silberkatalysatoren"	Schwerpunktprogramm 1091	Je 267/3-1	Deutsche Forschungsgemeinschaft	2004 - 2006	Dr. F. C. Jentoft	Prof. P. Claus	
"Role of redox processes for the catalytic activity of sulfated zirconia materials"	ELCASS	MAPAFHI 00001	MPG	2004 - 2005	Dr. F. C. Jentoft	Prof. Dr. F. Garin	Dr. D. S. Su
Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Advanced Technology in Catalytic Chemistry and Engineering for Novel Applications	ATHENA	PS 960	University of Glasgow	2003 - 2007	Prof. Dr. R. Schlögl Prof. H.-J. Freund Dr. A. Knop-Gericke		Prof. Dr. D. Jackson
Entwicklung, Charakterisierung und in situ-Katalyseverhalten neuartiger, nanostrukturierter Übergangsmetalloxid-Modell-Katalysatoren für Partialoxidationen	DFG-Schwerpunktprogramm 1091	HE 4515/1-1 HE 4515/1-2	Deutsche Forschungsgemeinschaft	21.10.2004 – 20.10.2006 2006-2008	Dr. C. Hess		



External Funds

Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Struktur, Dynamik und Reaktivität von Übergangsmetalloxid- Aggregaten	Sfb	Sfb 546	Sonder-Forschungs-bereich	2000 - 2005	Dr. D.S. Su	Prof. Dr. R. Schlögl	Prof. Dr. J. Sauer
Carbon Nanotubes for Applications in Electronics, Catalysis, Composites and Nano-Biology	CANAPE	PS 809	European Union	2.6.2004 – 1.6.2008	Dr. D. S. Su		Prof. Dr. J. Robertson
Electrocatalytic Gas-Phase Conversion of CO ₂ in Confined Catalysts	ELCAT 	PS 807	European Union	1.9.2004 – 31.8.2011	Dr. D. S. Su		Prof. Dr. G. Centi
Nanocarbon – Nanocarbon related materials in heterogeneous catalysis	ELCASS	MAPAFHI 00001	MPG	2004 - 2005	Dr. D. S. Su	Prof. G. Centi Prof. M. J. Ledoux Dr. C. Pham-Huu	Dr. D. S. Su
Electron microscopy study of one-dimensional II-VI semiconductor nanostructures grown by molecular-beam epitaxy	DAAD	PS 963	Deutscher Akademischer Austauschdienst DAAD	2004 - 2005	Dr. D. S. Su	 Deutscher Akademischer Austausch Dienst German Academic Exchange Service	DAAD
Cooperation Bao Partnergruppe in Dalian	Bao	MCHAFHI 00001	MPG	1.10.2000 – 30.9.2005	Dr. D. S. Su		Prof. Dr. Xinhua Bao
Cooperation Zagreb “TEM and Raman spectroscopy of nanostructured transition metal oxides”	Zagreb	K 500Z	MPG	2004 - 2006	Dr. D. S. Su		Dr. D. S. Su
Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Katalytisches System zur filterlosen kontinuierlichen Russpartikelverminderung bei Fahrzeugdieselmotoren	MAN 	Kst. 931	Bayerische Stiftung	2001 - 2004	Prof. Dr. R. Schlögl Dr. T. Ressler	Prof. Dr. Niessen	TU München
Brückenschläge zwischen idealen und realen Systemen in der Heterogenen Katalyse Projekt "Charakterisierung und Modifikation der aktiven Zentren für die heterogen katalysierte Partialoxidation von Methanol über Kupfer“	DFG-Schwerpunktprogramm 1091	SCHL 332/4-3	Deutsche Forschungsgemeinschaft 	2004	Dr. T. Ressler	Prof. Dr. R. Schlögl, Prof. Dr. A. Groß, Prof. Dr. R. Behm Dr. G. Dehm,	Prof. Dr. R. Imbihl
Nanochemie für zukünftige Automobiltechnik	Zeit-Stiftung 	PS 995	Zeit-Stiftung	2000 - 2003	Dr. T. Ressler		Dr. O. Gnad

External Funds

Project Name	Akronym	Referenz No.	Funds` Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Aufklärung des Mechanismus der BMA-Reaktion	Degussa-Hüls		Degussa-Hüls AG	01.09.1999 – 28.02.2001	Prof. Dr. R. Schlögl Dr. G. Mestl		Prof. Dr. R. Schlögl
1. Zusammenarbeit über Oxidhydrierung von Alkoholen 2. MSA-Katalysatoren in der n-Butan-Oxidation 3. n-Butan-Oxidation an VPO	BASF	Kst. 950	BASF 	01.02.1996 – 31.12.2001	Prof. Dr. R. Schlögl		Prof. Dr. R. Schlögl
Entwicklung von generischen Technologien zur kombinatorischen Katalyseforschung für anspruchsvolle katalytische Reaktionen		Kst. 916 	BMBF	2000 - 2003	Dr. F. C. Jentoft	Prof. J. A. Lercher	Prof. Dr. F. Schüth

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.

TU Berlin, Institute of chemistry, Department of anorganic and analytical Chemistry (SS and WS)

Instructors: T. Ressler

Lectures for Chemistry major course Dipl. Chem

„Kinetics of solids reactions- principles and experiments“

"Phase transitions and the influence on material properties"

„Introduction into x-ray structure analysis“

Seminars

„introduction into general and anorganic chemistry“ for students of chemistry as minor subject

"Anorganic Chemistry I", elementary course Dipl. Chem.

Humboldt Universität in Berlin, Institute of chemistry, Department of Anorganic Chemistry

Instructors: A. Trunschke

"Reaction Mechanisms in Heterogeneous Catalysis"

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 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.

Occupation practical course

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.

LetteVerein

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**.



Pupil practical course

Hallo,

*ich heiße **Nina K.** (16) und gehe auf das Paul- Natorp Gymnasium in Schöneberg. Dort besuche ich die 10. Klasse.*

In meiner näheren Umgebung befindet sich ein Institut der Max-Planck-Gesellschaft, dieses beschäftigt sich mit der Bildungsforschung.

Da ich mich aber für die Naturwissenschaften sehr interessiere, bewarb ich mich am Fritz- Haber- Institut für ein Schülerpraktikum. Man beschäftigt sich dort mit Katalysatoren und ihren Eigenschaften. Es gibt 5 verschiedene Abteilungen am FHI. Ich entschied mich für die Abteilung Anorganischen Chemie. Das Praktikum versprach, sehr vielseitig zu werden. Wie sich herausstellte, war ich fast jeden Tag mit einem neuen Thema beschäftigt. Ob es die Elektronenmikroskopie, XPS oder die Kalometrie war. In all diesen Bereichen und in noch viel mehr spielen Chemie und Physik eine große Rolle. Man war immer darauf bedacht, mir alles so gut wie es ging verständlich zu erklären. Ich denke, das dieses Praktikum mir einen sehr guten Einblick in das Arbeitsleben gegeben hat. So weiß ich vielleicht ein wenig mehr darüber in welchen Berufszweig ich einmal einsteigen möchte.



Lange Nacht der Wissenschaften

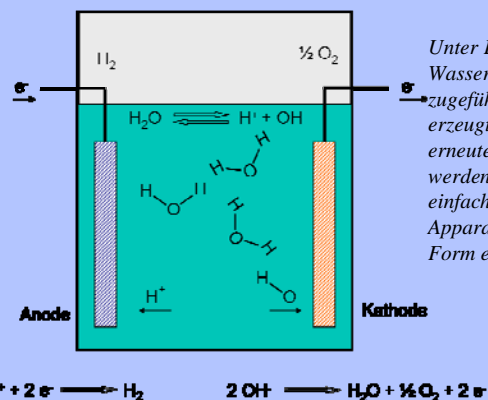


Wasserstofftechnologie

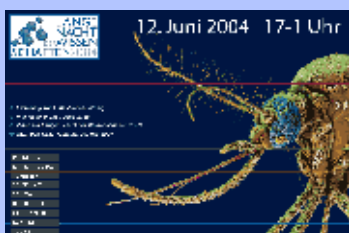
Anhaltende Diskussionen um die Gestaltung der zukünftigen Energieversorgung haben auch das allgemeine öffentliche Interesse erreicht. Innovative Ansätze umfassen dabei die unter dem Begriff *Wasserstofftechnologie* zusammengefassten Prozesse, dabei kommt der Brennstoffzellentechnologie eine zentrale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

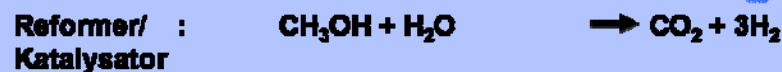


Unter Energiezufuhr kann Wasser in seine Bestandteile Wasserstoff und Sauerstoff gespalten werden. Die zugeführte Energie ist dann quasi in der Form des erzeugten Wasserstoffes gespeichert und kann bei erneuter Bildung von Wasser wieder freigesetzt werden. Die Spaltung des Wassers lässt sich am einfachsten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



Where does hydrogen come from ?

DMFC
Direct Methanol
Fuel Cell



Long Night of Science



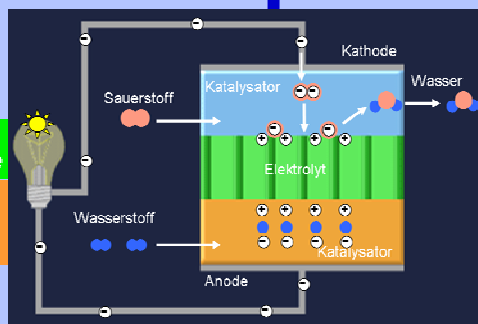
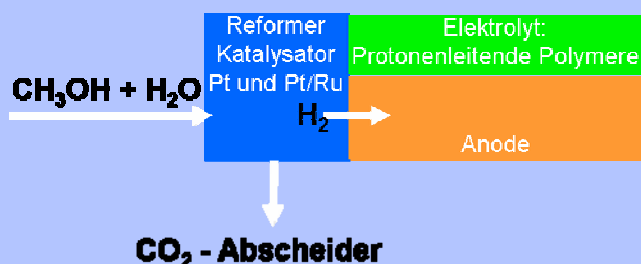
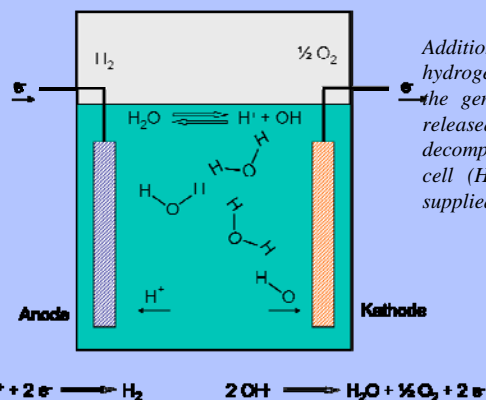
Hydrogen Technology

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>)

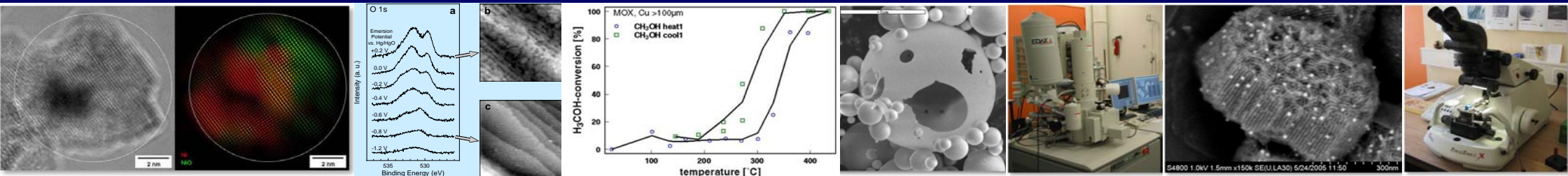


Function principle of a fuel cell

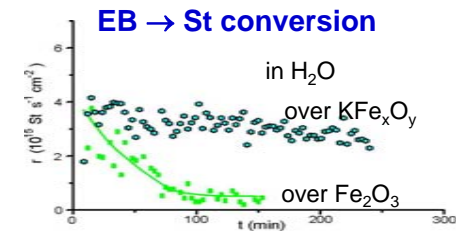
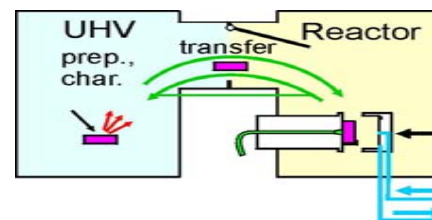
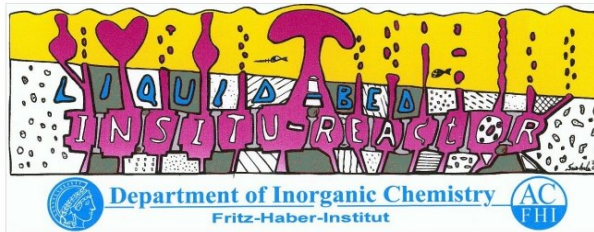
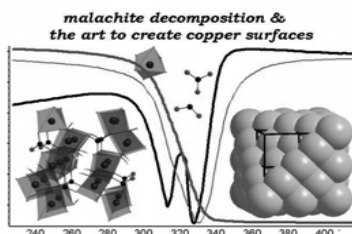
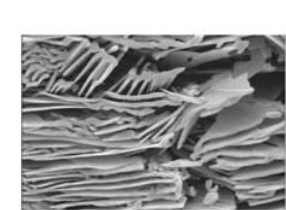


Notes





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



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