



DEPARTMENT OF



MAX-PLANCK-GESELLSCHAFT

INORGANIC CHEMISTRY



FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT

January 2009 / 4th Edition

Zr

H-C≡O-I

Prof. Jentoft accepted the offer of an associate professorship at the Univ. of Oklahoma

Mo

A+B → AB

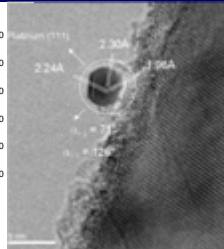
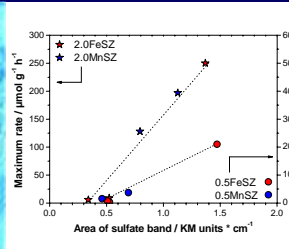
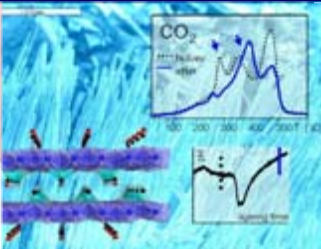
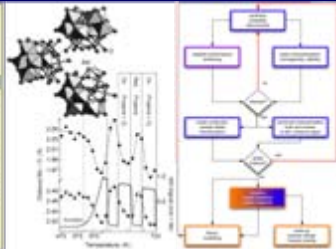
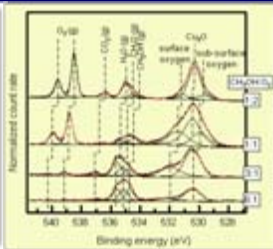
5 nm

C

CH₄ + O₂ → CH₂ → C₂H₂ → C₂H₄ → C₂H₆

CH₄ + O₂ → H₂O + CO₂ + CO + H₂

Platinum



The methane oxidation on Pt has been investigated on α -Al₂O₃ foam catalysts coated with Pt nanoparticles (reticulated pore structure, $d_{pore} = 300-500\mu m$)



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

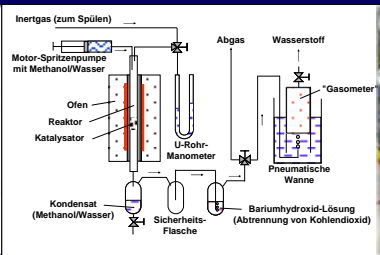
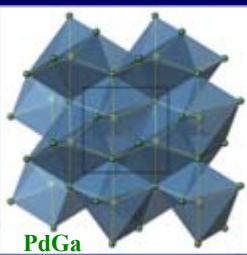
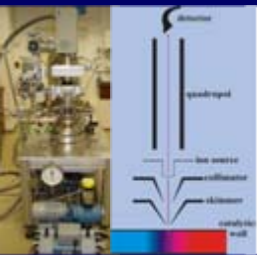
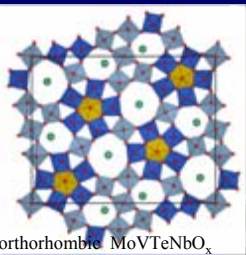
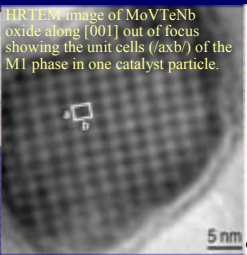



Table of Contents



- | | | | |
|----------|--|----------|---|
| A | History of the Fritz-Haber-Institut | I | FHI Library / Publications |
| B | How to reach the Institute | J | Patents |
| C | Preface | K | Guest-Lecturers |
| D | Internal Structure | L | External Funds |
| E | Miscellaneous | | - List of external funds |
| F | Instrumentation | | - Cluster of Excellence: “Unifying Concepts in Catalysis” |
| G | Understanding Catalysis | | - European Union: Network of Excellence / NoE |
| H | Scientific Progress | | - EnerChem: Nanochemical Concepts for a Sustainable Energy Supply |
| | - Molybdenum-Vanadium compounds in C3 and C4 selective oxidation | | - Collaborative Research Centers: SFBs, SFB 546, B2 |
| | - Copper and palladium catalysts in C1 chemistry | | - Palladium intermetallic compounds |
| | - Silver in partial oxidation reactions | M | Teaching Activities |
| | - Oxygenated ruthenium in CO-oxidation | N | Long Night of Science |
| | - Carbon in catalysis | O | Practical Courses |
| | - High temperature catalysis research | P | Notes |

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).

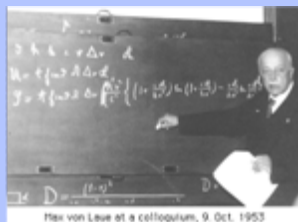
What is now called the Fritz-Haber-Institut of the Max-Planck-Gesellschaft was founded in 1911 as the Kaiser-Wilhelm-Institut for Physical Chemistry and Electrochemistry, together with the Kaiser-Wilhelm-Institut for Chemistry. These were in fact the first two institutes of the Kaiser-Wilhelm Society (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 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
- 2008 **Martin Wolf**, appointed director of Dept. of Physical Chemistry

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

Faradayweg 4 – 6

14195 Berlin

Germany



Preface

Director:

Prof. Dr. Robert Schlögl

Tel: 49 30 8413 4400

Fax: 49 30 8413 4401

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



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

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 been 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

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.

RS

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 and PL and main methodical activities.



REACTIVITY

GL: Dr. A. Trunschke

Tel: 49 30 8413 4457
E-mail: trunschke@fhi-berlin.mpg.de

Mo-V compounds in C3 and C4 oxidation

16 members

Synthesis, vibrational and UV-vis spectroscopy, reactor technology and catalytic testing

NANOSTRUCTURES

GL: Dr. M. Behrens

Tel: 49 30 8413 4408
E-mail: behrens@fhi-berlin.mpg.de

Cu, Pd in C1 chemistry

12 members

Synthesis, Elemental analysis, X-Ray and neutron diffraction, TG, DSC, EXAFS



ELECTRONIC STRUCTURE and ADSORPTION

GL: Dr. A. Knop-Gericke

Tel: 49 30 8413 4422
E-mail: knop@fhi-berlin.mpg.de

Metals in sel oxidation

Emmy Noether / PL: Dr. R. Horn

20 members

Photoelectron spectroscopy, TP desorption, TP reaction, Raman, Calorimetry, BET, MBMS, Laser spectroscopy, BESSY II

MICRO- AND NANOSTRUCTURE

GL: Dr. D. S. Su

Tel: 49 30 8413 5406
E-mail: dangsheng@fhi-berlin.mpg.de

Nanocarbon in energy chemistry

C-OH chemistry / PL: J. P. Tessonnier

TEM service group: Dr. D. S. Su

20 members

TEM, SEM, ELNES, RFA, Nanoreaction



Miscellaneous

Emmy-Noether-Group "High Temperature Catalysis"
Dr. Raimund Horn; horn_r@fhi-berlin.mpg.de



Beginning July 1st 2008, Dr. Raimund Horn has been awarded the funding of a Junior Research Group within the Emmy Noether Program of the German Research Foundation (DFG). Funding is granted for five years, provided that the project is evaluated positively at the end of the third year. The research in the High Temperature Catalysis Group aims at a mechanistic understanding of chemical and physical surface gas interactions in catalytic alkane oxidations on various catalysts (metals, oxides) under high temperature (up to 1300 °C) and high pressure (up to 5 MPa) conditions.



Prof. Dr. Christian Hess accepted the offer of a full professorship at the Technische Universität Darmstadt, Germany from March. 1, 2008.

New affiliation:

Eduard-Zintl-Institut für Anorganische u. Physikalische Chemie; Technische Universität Darmstadt
Petersenstr. 20, 64287 Darmstadt, Germany

Tel.: +49 (0)6151 164925/164945

Fax: +49 (0)6151 164995

Email: hess@pc.chemie.tu-darmstadt.de

www1.tu-darmstadt.de/fb/ch/Fachgebiete/PC/AKHess



Prof. Dr. Friederike C. Jentoft accepted the offer of an associate professorship at the University of Oklahoma, USA from Oct. 1, 2008.

New affiliation:

Associate Professor of Chemical Engineering; School of Chemical, Biological & Materials Engineering
University of Oklahoma

100 East Boyd Street, Sarkeys Energy Center
Norman, OK 73019-1004, USA

Phone: (405) 325-0465, Fax: -5813

Email: fcjentoft@ou.edu

www.cbme.ou.edu

Group leader: GL Project leader: PL

Instrumentation

REACTIVITY

Dr. A. Trunschke



Contact:
Dr. A. Trunschke
trunschke@fhi-berlin.mpg.de

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 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 **automated laboratory reactor systems for precipitation and hydrothermal synthesis** equipped with probes for measuring pH, conductivity, turbidity, viscosity, pressure, temperature, and UV-vis spectra. The thermal treatments are performed in rotating furnaces under controlled atmosphere.

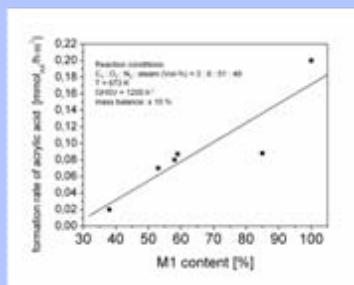
Molecular spectroscopy is used to understand catalyst synthesis. The nature and number of the active sites on the catalyst surface and the reaction mechanism are addressed by adsorption of reactants and probe molecules in static or flow operation at 77-873K, in-situ spectroscopic experiments, and **microreactor** studies.

Examples of the technical equipment:

- Automated laboratory reactor system (Mettler-Toledo Labmax®), analytic autoclave HPM-PT-040 (Premex), parallel microwave reactors Speedwave MWS-3 (Berghof)
- Lambda 650 UV-vis spectrometer (Perkin Elmer) with Harrick DR accessory
- IFS 66 FTIR (Bruker) and Spectrum 100 FTIR (Perkin Elmer) for in-situ measurements in transmission, diffuse reflectance and ATR
- Single-tube and parallel (ILS) fixed-bed reactors for gas phase oxidation equipped with GC-MS, GC (Agilent), and MS OmniStar™ (Pfeiffer)



Analytic autoclave HPM-PT-040
(Premex Reactor GmbH)



Oxidation of propane to acrylic acid over crystalline MoVTeNb oxides composed of different fractions of the phase „M1“

ELECTRONIC STRUCTURE AND ADSORPTION

Dr. A. Knop-Gericke



Contact:
Dr. A. Knop-Gericke,
knop@fhi-berlin.mpg.de

ISS: Soft X-ray station at BESSY :

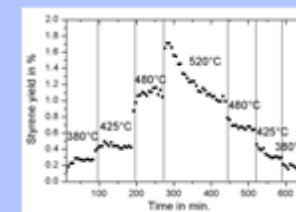


In situ XPS endstation of the ISS beamline

BESSY and the FHI installed the facility ISS (Innovative Station for In Situ Spectroscopy). ISS 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. This facility allows measurements of XP and XA spectra in the soft energy range under reaction conditions (mbar pressure range, T < 600°C.) One aim of these investigation is the identification of correlation between the electronic surface structure of a working catalyst and its catalytic performance. Subsurface species were observed under reaction conditions by the help of photon energy variation (depth profile).

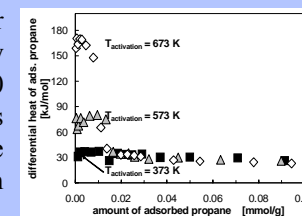
Combined TDS, XPS and reactivity studies of low surface area (model) catalysts

Combining thermal desorption (TDS) with the surface and element sensitive method XPS and a micro flow reactor yield a powerful investigation toolset of low surface area (model) catalysts. The figure shows the yield of styrene in the oxidative dehydrogenation (ODH) of ethylbenzene over ~0.03mg carbon nanotube on highly oriented pyrolytic graphite, HOPG.



Measurement of isotherms & differential heats of adsorption by microcalorimetry

Catalytically active sites can be identified by their interaction with the reactant or a chemically closely related molecule. SETARAM MS80 and HT1000 Calvet-type microcalorimeters with all-metal cells connected to vacuum and gas-dosing systems (figure shows differential heats of propane adsorption on differently dehydrated 10wt% V_xO_y/SBA15 at 313 K)



Instrumentation

NANOSTRUCTURES

Dr. M. Behrens



Contact:
Dr. M. Behrens
behrens@fhi-berlin.mpg.de

Scaleable and reproducible preparation under controlled conditions is a prerequisite for knowledge-based catalyst design. Precursor phases, intermediates during the preparation process and the final catalyst have to be submitted to comprehensive characterization using various analytical tools. The facilities in the group include:

- **Automated laboratory reactor system** (Mettler-Toledo Labmax, photo) for controlled precipitation. Chemistry in solution and suspension can be monitored in-situ using probes for pH, conductivity, turbidity and UV-vis spectroscopy
- Lab scale (Mini Büchi B-191) and pilot plant scale (Niro Minor Mobile, photo) **spray dryer** for drying and solidification.
- **Particle size distributions** and **zeta potentials** of suspensions are determined using a Malvern Zetasizer Nano.



- **Gloveboxes** for handling of samples in inert atmosphere
- **Thermal analysis** in a thermobalance (Netzsch STA 449C Jupiter) with coupled mass spectrometry (Pfeiffer Omnistar) or with high pressure differential scanning calorimetry (HP DSC 827e, Mettler-Toledo)
- **Temperature programmed desorption or reaction** in various gas atmospheres (TPDRO 1100, CE instruments) with thermal conductivity detector or coupled mass spectrometry (Pfeiffer Omnistar)

- **X-ray diffraction (XRD)** in transmission (STOE Stadi-P with autosampler) or reflection geometry (Bruker D8 Advance, photo)
- **In-situ X-ray diffraction** on a STOE theta-theta diffractometer equipped with a high temperature reactor chamber (Anton Paar XRK 900) with coupled mass spectrometry (Pfeiffer Omnistar)



MICROSTRUCTURE

Dr. D. S. Su



Contact:
Dr. D. S. Su,
dangsheng@fhi-berlin.mpg.de

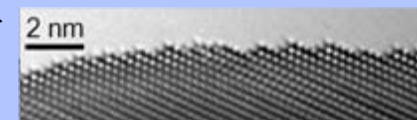
For microstructural investigations, 5 electron microscopes are available.

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-Ångström 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.

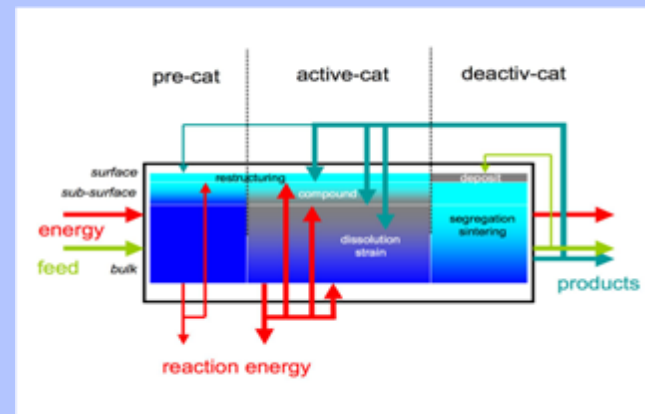
A **concept** of heterogeneous catalysts is developed linking the surface chemistry of the substrate (the desired process) with the material chemistry of the catalyst (an „invisible“ process).

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 target of the Department that will be pursued in four of the research areas and one of the associated group:

Reactivity / Oxides: *“Mo-V compounds for C3,C4 oxidation”*

Nanostructures / Bulk structure : *“Cu, Pd in C1”*

Electronic Structure and Adsorption / Metals: *“Metals in sel oxidation”*

Micro-and Nanostructure / Carbon: *“Nanocarbon in energy chemistry”*

Emmy-Noether-Group: *“High Temperature Catalysis”*

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.

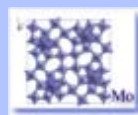
Research concept



- We study non-equilibrium systems: kinetics is all-important:
 - optimize synthesis
 - document quantitatively the synthesis (in-situ observations)
 - thorough multi-method characterization including reactivity (probe molecule adsorption, thermal methods).
- We are interested in generic effects: always reproduction of every single experiment.
- We need quantitative results:
 - multiple steady state kinetics
 - pressure gaps, wide variations of process conditions
 - quantification of structural data.
- We want high-quality representation of results in graphics and images.

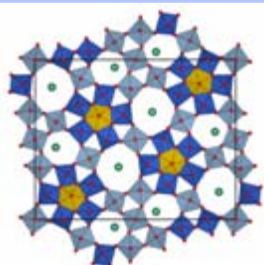
Scientific Progress

Molybdenum-Vanadium compounds in C3 and C4 selective oxidation

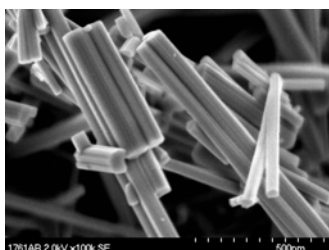


Background and objective

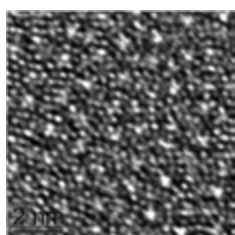
Selective oxidation of light alkanes with molecular oxygen to aldehydes or acids provides alternative access to chemical intermediates by utilization of natural gas or renewable feedstock as a replacement for olefin-based petrochemistry. However, the catalytic activation of C-H bonds in alkanes requires 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.



1 Structural model of an orthorhombic MoVTeNbO_x phase



2 SEM image of phase-pure M1

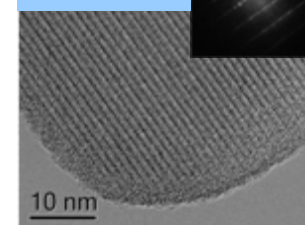


3 HRTEM image of M1 viewed along the <001> zone axis

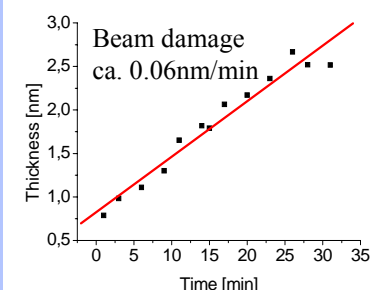
Results

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 photoelectron 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.

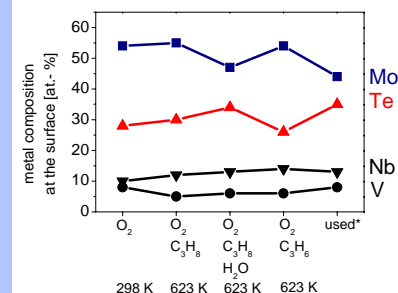
Zone axis
~<012>



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

Contact:

Dr. Annette Trunschke
trunschke@fhi-berlin.mpg.de

External collaborations:

University Malaya, Kuala Lumpur, Malaysia (Ass. Prof. Dr. Sharifah Bee Abd Hamid)
TU Berlin (Prof. Dr. R. Schomäcker), TU München (Prof. Dr. J.A. Lercher)

Financial support:
Südchemie AG

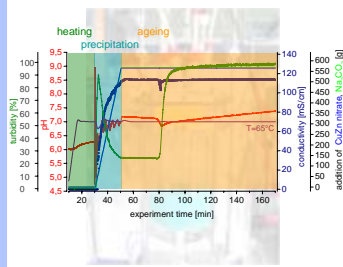
Scientific Progress

Copper and palladium catalysts in CI chemistry

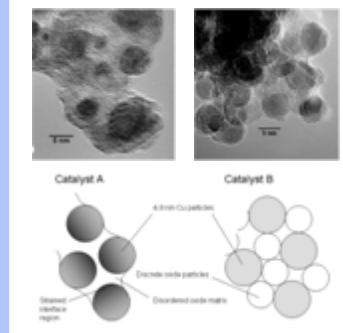


1 Methanol steam reforming
 $\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + 3\text{H}_2$
Methanol synthesis
 $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$

2 Precursor preparation



3 Cu/ZnO/Al₂O₃ microstructure



Introduction

Methanol is one of the most important basic chemicals. In the future, it might also serve as a chemical hydrogen carrier for mobile applications of fuel cells via the methanol synthesis and steam reforming reaction network (1). Nanostructured copper zinc oxide catalysts are employed in industrial methanol synthesis and are also active in methanol steam reforming as are palladium-based intermetallic compounds. The increasing worldwide demand for methanol requires further optimization of the industrially applied Cu/ZnO system. The challenge in preparation of palladium intermetallic compound catalysts lies in the generation and stabilization of high metallic surface areas in a homogeneous microstructure.

Our approach to these systems is to characterize the nanostructured ensemble present in highly active “real” catalysts in order to identify relevant features for catalytic performance. Simultaneously, catalyst synthesis is investigated in detail to understand the relations of precursor properties and catalytic activity of the final product. The preparative strategy of the group aims at rationalization of this so-called “chemical memory” by optimization of well-established synthetic routes as well as development of novel preparation methods (2).

External collaborations (Cu):

Technical University Berlin (T. Ressler, R. Schomäcker)
Ruhr-University Bochum (M. Muhler)
University Malaya, Kuala Lumpur (Sharifah Bee Abd Hamid)
Süd-Chemie AG, Bruckmühl

Results

Cu/ZnO/Al₂O₃ catalysts of industrially relevant composition can be prepared with different microstructure of the oxide phase (3): the typical nanoparticulate arrangement (B) and a continuous amorphous oxide matrix with partially embedded Cu nanoparticles (A). Interestingly, the methanol synthesis activity of sample A was higher despite a 30% lower accessible Cu surface area (4). This result suggests enhancement of the beneficial metal/oxide interface interaction by partial embedding of Cu particles.

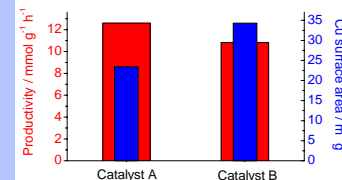
Very small embedded Cu particles can also be prepared via hydrotalcite-like CuZnAl precursors. Here, the specific surface area of precursor and oxide intermediate is generally lower compared to the technically applied synthesis via malachite-like precursors. Using a microemulsion technique, the BET surface area can be increased almost by a factor of two compared to a co-precipitated sample (5).

Co-precipitation methods are explored as routes to Pd-based intermetallic catalysts for methanol steam reforming, which are active and selective also in hydrogenation reactions (section: L, Pd intermetallic compounds). As preliminary results e.g. nanostructured Pd-Ga-Mg precursor phases were obtained, which after decomposition yield nanostructured oxides (6). After reduction intermetallic Pd-Ga phases may be obtained at the oxide interfaces.

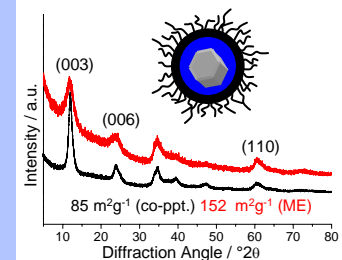
External collaborations (Pd):

MPI for Chemical Physics of Solids (Y. Grin, M. Armbrüster)
University of Innsbruck (B. Klötzer, S. Penner)
Technical University Vienna (G. Rupprechter)

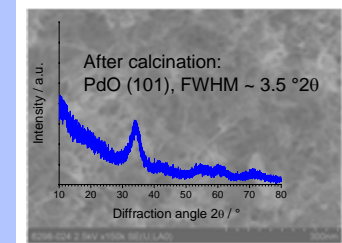
4 Catalytic activity



5 Microemulsion precursors



6 Pd-Ga-Mg precursors

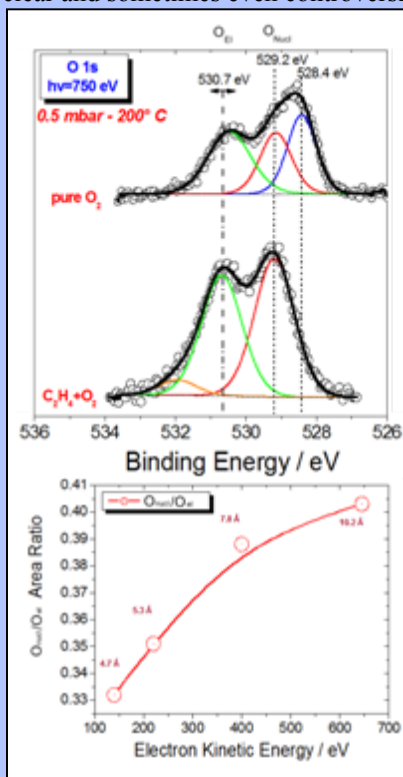


Contact:
Dr. Malte Behrens
behrens@fhi-berlin.mpg.de

Scientific Progress

Silver in partial oxidation reactions

The remarkable catalytic activity of silver in partial oxidation reactions is known for decades. Particularly, the ethylene epoxidation and formaldehyde synthesis reactions are two industrially important reactions which received most attention. However, apart from the great effort done in the past years, there are still open questions about the mechanistic details of these reactions. It is well known that silver can accommodate many oxygen species depending on the temperature, partial pressure of gas feed, the structure and morphology of the silver catalyst, nevertheless, the role of these different species as active sites or spectators in the catalytical reactions is not clear and sometimes even controversial in the literature.



In order to shed some light on these questions, we have investigated the methanol oxidation to formaldehyde and ethylene epoxidation reactions under realistic temperatures (180 – 650°C) in the mbar range (0,1 - 1 mbar) by in situ XPS combined with time-resolved online MS. Different catalyst materials have been used, silver foils, powders with few to hundreds microns in grain sizes and supported nanometer sized catalysts.

The upper panel in the figure shows oxygen 1s spectra from silver powder during ethylene epoxidation at 0.5 mbar and 200°C. From the three oxygen species presented under O2 atmosphere, only two survive under steady state reaction conditions, the so called, electrophilic (Oel) and nucleophilic (Onucl) oxygen species. The ratio between these two species (Oel/Onucl) measured at different particle sizes was found to correlate with the catalytic activity. Moreover, XPS measurements with different excitation energies revealed that the Oel is more surface localized than the Onucl (lower panel).

Contact:

Dr. Axel Knop-Gericke
knop@fhi-berlin.mpg.de

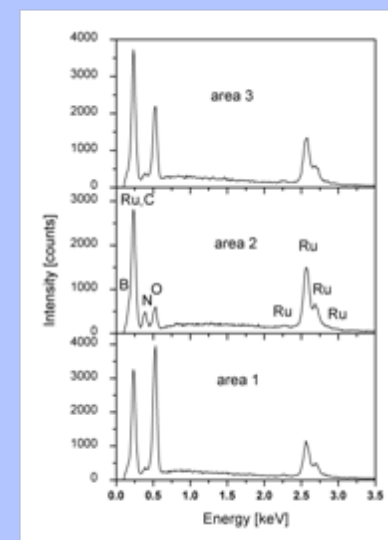
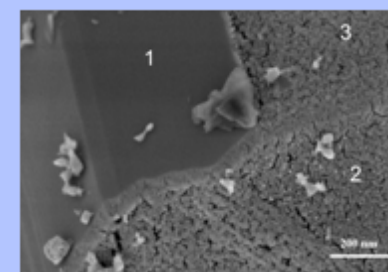
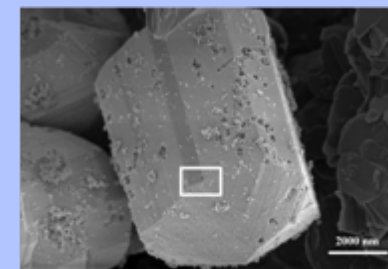


Scientific Progress

Oxygenated Ruthenium in CO-oxidation

Ruthenium was believed to be an outstanding example for the pressure gap; very high activity under ambient pressure faced low activity in UHV. Two different phenomena were identified as reasons for this pressure gap by different research groups in the literature: the kinetically inhibited growth of RuO₂, namely the (110) surface and the also inhibited growth of a complete (1x1) oxygen monolayer.

To shed some light on this highly controversial discussion we started our experiments with fully oxidized RuO₂ powder. This powder is completely inactive in the CO-oxidation. Only long treatment in reducing atmosphere (CO:O₂=14:1) activates the catalyst. In-situ XRD reveals the bulk state of the catalyst still as RuO₂. High resolution SEM micrographs with high surface sensitivity (low accelerating voltage) are shown in figure 1, figure 2 is a magnification of the marked area in fig.1: All apical facets (numbered 2) and only one lateral facet (3) are roughened, while most of the lateral facets remain smooth. Furthermore EDX (figure 3) shows a lower oxidation degree from the apical facets over the roughened lateral facet to the smooth facets. From this we conclude that the reaction starts selectively at the apical facets and the first activation step is reduction. Since reduction to Ru metal with the still fully oxidized bulk is rather unlikely we believe that the activity owes to the existence of subsurface oxygen species.



Contact:

Dr. D. Rosenthal, Dr. F. Girgsdies, Dr. R. Blume
dirkrose@fhi-berlin.mpg.de, girgsdie@fhi-berlin.mpg.de, raoul@fhi-berlin.mpg.de

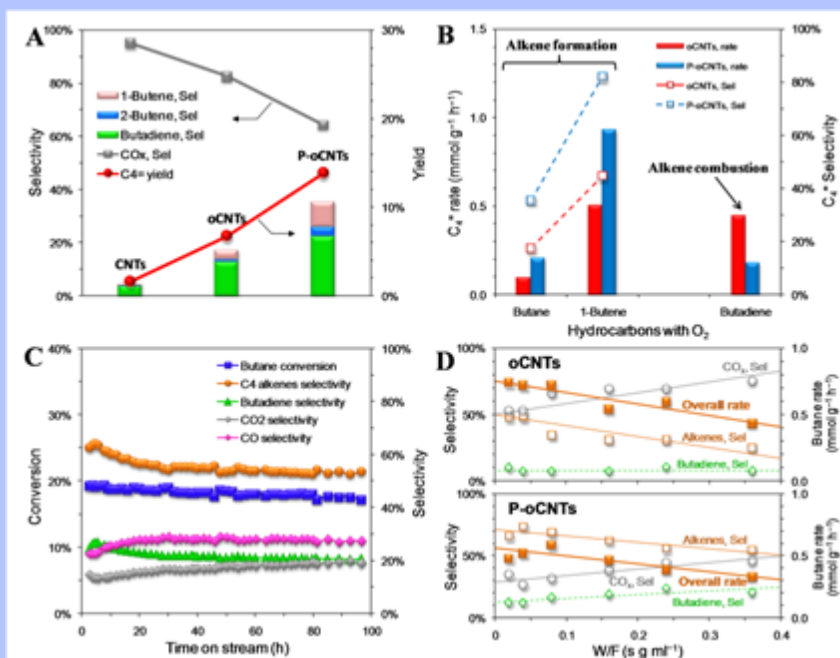
Scientific Progress

Carbon in catalysis



Surface-Modified Carbon Nanotubes for Oxidative Dehydrogenation of *n*-Butane:

We show that carbon nanotubes with modified surface functionality efficiently catalyze the oxidative dehydrogenation of *n*-butane to butenes, especially butadiene. This process is mildly catalyzed by ketonic C=O groups and occurs via a combination of parallel and sequential oxidation steps. A small amount of phosphorus greatly improved the selectivity by suppressing the combustion of hydrocarbons. (Science Vol. 322, 73-77 (2008))



(A) ODH activities of various CNTs.

(B) Performance of modified CNTs in ODH of butane and 1-butene and in combustion of butadiene.

(C) Stability of P-oCNTs in ODH.

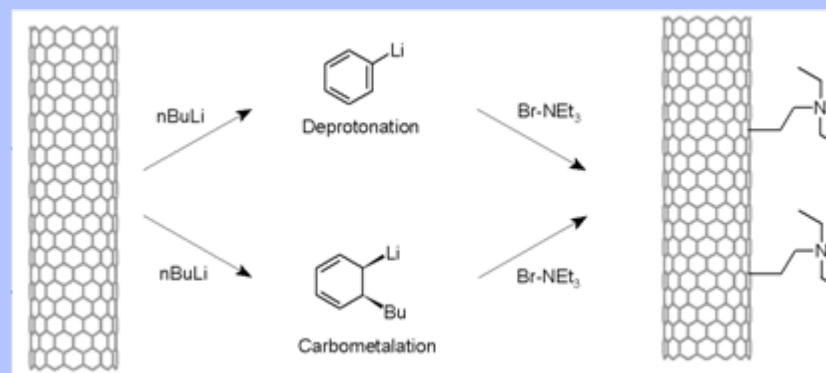
(D) Dependence of product selectivity and reaction rate on residence time.

Fe-Co Alloy Nanoparticles on Carbon Nanotubes for Ammonia Decomposition:

Fe-Co alloy nanoparticles were synthesized inside the tubular channel of CNTs. The prepared system shows an unusual synergism in alloy catalysis. The alloy nanoparticles with widely varying Co/Fe ratio are kept as active as Co for the H₂ production from NH₃ decomposition. The stability of Co was significantly improved by alloying with Fe. (Nano Letters, Vol. 8, 2738-2743 (2008))

Covalent Functionalization of Carbon Nanotubes with Amines and the Application as Basic Heterogeneous Catalyst for Biomass Conversions:

Amino groups have been grafted on CNTs by a simple, one-pot, deprotonation/carbometalation reaction followed by an electrophilic substitution. This produces very homogeneous samples with a high number of easily accessible basic groups. The concentration of the basic groups is closed to the concentration of Brønsted acid sites in zeolites, without any optimization of the grafting procedure. The obtained samples are active for a typical biomass conversion to biodiesel.



Functionalization of CNTs by deprotonation/carbometalation followed by the electrophilic attack of the bromo-triethylamine.

Contact:

Dr. Dangsheng Su

dangsheng@fhi-berlin.mpg.de

External collaborations:

European Laboratory for Catalysis and Surface Science (ELCASS)

further collaborations under L „External Funds“

Financial support:

European Union

Deutsche Forschungsgemeinschaft

Scientific Progress

High temperature catalysis research

The one step transformation of natural gas components like methane and ethane into valuable chemicals like methanol, formaldehyde, ethylene or synthesis gas (Fig. 1), is a formidable challenge for catalysis research and chemical engineering in the 21st century. Heterogeneous catalytic alkane oxidations at high temperatures and pressures might be a way to accomplish these transformations provided that it is possible to optimize the interaction between reactions at the catalyst surface and in the surrounding gas phase and to maximize the kinetically controlled formation of partial oxidation products.

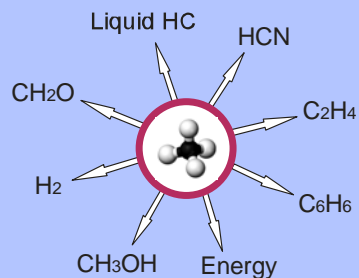


Fig. 1

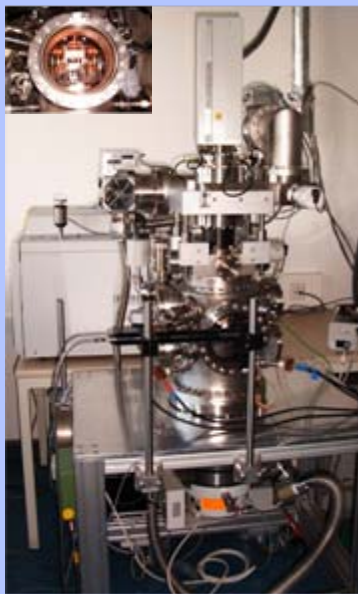


Fig. 2

The research in our high temperature catalysis project aims at a mechanistic understanding of chemical and physical surface gas interactions in catalytic alkane oxidations on various catalysts (metals, oxides) under high temperature (up to 1300 °C) and high pressure (up to 5 MPa) conditions. Novel in-situ diagnostic techniques like Spatial Profile Measurements, Raman Spectroscopy, Cavity Ringdown Spectroscopy and Molecular Beam Mass Spectrometry (MBMS, Fig.2) are developed and applied in the project to provide insight into surface and gas phase chemistry under high temperature, high pressure reaction conditions. In the future, experimental results will be compared to microkinetic numerical simulations coupling detailed surface and gas phase reaction models with physical transport mechanisms of mass, heat and momentum.

Contact:

Dr. Raimund Horn

horn_r@fhi-berlin.mpg.de

External collaborations:

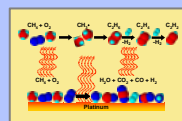
Cluster of Excellence „Unifying Concepts in Catalysis – UniCat“

Prof. Lanny D. Schmidt, Department of Chemical Engineering and Materials Science, University of Minnesota, USA

Financial support:

BMBF

German Research Foundation



Results: The methane oxidation on Pt has been investigated both, on α -Al₂O₃ foam catalysts coated with Pt nanoparticles (reticulated pore structure, $d_{\text{pore}} \approx 300$ -500 μm , Fig. 3) and polycrystalline Pt tubes with 4.4mm inner diameter (Fig. 4).

Reactor measurements on the foam catalysts with a geometric surface to volume ratio of about 160cm⁻¹ show H₂, CO, H₂O and CO₂ as reaction products. Spatially resolved species and temperature profiles (Fig. 5) reveal that these products are formed at the Pt surface by partial and total oxidation of methane followed by steam reforming. CO₂ reforming is not observed.

Methane oxidation in a Pt tube with only $\sim 7\text{cm}^{-1}$ surface to volume ratio leads at temperatures below 1100°C also to H₂, CO, H₂O and CO₂. However, above 1100°C surface temperature, a sudden formation of C2 products (C₂H₆, C₂H₄, C₂H₂) is observed (Fig. 6). Quantitative measurements of gas phase CH₃· radicals reveal the onset of gas phase chemistry at this point. C2 products are obviously formed by coupling of CH₃· radicals in the gas phase and subsequent dehydrogenation. H₂, CO, H₂O and CO₂ are formed by surface oxidation reactions supplying heat to drive the gas phase chemistry.

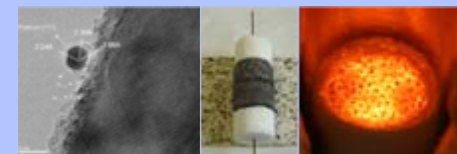


Fig. 3



Fig. 4

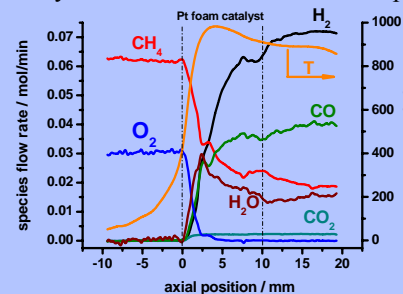


Fig. 5

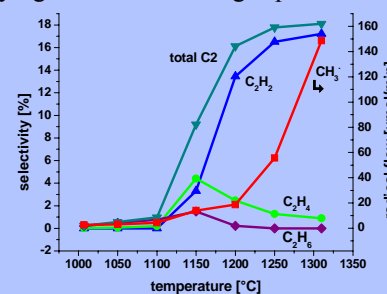


Fig. 6

FHI library / Publications



FHI Library

collects special literature covering the research fields of the institute. The library has about 15.500 monographs and 28.600 journal volumes. In addition, the library offers about 20.000 currently subscribed electronic journals, most of them based on central MPG agreements. The range of electronic services of the FHI Library includes various databases, access terms and conditions for e-journals as well as catalogues. Therefore, the qualified library personnel will remain indispensable also in the new age of electronic „libraries without walls“. The acceptance of electronic media is very high within the FHI due to constant efforts and the regular training of the users.

The traditional services as interlibrary loan service, acquisition of books and other information material, literature searches and reader service are also available. Furthermore, the library participates in the development and maintenance of the Max Planck Virtual Library (VLib).

Max Planck Virtual Library (VLib)



This system is a portal to various information resources available to members and guests of the Max Planck Society. To support that system the library is giving feedback to VLib by intensely testing the user interface and integrating library catalogs that run with the library system Allegro. In addition, the library prepares manuals and offers seminars for colleagues (train the trainer) and for FHI scientists.

Contact:
Uta Siebeky
siebeky@fhi-berlin.mpg.de

Open Access



The library is constantly monitoring the publication market, especially in respect of to new trends, e.g. Open Access. The FHI is practicing open access to scientific results as stated in the „Berlin Declaration on Open Access to the Knowledge in the Sciences and Humanities“ in two ways: Publication in Open Access Journals and institutional self-archiving on the eDoc Server. Currently about 1000 open access documents from FHI scientists are available on the eDoc Server.

eDoc Server



eDoc is the electronic repository of the Max Planck Society and provides the possibility to represent the research output of the Institutes.

The library assists the scientists by offering seminars and regular training courses on how to make best use of the eDoc Server.

The library has been testing the eDoc Server System thoroughly since its implementation. Presently the Max Planck Digital Library (MPDL) is preparing a new publication management system with additional tools. The FHI is one of the pilot institutes in the eSciDoc Project and the library operates for further development in close cooperation with the MPDL.

The following publication list 2006 – Nov. 2008

is generated by eDoc.

<http://edoc.mpg.de>

Publications

2006

Max Planck Society
eDoc Server

eDoc

2006

Bauer, F., H. G. Karge: Characterization of Coke on Zeolites. In: Molecular Sieves – Science and Technology, Volume 5, Chapter 5. Ed. by 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 MoVTaNb mixed oxide catalyst. *Applied Catalysis A: General* **307**, 137-147 (2006).

Bentrup, U., A. Brückner, M. Fait, B. Kubias and J. B. Stelzer: Structure–reactivity relationships in VO_x/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.-G. Willinger, D. S. Su and X. Bao: Facile Autoredox 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).

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., 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 ZrTiO₄ by solid state reaction in equimolar mixture of TiO₂ and ZrO₂. *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. Schafrank, 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).

Publications

2006

Gassenbauer, Y., R. Schafrank, 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. Schafrank, 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), 1263-1263 (2006).

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).

Max Planck Society
eDoc Server



2006

Hoang, D. L., S. Farage, A. Dittmar, A. Trunschke, H. Lieske and A. Martin: Studies on CrO_x/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** (5), 054102-054102-9 (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).

Jentoft, F. C.: UV-vis-NIR Spectroscopy in Catalysis: Theory, Experiment, Analysis and Application under Reactive Conditions. *Advances in Catalysis*, invited article, accepted to editorial office 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).

Publications

2006

Max Planck Society
eDoc Server

eDoc

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).

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 Jahresbericht 2006, 1347-1348 (2006).

Ličina, V., Gajović, A., Muguš-Milanković, I. Djerđj, N. Tomašić and D. S. Su: Correlation between the microstructure and the electrical properties of ZrTiO₄ ceramics.

Journal of American Ceramics Society **89** (7), 2196-2205 (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/VO_x 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-VO_x 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).

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.

In: 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. In: 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, 1-47 (2006).

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 **20**, 7-7 (2006).

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).

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).

Publications

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. Ntaftos 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. Gulians, A. Knoester and H. Brongersma: Surface analysis of the ab-plane of MoVTeNbO_x catalysts for propane (amm) oxidation by low energy ion scattering (LEIS). In: 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. Baldwin: Caterpillar-elicited methanol emission: a new signal in plant-herbivore interactions? *The Plant Journal* **46** (6), 948-960 (2006).

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**, 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).

Max Planck Society
eDoc Server



2006 / 2007

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/TiO₂ 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 CH₃OH 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).

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).

Bauer, F. and H. G. Karge: Characterization of Coke on Zeolites. In: Characterization II. (Eds.) Karge, Helmut G.; Weitkamp, Jens. *Molecular Sieves - Science and Technology* **5**. Springer-Verlag, Berlin (2007) 249-364.

Bluhm, H., M. Hävecker, A. Knop-Gericke, M. Kiskinova, R. Schögl and M. Salmeron: In situ x-ray photoelectron spectroscopy studies of gas-solid interfaces at near-ambient conditions. *Materials Research Society Bulletin* **32**, 12, 1022-1030 (2007).

Publications

2007

Max Planck Society
eDoc Server



2007

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).

Blume, R., M. Hävecker, S. Zafeiratos, D. Teschner, A. Knop-Gericke, R. Schlögl, P. Dudin, A. Barinov and M. Kiskinova: Oxidation of methanol on Ru catalyst: Effect of the reagents partial pressures on the catalyst oxidation state and selectivity.

Catalysis Today **124**, 1-2, 71-79 (2007).

Breitkopf, C., H. Papp, X. Li, R. Olindo, J. A. Lercher, R. Lloyd, S. Wrabetz, F. C. Jentoft, K. Meinel, S. Förster, K.-M. Schindler, H. Neddermeyer, W. Widdra, A. Hofmann and J. Sauer: Activation and Isomerization of n-Butane on Sulfated Zirconia Model Systems - An Integrated Study Across the Materials and Pressure Gaps.

Physical Chemistry Chemical Physics **9**, 3600-3618 (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).

Clavel, G., M.-G. Willinger, D. Zitoun and N. Pinna: Solvent Dependent Shape and Magnetic Properties of Doped ZnO Nanostructures.

Advanced Functional Materials **17**, 16, 3159-3169 (2007).

Delgado, J. J., X. Chen, D. S. Su, S. B. Abd Hamid and R. Schlögl: A Novel Catalyst for Synthesis of Styrene: Carbon Nanofibers Immobilized on Activated Carbon.

Journal of Nanoscience and Nanotechnology **7**, 10, 3495-3501 (2007).

Denkwitz, 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).

Dennstedt, A., N. Frenzel, M. Behrens, A. Trunschke, R. Schlögl, M. Lerch and T. Ressler: Cu on Zirconia and Zirconium Oxynitride as Catalyst for Methanol Steam Reforming. HASYLAB Jahresbericht 2007, Annual Report 1, 513-514 (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).

Ethiraj, A. S., S. Kharrazi, N. Hebalcar, J. Urban, S. R. Sainkar and S. K. Kulkarni: Highly photostable dye entrapped core-shell particles.

Materials Letters **61**, 25, 4738-4742 (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).

Gabasch, H., K. Hayek, B. Klötzer, W. Unterberger, E. Kleimenov, D. Teschner, S. Zafeiratos, M. Hävecker, A. Knop-Gericke, R. Schlögl, B. Aszalos-Kiss and D. Zemlyanov: Methane oxidation on Pd(111): In situ XPS identification of active phase.

Journal of Physical Chemistry C **111**, 22, 7957-7962 (2007).

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).

Guo, J. S., G. Q. Sun, Z. M. Wu, S. G. Sun, S. Y. Yan, L. Cao, Y. S. Yan, D. S. Su and Q. Xin: The durability of polyol-synthesized PtRu/C for direct methanol fuel cells.

Journal of Power Sources **172**, 2, 666-675 (2007).

Gutel, T., J. Garcia-Antón, 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 **17**, 3290-3292 (2007).

Hensel, N., G. Franz, M. Riedl, M. Gottschalk, B. Wunder, F. Galbert and J. Nissen: Polymorphism and solid solution in the system SiO₂-AlPO₄(-H₂O): a review and new synthesis experiments up to 3.5 GPa and 1573 K.

Neues Jahrbuch für Mineralogie-Abhandlungen **184**, 2, 131-149 (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).

Hess, C., G. Tzolova-Müller and R. Herbert: The influence of water on the dispersion of vanadia supported on silica SBA-15: A combined XPS and Raman study.

Journal of Physical Chemistry C **111**, 26, 9471-9479 (2007).



Publications

2007

Max Planck Society
eDoc Server



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).

Imbihl, R., A. Scheibe, Y. F. Zeng, S. Günter, R. Kraehnert, V. A. Kondratenko, M. Baerns, W. K. Offermans, A. P. J. Jansen and R. van Santen: Catalytic ammonia oxidation on platinum: mechanism and catalyst restructuring at high and low pressure. *Physical Chemistry Chemical Physics* **9**, 27, 3522-3540 (2007).

Janetzky, M., E. Rödel, C. Pietzonka, U. Müller, T. Ressler and B. Harbrecht: The valence problem of Pd₄Br₄Te₃. *Chemistry - A European Journal* **13**, 35, 9882-9891 (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).

Kasatkin, I., P. Kurr, B. Kniep, A. Trunschke and R. Schlögl: Role of Lattice Strain and Defects in Copper Particles on the Activity of Cu/ZnO/Al₂O₃ Catalysts for Methanol Synthesis. *Angewandte Chemie* **119**, 38, 7465-7468 (2007).

Kondratenko, V. A. and M. Baerns: Effect of different oxygen species originating from the dissociation of O₂, N₂O and NO on the selectivity of the Pt-catalysed NH₃ oxidation. *Catalysis Today* **121**, 3-4, 210-216 (2007).

Kondratenko, V. A. and M. Baerns: Mechanistic insights into the formation of N₂O and N₂ in NO reduction by NH₃ over a polycrystalline platinum catalyst. *Applied Catalysis B: Environmental* **70**, 1-4, 111-118 (2007).

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

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* **8**, 420-427 (2007).

Kovnir, K., D. Teschner, M. Armbrüster, P. Schnörch, M. Hävecker, A. Knop-Gericke, Y. Grin and R. Schlögl: Pinning the catalytic centre: A new concept for catalysts development. *BESSY Highlights* **2007**, 22-23 (2007).

Kraehnert, R. and M. Baerns: Morphology changes of Pt-foil catalyst induced by temperature-controlled ammonia oxidation near atmospheric pressure. *Applied Catalysis A: General* **327**, 1, 73-81 (2007).

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 (2007).

Kustov, A. L., T. W. Hansen, M. Kustova and C. H. Christensen: Selective catalytic reduction of NO by ammonia using mesoporous Fe-containing HZSM-5 and HZSM-12 zeolite catalysts: An option for automotive applications. *Applied Catalysis B* **76**, 3-4, 311-319 (2007).

Li, H., G. Sun, N. Li, S. Sun, D. S. Su and Q. Xin: 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).

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

Mastalir, A., A. Patzko, B. Frank, R. Schomäcker, T. Ressler and R. Schlögl: Steam reforming of methanol over Cu/ZnO/Al₂O₃ modified with hydrotalcites. *Catalysis Communication* **8**, 11, 1684-1690 (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).

Paál, Z., N. Györfy, A. Wootsch, L. Tóth, I. Bakos, S. Szabó, U. Wild and R. Schlögl: Preparation, physical characterization and catalytic properties of unsupported Pt-Rh catalyst. *Journal of Catalysis* **250**, 2, 254-263 (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. In: *Nanoparticles and Catalysis*. (Eds.) Astruc, Didier. Wiley-VCH Verlag, Weinheim (2007) 555-622.

Perathoner, S., R. Passalacqua, G. Centi, D. S. Su and G. Weinberg: Photoactive titania nanostructured thin films: Synthesis and characteristics of ordered helical nanocoil array. *Catalysis Today* **122**, 3-13 (2007).

Pestryakov, A. N., N. Bogdanchikova, A. Simakov, I. Tuzovskaya, F. C. Jentoft, M. Farias and A. Diaz: Catalytically active gold clusters and nanoparticles for CO oxidation. *Surface Science* **601**, 18, 3792-3795 (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).

Publications

2007

Max Planck Society
eDoc Server

eDoc

2007

Pozdnyakova-Tellingner, 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. In: 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).

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. and S. Wrabetz: Department of Inorganic Chemistry - Fritz-Haber-Institut der Max-Planck-Gesellschaft. 3rd Edition Department of Inorganic Chemistry / FHI, Berlin (2007) Total Numbers of Pages 48 p.

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).

Selvam, T., M. Kostner, G. Mabande, W. Schwieger, N. Pfänder and R. Schlögl: Synthesis, characterization and catalytic properties of mesoporous Al-FSM-16 materials. Journal of Porous Materials **14**, 3, 263-272 (2007).

Soerijanto, H., E. Rödel, U. Wild, M. Lerch, R. Schomäcker, R. Schlögl and T. Ressler: The impact of nitrogen mobility on the activity of zirconium oxynitride catalysts for ammonia decomposition. Journal of Catalysis **250**, 19-24 (2007).

Su, D. S. and X. Chen: Natural Lavas as Catalysts for Efficient Production of Carbon Nanotubes and Nanofibers. In: Angewandte Chemie International Edition **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 supported catalyst.

Physica Status Solidi B **244**, 11, 3916-3919 (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-Tellingner, 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-Tellingner, 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).

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. In: Journal of the American Chemical Society, submitted (2007).

Titirici, M. M., A. Thomas, S.-H. Yu, J.-O. Müller and M. Antonietti: A Direct Synthesis of Mesoporous Carbons with Bicontinuous Pore Morphology from Crude Plant Material by Hydrothermal Carbonization. Chemistry of Materials **19**, 17, 4205-4212 (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).

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).



Publications

2007 / 2008

Max Planck Society
eDoc Server



2008

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).

Zenkovets, G. A., G. N. Kryukova, V. Y. Gavrilov, S. V. Tsybulya, V. A. Anufriyenko, 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., 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.: Surface effects in the energy loss near edge structure of different cobalt oxides. *Ultramicroscopy* **107**, 8, 598-603 (2007).

Baerns, M. and E. V. Kondratenko: Oxidative coupling of methane. In: *Handbook of Heterogeneous Catalysis: 2nd Edition in 8 Volumes*. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 3010-3023.

Berthoud, R., A. Baudouin, B. Fenet, W. Lukens, K. Pelzer, J.-M. Basset, J.-P. Candy and C. Copéret: Mono-nuclear Ru hydride species vs. Ru nanoparticles: the effect of silane functionalities on silica surfaces. *Chemistry - A European Journal* **14**, 12, 3523-3526 (2008).

Bron, M., D. Teschner, U. Wild, B. Steinhauer, A. Knop-Gericke, C. Volckmar, A. Wootsch, R. Schlögl, P. Claus: Oxygen-induced activation of silica supported silver in acrolein hydrogenation. *Applied Catalysis A: General*, **341**, 1-2, 127-132 (2008)

Fu, Q., G. Weinberg and D. S. Su: Selective filling of carbon nanotubes with metals by selective washing. *New Carbon Materials* Volume, **23**, 1, 17-20 (2008).

Gajović, A., D. Gracin, I. Djerdj, N. Tomašić, K. Juraić and D. S. Su: Nanostructure of thin silicon films by combining HRTEM, XRD and Raman spectroscopy measurements and the implication to the optical properties. *Applied Surface Science* **254**, 2748-2754 (2008).

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 (2008).

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* **456**, 1-2, 313-319 (2008).

Grillo, M. E., M. W. Finnis and W. Ranke: Surface structure and water adsorption on Fe₃O₄(111): Spin-density functional theory and on-site Coulomb interactions. *Physical Review B* **77**, 7, 075407-1-075407-2 (2008).

Hébert, C., D. S. Su and P. Pongratz: Mechanism for the reduction of V₂O₅ to VO by electron irradiation. *Philosophical Magazine*, submitted (2008).

Huang, Y., A. Wang, L. Li, X. Wang, D. S. Su and T. Zhang: "Ir-in-ceria": A highly selective catalyst for preferential CO oxidation. *Journal of Catalysis* **255**, 2, 144-152 (2008).

Jentoft, F. C.: Oxo-Anion Modified Oxides. In: *Handbook of Heterogeneous Catalysis Vol. I*. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH, Weinheim (2008) 262-278.

Karge, H. G.: Solid-state ion exchange in zeolites. In: *Handbook of Heterogeneous Catalysis*. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 484-510.

Kondratenko, V. A., U. Bentrup, M. Richter, T. W. Hansen and E. V. Kondratenko: Mechanistic aspects of N₂O and N₂ formation in NO reduction by NH₃ over Ag/Al₂O₃: the effect of O₂ and H₂. *Applied Catalysis B: Environmental*, submitted (2008).

Kornelak, P., D. S. Su, C. Thomas, J. Camra, A. Weselucha-Birczyńska, M. Toba and M. Najbar: Surface species structure and activity in NO decomposition of an anatase-supported V–O–Mo catalyst. *Catalysis Today* **137**, 2-4, 273-277 (2008).

Kovnir, K., D. Teschner, M. Armbrüster, P. Schnörch, M. Hävecker, A. Knop-Gericke, Y. Grin and R. Schlögl: Pinning the catalytic centre: A new concept for catalysts development. *BESSY Highlights 2007*, 22-23 (2008).

Kraehnert, R. and M. Baerns: Kinetics of ammonia oxidation over Pt foil studied in a micro-structured quartz-reactor. *Chemical Engineering Journal* **137**, 2, 361-375 (2008).

Publications

2008

Max Planck Society
eDoc Server

eDoc

2008

Kubias, B., M. J. G. Fait and R. Schlögl: Mechanochemical Methods. In: Handbook of Heterogeneous Catalysis. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 571-583.

Ličina, V., A. Gajović, A. Moguš-Milanković, I. Djerdj, N. Tomašić and D. S. Su: Correlation between the microstructure and the electrical properties of ZrTiO₄ ceramics. Journal of American Ceramic Society **91**, 1, 178-186 (2008).

Liu, Y., D. Ma, X. Han, X. Bao, W. Frandsen, D. Wang and D. S. Su: Hydrothermal synthesis of microscale boehmite and gamma nanoleaves alumina. Materials Letters **62**, 1297-1301 (2008).

Liu, X., D. S. Su and R. Schlögl: Oxidative dehydrogenation of 1-butene to butadiene over carbon nanotube catalysts. Carbon **46**, 544-561 (2008).

Moehmel, S., N. Steinfeldt, S. Engelschalt, M. Holena, S. Kolf, M. Baerns, U. Dingerdisen, D. Wolf, R. Weber and M. Bewersdorf: New catalytic materials for the high-temperature synthesis of hydrocyanic acid from methane and ammonia by high-throughput approach. Applied Catalysis A: General **334**, 1-2, 73-83 (2008).

Osswald, J., R. Giedigkeit, R. E. Jentoft, M. Armbrüster, F. Girgsdies, K. Kovnir, T. Ressler, Y. Grin and R. Schlögl: Palladium Gallium Intermetallic Compounds for the Selective Hydrogenation of Acetylene Part I: Preparation and Structural Investigation Under Reaction Conditions. Journal of Catalysis **258**, 1, 210-218 (2008).

Osswald, J., K. Kovnir, M. Armbrüster, R. Giedigkeit, R. E. Jentoft, U. Wild, Y. Grin and R. Schlögl: Palladium Gallium Intermetallic Compounds for the Selective Hydrogenation of Acetylene Part II: Surface Characterization and Catalytic Performance. Journal of Catalysis **258**, 1, 219-227 (2008).

Celaya Sanfiz, A., T. W. Hansen, A. Sakthivel, A. Trunschke, R. Schlögl, A. Knoester, H. H. Brongersma, M. H. Looi, S. B. A. Hamid: How important is the (001) plane of M1 for selective oxidation of propane to acrylic acid? Journal of Catalysis **258**, 1, 35-43 (2008).

Schlögl, R.: Ammonia Synthesis. In: Handbook of Heterogeneous Catalysis. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 2501-2575.

Schlögl, R.: Carbon. In: Handbook of Heterogeneous Catalysis. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 357-427.

Schlögl, R.: Fused Catalysts. In: Handbook of Heterogeneous Catalysis. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 81-92.

Schlögl, R.: In situ powder X-ray diffraction: a basic tool for characterisation of heterogeneous catalysts. Advances in Catalysis **52**, accepted (2008).

Su, D. S., X. Chen, X. Liu, J. Delgado, R. Schlögl and A. Gajović: Mount Etna lava supported nanocarbons for oxidative dehydrogenation reactions. Advanced Materials **20** (19), 3597-3600 (2008).

Su, D. S., T. Jacob, T. W. Hansen, D. Wang, R. Schlögl, B. Freitag and S. Kujawa: Surface Chemistry of Ag Particles: Identification of Oxide Species by Aberration-Corrected TEM and by DFT Calculations. Angewandte Chemie International Edition **47**, 27, 5005-5008 (2008).

Su, D. S., A. Serafino, J.-O. Müller, R. E. Jentoft, R. Schlögl and S. Fiorito: Cytotoxicity and Inflammatory Potential of Soot Particles of Low-Emission Diesel Engines. Environmental Science and Technology **42**, 5, 1761-1765 (2008).

Teschner, D., J. Borsodi, A. Wootsch, Zs. Revay, M. Hävecker, A. Knop-Gericke, S. D. Jackson and R. Schlögl: The Roles of Subsurface Carbon and Hydrogen in Palladium-Catalyzed Alkyne Hydrogenation. Science **320**, 5872, 86-89 (2008).

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 (2008).

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 (2008).

Wang, D., A. Villa, F. Porta, L. Prati and D. S. Su: Bimetallic Gold/Palladium Catalysts: Correlation between Nanostructure and Synergistic Effects. Journal of Physical Chemistry C **112**, 23, 8617-8622 (2008).

Xu, Y.-J., G. Weinberg, X. Liu, O. Timpe, R. Schlögl and D. S. Su: Nano-architecturing of Activated Carbon: New Facile Strategy for Chemical Functionalization of the Surface of Activated Carbon. Advanced Functional Materials, accepted (2008).

Zhang, J., Y.-S. Hu, J.-P. Tessonnier, G. Weinberg, J. Maier, R. Schlögl and D. S. Su: CNFs@CNTs: Superior Carbon for Electrochemical Energy Storage. Advanced Materials **20**, 8, 1450-1455 (2008).

Zhang, J., X. Liu, R. Blume, a. Zhang, R. Schlögl and D. S. Su: Surface-Modified Carbon Nanotubes Catalyze Oxidative Dehydrogenation of n-Butane. Science **322**, 5898, 73-77 (2008).

Zhang, J., J.-O. Müller, W. Zheng, D. Wang, D. S. Su and R. Schlögl: Individual Fe-Co Alloy Nanoparticles on Carbon Nanotubes: Structural and Catalytic Properties. Nano Letters, accepted (2008).

Zhang, Z. and D. S. Su: Behaviour of TEM metal-grids during in-situ heating experiments. Ultramicroscopy, submitted (2008).

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

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. Schlögl, 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. Schlögl

EP2005/008022, July 22, 2005

"Metal oxide catalyst and method for the preparation"

Inventors: R. Schlögl, O. Timpe, S.B. Abd Hamid

EP2005/007619, 2005

"Carbon nanotubes fixed on activated carbon"

Inventors: R. Schlögl, S.B. Abd Hamid

DE 102004 034 630.5, 2004, 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; WO2007104569, 2007;

USA, Japan, China, Malaysia, Singapur, Indonesien, Kanada, 2008

"Palladium-Gallium intermetallic compounds as catalysts for the selective hydrogenation of acetylene"

Inventors: J. Grin, R. Schlögl, J. Osswald

EP2006/00346, April 13, 2006; USA, China, Japan 2008

"Nanocarbon-activated carbon composites"

Inventors: R. Schlögl, S.B. Abd Hamid

EP07018368, 2007

"Use of a mixture of an ordered intermetallic compound and an inert material as a catalyst and corresponding hydrogenation processes"

Inventors: M. Armbrüster, M. Schmidt, K. Kovnir, M. Friedrich, K. Weinhold, Yu. Grin, R. Schlögl

EP07021904.3, 2007

"Preparation of intermetallic compounds via gas phase and nanoparticle synthesis"

Inventors: M. Armbrüster, M. Schmidt, K. Kovnir, M. Friedrich, K. Weinhold, Yu. Grin, R. Schlögl

EP07019469.1, 2007; PCT/EP2008/008383

"A new assembly of nanocarbon structure for energy storage"

Inventors: DS. Su, J. Zhang, R. Schlögl, J. Maier

PCT/EP2007/063523, 2007

"Novel synthetic route to mesostructured MoVTe mixed oxide"

Inventors: R. Schlögl, A. Trunschke

Submission USA 2008

"Phase-enriched MoVTeNB mixed oxide catalyst and methods for the preparation"

Inventors: O. Timpe, S. Ayyamperiumal, A. Trunschke, R. Schlögl

EP submission 08167109.1, 10/ 2008

"P-modified Mo-V-Nb mixed oxide catalyst"

Inventors: R. Schlögl, A. Trunschke, O. Timpe, A.C. Sanfiz

EP submission 08167110.9, 10/ 2008

"Bi-modified Mo-V-Nb mixed oxide catalyst"

Inventors: R. Schlögl, A. Trunschke, O. Timpe, A.C. Sanfiz

Int. submission, 10/2008

"Hydrogenation process using mixture of an ordered IMC and inert material"

Inventors: M. Armbrüster, M. Schmidt, K. Kovnir, M. Friedrich, K. Weinhold, Yu. Grin, R. Schlögl

Int. submission based on EP07021904.3, 2008

"Preparation of intermetallic compounds via gas phase and nanoparticle synthesis"

Inventors: M. Armbrüster, M. Schmidt, K. Kovnir, M. Friedrich, K. Weinhold, Yu. Grin, R. Schlögl

Guest - lectures

2003 - 2008

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 & Ortsaufgelöste 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 - 2008

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 ₂ O 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	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 - 2008

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 Bruxelles	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, Université Montpellier	Toxicity of Carbon nanoparticles towards human cells
30.03.2006	Dr. Cécile Hébert Inst. f. Festkörperphysik, TU Wien	Low Loss EELS and the measurement 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 - 2008

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 nanoparticles
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, Boriskov Institute of Catalysis, Novosibirsk, Russia 	Size effects of supported nanoparticles in catalysis
12.12.2007	Dr. Juan P. Holgado Vázquez Instituto de Ciencia de Materiales de Sevilla (Univ. Sevilla - CSIC) 	Strategies for design nanostructured catalysts: from real materials to model systems

Date	Speaking Guest	Titel
21.02.2008	Prof. Lanny D. Schmidt Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis	Catalytic Autothermal Reforming of Renewable Fuels at Millisecond Times
13.03.2008	Dr. Nicola Pinna Laboratorio Associado CICECO Universidade de Aveiro Campus Universitario de Santiago	Non-aqueous sol-gel routes to nanostructured metal oxides
02.04.2008	Dr. Stephan Hofmann Centre for Advanced Photonics and Electronics, Uni. of Cambridge, UK	Catalyst Dynamics during Carbon Nanotube and Si Nanowire CVD
16.04.2008	Prof. E. Joseph Nordgren Uppsala University, Physics Dept., Sweden 	Soft X-ray fluorescence and resonant inelastic scattering for materials and chemical physics
28.04.2008	Dr. Jan Haubrich Dept. of Chemistry and Chemical Biology, Harvard University	Adsorption, Wechselwirkung und Reaktivität von Aldehyden und Alkenen mit Legierungsoberflächen und Oxiden










Guest - lectures

2003 - 2008

Date	Speaking Guest	Titel
30.04.2008	Prof. Theodor Doll Johannes Gutenberg-Universität Mainz und dem Institut für Mikrotechnik Mainz GmbH	The Electroadsorptive Effect in Fully Depleted Metal Oxide Film Gas Sensors
11.06.2008	Dr. Fachri Atamny OC Oerlikon Balzers Ltd, Solar	Photovoltaic Solar: Market and Technology Trends
02.07.2008	Dr. Wolfgang Kleist Institut für Chemie- / Bioingenieur- wiss., ETH Zürich, Schweiz	Modified Metal-Organic Frameworks - Synthesis, Properties and  Potential in Catalysis
09.07.2008	Prof. Michael Smith Villanova University, Villanova, PA, USA	Order on what scale? Studies in the structure of porous carbons and mesoporous silicates
10.07.2008	Prof. Shriram Ramanathan School of Engineering and Applied Sciences, Harvard Uni., Cambridge	Structure-Property relations in ultra-thin fluorite metal-oxides
29.07.2008	Prof. Laurent Duda Uppsala University, Sweden	Resonant inelastic soft x-ray scattering as a tool for studying chem. processes in situ
30.07.2008	Prof. Josef Breu Lehrstuhl fuer Anorganische Chemie I, Uni. Bayreuth, Germany	Colloids and Hybrids
13.08.2008	Dr. Karen Wilson Uni. of York, Dept. of Chemistry	Recent developments in environmental catalysis
27.08.2008	Prof. Konstantin I. Hadjiivanov Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences	IR Spectroscopy of Isotopically Labeled Surface Species 
03.09.2008	Prof. Jean Marie Basset  Laboratoire de Chimie Organométallique de Surface, Villeurbanne, France	Surface organometallic chemistry: a predictive approach of heterogeneous catalysis?





Date	Speaking Guest	Titel
17.09.2008	Prof. Leon Lefferts University of Twente, Catalytic Processes and Materials Group	Heterogeneous catalysis in liquid phase; Fundamental and engineering challenges
01.10.2008	Prof. Robert Glaum Institut für Anorganische Chemie, Universität Bonn, Germany	Ein Festkörperchemiker auf Abwegen
22.10.2008	Prof. Rüdiger Kniep MPI für chemische Physik fester Stoffe, Dresden/Germany	Apatit-Gelatine-Nanocomposites (aus dem Reich der Borophosphate) 
05.11.2008	Prof. Juri Grin Chemische Metallkunde, MPI für chemische Physik fester Stoffe, Dresden/Germany 	Intermetallic compounds and redox reactions
09.12.2008 10.12.2008	Prof. Gabor A. Somorjai Department of Chemistry and Lawrence Berkeley National Laboratory, University of California, Berkeley, USA	Winner of the Gerhard Ertl Lecture Award 2008 Molecular Foundations of Heterogeneous Metal 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 - 2009	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 - 2009	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 	M.IF.A.FHI 08025	MPG 	2005 - 2010	Prof. R. Schlögl Dr. D. S. Su	Prof. F. Schüth (MPI für Kohleforschung), Prof. J. Maier (MPI für Festkörperforschung), Prof. K. Müllen (MPI für Polymerforschung)	Verbundprojekt
Entwicklung von Methanolsynthesekatalysatoren als Basis für nachhaltige Ressourcennutzung – TP3	BMBF	PSFHI 102	BMBF 	1.7.2005 – 31.12.2008	Prof. R. Schlögl Dr. M. Behrens 	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 Forschungsgemeinschaft	23.10.2006 continuing	Prof. R. Schlögl	Prof. M. Lerch Prof. R. Schomäcker	Prof. T. Ressler
Mischoxide		PSFHI 253	Südchemie	2007 - 2009	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 Teilprojekt AP1: "Aufklärung, Reaktionsmechanismus und Optimierung des bestehenden Katalysators"	CarboScale	PSFHI 105	BMBF 	2007 - 2012	Prof. Dr. R. Schlögl Dr. J. P. Tessonnier	TU Berlin Ruhr-Uni. Bochum Univ. Erlangen Univ. Clausthal Future Carbon GmbH Bayer Ehrfeld Mikrotechnik - BTS GmbH Leibnitz-Inst, Dresden TU Ilmenau Fraunhofer-Gesellschaft München H. C. Starck GmbH	Dr. D.S. Su Dr. J. P. Tessonnier
"Unifying Concepts in Catalysis", application to become Cluster of Excellence 	CoE Unicat	PSFHI 770	German Federal and State Governments to Promote Science and Research at German Univ.	starting 2007	Prof. R. Schlögl Prof. H.J. Freund Prof. G. Meijer Prof. M. Scheffler	http://www.unicat.tu-berlin.de	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 Dr. M. Behrens (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)
Elektroden-Charakterisierung	FuEV	PSFHI 254	Bayer AG 	1.7.2007 – 20.6.2009	Prof. R. Schlögl	Prof. R. Schlögl (FHI der MPG) Prof. R. Schomäcker (TU Berlin)	
Identification of local environment of transition metal promoter cations in zirconia-based heterogeneous catalysts.	DFG	436 MOL	Deutsche Forschungsgemeinschaft	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 Forschungsgemeinschaft	2004 – 2008	Dr. F. C. Jentoft	Prof. V. Kazansky (RAS Moscow, Russian)	
PROX catalysts	PROX		MPG	2004 – 2006 continuing	Dr. F. C. Jentoft	Dr. A. Knop-Gericke Dr. A. Woosch (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
Struktur, Dynamik und Reaktivität von Übergangsmetalloxid- Aggregaten	Sfb	Sfb 546	Sonderforschungsbereich	2000 - 2009	Dr. D.S. Su Dr. K. Pelzer (Aug. 2008)	Prof. Dr. R. Schlögl	Prof. Dr. J. Sauer
Electrocatalytic Gas-Phase Conversion 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 molecular-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 continuing	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 – 2009	Dr. D. S. Su	Prof. Dr. M. Najbar	Dr. D. S. Su
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 Forschungsgemeinschaft	15.10.2007 – 14.10.2009	Dr. D. S. Su	Prof. R. Nießner Dr. N. Ivleva	Prof. R. Schlögl

External funds

Project Name	Akronym	Referenz No.	Funds' Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
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
Pd model catalysts in oxidation reactions			MPG	2004 - 2008	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-Nachwuchsgruppe	HE 4515/1-1 HE 4515/1-2	Deutsche Forschungsgemeinschaft	2004-2008	Dr. C. Hess		
Functional analysis of noble metal catalysts in selective hydrogenation	Partner Group	M.PG.A.FHI00002	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	
Interaction of Surface and Gas Reactions in High Temperature (max ca. 1300°C) High Pressure (max. ca. 5 M Pa) Catalytic Alkane Oxidations	Emmy-Noether-Nachwuchsgruppe	EM.FHI 707	Deutsche Forschungsgemeinschaft	2007 - 2012	Dr. R. Horn		

Cluster of Excellence CoE

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



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).

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



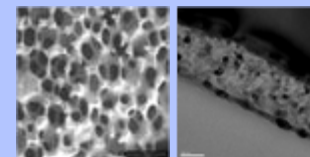
Coordinator of the FHI der MPG, Dept. of AC:

Dr. Axel Knop-Gericke
knop@fhi-berlin.mpg.de

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

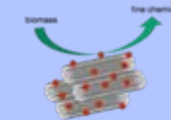
The projects of FHI / Dept. of AC within UniCat Research area A: Bridging the materials gap in complex catalysis

1. Direct oxidative coupling of methane to ethylene on Li-MgO foam catalysts
(Dr. Ulyana Zavyalova, Oliver Korup, Dr. Isabella Oprea, Dr. Raimund Horn)
Goal: Understanding of mechanistic details of the methane activation towards design of tailored basic oxide catalysts. Comprehensive study of the heterogeneous-homogeneous reaction mechanism on Li/MgO foam catalysts with various surface-to-volume ratios.



2. Molybdenum molecular compounds for modeling active sites of selective oxidation catalysts
(Kazuhiko Amakawa)
Goal: Study of the structure-reactivity relationship in metastable MoO_x based catalysts for selective oxidation reactions.

3. Conversion of biomass on the MWCNT-supported metallic nanoparticles
(Sylvia Reiche)
Goal: Design and application of MWCNT-supported metallic catalysts for conversion of biomass into building blocks for the production of biodegradable polymers.



What is BIG-NSE?



The Berlin International Graduate School for Natural Sciences and Engineering (BIG-NSE) is the graduate program of the UniCat Cluster of Excellence. With the founding of BIG-NSE, UniCat aims to recruit gifted students and young researchers from all over the world and offer them a broad, high level structured educational program in order to prepare them for the high-ranking research performed at the cluster. Within a so-called "Initial Phase" of three months, basic lectures are given on topics of all three areas of the cluster. In addition soft skill courses, such as language courses, training in personal skills (presentation, communication), counseling on setting up a business, project management, funding acquisition etc., as well multiple excursions to scientific institutes and industrial enterprises complete the educational program.



<http://www.big-nse.tu-berlin.de>



European Union - Network of Excellence / NoE



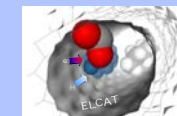
What is the SIXTH FRAMEWORK PROGRAMME (FP6) ?

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>



CANAPE
completed in 2008



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.

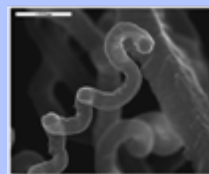
<http://idecat.org>

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 CO₂ 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 CO₂ 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 CO₂ to chemicals.
- Use the confinement effect in nanomaterials to promote unconventional catalytic reactions.

<http://www.elcat.org>

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.



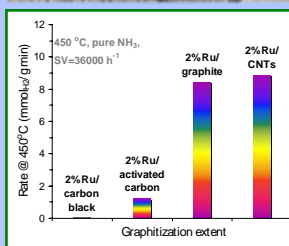
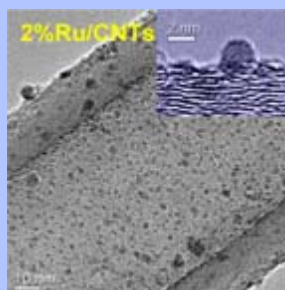
The world energy consumption is at present based nearly to 90% on fossil sources of energy (coal, oil, natural gas). Low efficiency of energy utilization has speeded up the depletion of fossil fuels and global warming. With the establishment of "nano-chemical concepts of lasting power supplies – EnerChem", 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

Ammonia decomposition ($2\text{NH}_3 \rightarrow \text{N}_2 + 3\text{H}_2$) is free of CO_x and environmentally benign. Conversion of nearly 100% can be achieved at 400°C on the supported metals. Carbon nanotube is the best support due to its high electric conductivity and thermal/chemical stabilities. The graphitic structure as the electron reservoir greatly enhances the reaction rate via optimizing electron exchange on the local domain of active sites.

Structure of carbon was found to determine the activity of supported metals, *i.e.* the higher the graphitization, the higher the activity. As revealed by *in-situ* XPS at a near-ambient pressure, the decomposition activity shows a positive dependency on the efficiency of electron transfer inside the "Ru-C-promoter" ternary interfaces. Advantage of CNTs is only found on its confinement on the stability.



Contact:

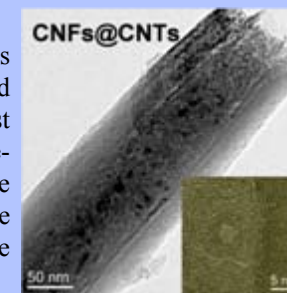
Dr. Jain Zhang
jian@fhi-berlin.mpg.de

External collaborations:

MPG-Colloid and Interfaces (Golm), MPI-Coal Research (Muelheim),
MPI-Polymer Research (Mainz), MPI-Solid State Science (Stuttgart),

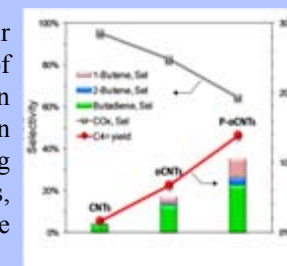
2. Novel nanocarbons for electrochemical energy storage

Li-ion rechargeable batteries are not only consumer electronics but, most importantly, green carrier of electricity in hybrid electric vehicles. Carbon as a richly available and low-cost resource is a promising electrode material. Carbon nanotube-encapsulated nanofibers (CNFs@CNTs) as a superior electrode material provides a long-term stability at a high storage capacity. Facile fabrication benefits it a great potential to be commercialized.



3. Carbon-based metal-free catalysis

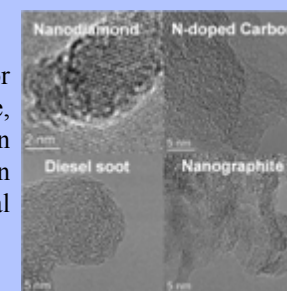
Traditional metal catalysts are deeply involved in their chemical complexity, such as lattice oxygen, various forms of polyvalent metals, parallel coke formation, etc. We use carbon with nanostructure to catalyze oxidative dehydrogenation reactions of propane, butane and ethylbenzene, producing important industrial monomers including propene, butenes, butadiene, and styrene. A superior selectivity to alkenes can be observed for a long period of time, *e.g.* 500 h.



This catalytic process is mediated by surface ketonic carbonyl groups embedding in graphitic substrate. The turnover over local active sites is simplified as: $>\text{C}=\text{O} + \text{alkane} \rightarrow \geq\text{C}-\text{OH} + \text{alkene}$. The selectivity can be further improved by the addition of B or P to passivate the sites for total combustion. We note that the reaction is generally coke-free.

4. Structural characterization of novel nanocarbons

There is a great amount of carbons with novel structures, for example nanodiamond, nanographite, nano-onion, graphene, diesel engine soot, N-doped carbon, *etc.* We focus on characterizing the effect of their structural parameters on practical uses in electrochemistry, catalysis and environmental science.



Financial support:
MPG

Collaborative Research Centre

Collaborative Research Centers are long-term university research centers in which scientists and researchers work together within a cross-disciplinary research program.

What is a Collaborative Research Centre ?

Under the Collaborative Research Centre Program, funding may be provided for Collaborative Research Centers (SFBs), which are generally based at up to three universities.

In addition to the scientific projects funded in the SFB programs, specific project modules may also be incorporated. Examples include transfer projects, PR projects, integrated Research Training Groups, projects on information infrastructure and research service projects. Independent junior research groups that are funded in the Emmy Noether Program may be integrated in an SFB. International cooperation is also promoted in a variety of forms.

What aims the SFB 546 ?

Transition metal oxides find applications in many areas. The aim of the collaborative research centre 546 is focused on the relation between structures of transition metal oxides in different aggregation states and their functions. For this purpose gas-phase and solid state studies are combined: in the gas-phase diatomic molecules and small clusters are generated, characterized, and their reactivity is studied. Comparison is made with clusters deposited on surfaces as well as with epitaxial films and single crystal surfaces. Finally, "real" transition metal catalysts on supports will be studied.

Part of the SFB 546 are currently:



Spokesperson:

Prof. Dr. Joachim Sauer
Institut für Chemie
Humboldt-Universität
Unter den Linden 6
10099 Berlin
js@chemie.hu-berlin.de

SFB 546:

Structure, Dynamics and Reactivity of Aggregates of Transition Metal Oxides

Sub-project B2:

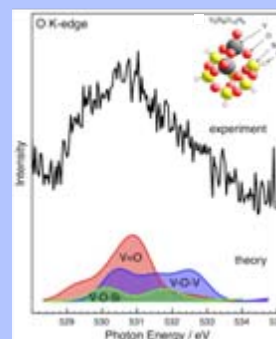
Partial oxidation of small hydrocarbon molecules with microscopic amounts of vanadia catalysts

Program Summary

Project B2 aims at establishing structure-activity relations for partial oxidation reactions of small alkane molecules using small V_xO_y particles and supported V_xO_y aggregates. An understanding of structure-activity relations requires on one hand the development of well-defined, realistic model systems, on the other hand the thorough characterization before and during reaction. The findings from the last funding period regarding the structural properties of V_xO_y /SBA-15 catalysts provide an excellent basis for future in situ investigations as well as the targeted development of novel synthetic strategies.

The objectives of AC in the SFB are:

All B projects dealing with polycrystalline materials (Poly B), i.e. sub-projects B2, B3, B6 and B7, will strongly focus on the **common goal to understand and maximize the selectivity in propane selective oxidation**. This approach is expected to yield synergistic effects as each sub-project will strongly focus on its area of expertise. The common sample pool begins with up scaling SBA-15 samples in order to provide SBA-15/V series, then SBA-15 modified samples and in parallel V on carbon nanotubes.



Theorie compared to experiment

In collaboration with Prof. Dr. Klaus Hermann (FHI), an experimental in-situ oxygen K-NEXAFS spectrum of 10.8 wt% V/SBA-15 has been compared to theoretical spectra of different oxygen coordinations. The theoretical spectra have been obtained by DFT calculations for a $V_2Si_6O_{14}H_6$ cluster as shown in the Figure. This comparison suggests the presence of V-O-V bridging bonds in the VO_x species on SBA-15.

Contact:
Dr. Katrin Pelzer
pelzer@fhi-berlin.mpg.de

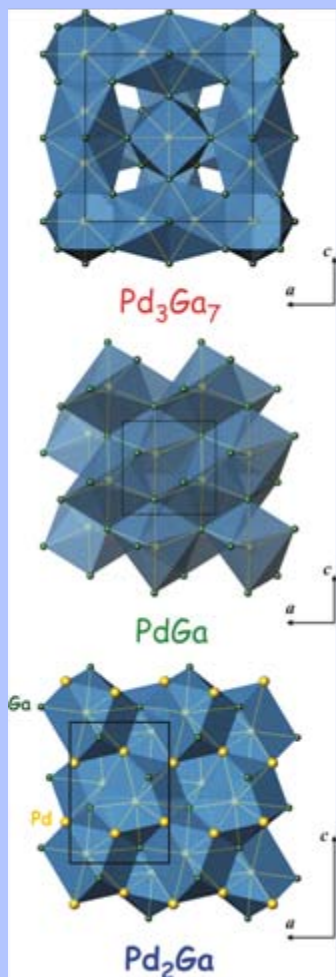
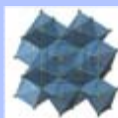
<http://www.chemie.hu-berlin.de/sfb546/index.html>



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Scientific Progress

Palladium intermetallic compounds



Selective hydrogenation is an important industrial process, for example to remove trace amounts of acetylene in ethylene feed for the production of polyethylene. Because acetylene poisons the polymerization catalyst, the acetylene content in the feed has to be reduced to the low ppm range. Moreover, economic efficiency requires high selectivity of the acetylene hydrogenation to prevent the hydrogenation of ethylene to ethane. Typical catalyst contain palladium, however its selectivity and long term stability is a critical issue.

To circumvent these problems we introduced a new family of Pd-based materials to hydrogenation chemistry. These new materials are intermetallic compounds (IMC) that are chemical compound of two or more metallic elements and adopts an ordered crystal structure that differs from those of the constituent metals. Intermetallic compounds are single phase materials.

Figure 1 illustrates three Pd-Ga intermetallic compounds with different stoichiometry. Here, the atomic environment of the catalytically active metal is pinned in the crystal structure. Quantum chemical calculations suggest that their Pd d band is further filled and shifted to higher binding energy by the chemical bonding between Ga and Pd (Fig. 2). This leads to a homogeneous distribution of the possible active sites to a

Fig.1 Palladium intermetallic compounds

significantly reduced segregation and to negligible sub-surface chemistry.

The intermetallic compounds have been prepared by mixing the two molten metals followed by milling of the intermetallic compound.

The IMC show considerably higher selectivity in the hydrogenation of acetylene to ethylene compared to the reference catalysts (Fig. 3). Moreover, they exhibit a remarkable catalytic long-term stability, because of the isolation of the active Pd sites, thus preventing polycondensation side-reactions.

In situ X-ray photoelectron spectroscopic experiment, which is biased toward the surface, confirmed the modified electronic structure of Pd and its stability in hydrogenation environment.

Filling of the Pd d-band and the covalent Pd-Ga interaction prevents the formation of subsurface hydrides, as confirmed by the bulk-sensitive Prompt Gamma Activation Analysis under reaction conditions. The geometrical isolation of Pd sites and the complete suppression of subsurface hydrogen are two key parameters for the superior catalytic properties.

Recently we are exploring the possibility to apply concept of IMC in different catalytic reactions. Our new target reaction is steam reforming of low carbon chain alcohols to produce hydrogen.

Fig.2 Electron density of states of elemental Pd and PdGa

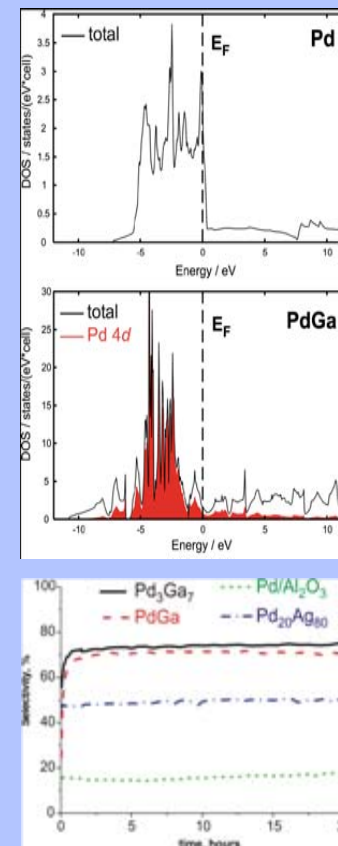


Fig.3 Selectivity in acetylene hydrogenation

Contacts:

Dr. Malte Behrens, behrens@fhi-berlin.mpg.de
Dr. Marc Armbrüster, research@armbruester.net

External collaborations:

Max-Planck-Institut für Chemische Physik fester Stoffe
(Prof.Dr. Y. Grin)

Teaching Activities

Staff scientists are regularly involved in the course programme of the Freie Universität, Humboldt Universität and Technische 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, Annette Trunschke 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.



Coordinator (coordinator@imprs-cs.mpg.de):

Dr. Thomas Risse; FHI; Dept. of Chemical Physics

<http://www.imprs-cs.mpg.de>

The International Max Planck Research School on "Complex Surfaces in Material Science" aims at combining the expertise of several strong research groups in the Humboldt Universität zu Berlin, the Freie Universität Berlin, and the Fritz-Haber-Institut der Max-Planck-Gesellschaft, creating a unique opportunity for foreign and German students in terms of cutting-edge research and a thorough training in the methods, concepts, and theoretical basis of the physics and chemistry of surfaces. The Research School provides an interdisciplinary environment, and a wealth of methods using state-of-the-art equipment.



Chair: Prof. Dr. Matthias Driess (matthias.driess@tu-berlin.de)

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

UniCat is the acronym for a new initiative on the area of catalysis research in the Berlin-Brandenburg area (Germany). UniCat is a Cluster of Excellence and BIG-NSE is its graduate school (<http://www.big-nse.tu-berlin.de>). UniCat has been developed within the Excellence Initiative started by the German Federal and State Governments, under the supervision of the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG).

Physical Chemistry Laboratory Class (WS only)

Instructor: 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.

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"

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. of AC

Instructors: D. S. Su, Dr. Di Wang

"Basics Course on Electron Microscopy and Its Applications"

lange Nacht der Wissenschaften



Wasserstofftechnologie

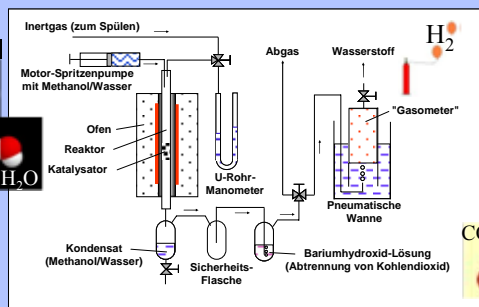
Anhaltende Diskussionen um die Gestaltung der zukünftigen Energieversorgung haben auch das allgemeine öffentliche Interesse erreicht. Innovative Ansätze umfassen dabei die unter dem Begriff *Wasserstofftechnologie* zusammengefassten Prozesse, dabei kommt der Brennstoffzellentechnologie eine zentrale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

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.

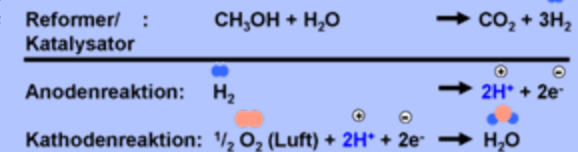
Woher kommt der Wasserstoff / Where does hydrogen come from?

z.B. aus Methanol CH_3OH



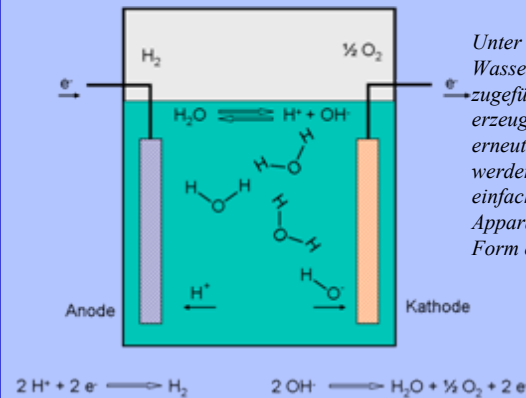
DMFC – Direct Methanol Fuel Cell

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.



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.



Long Night of Science



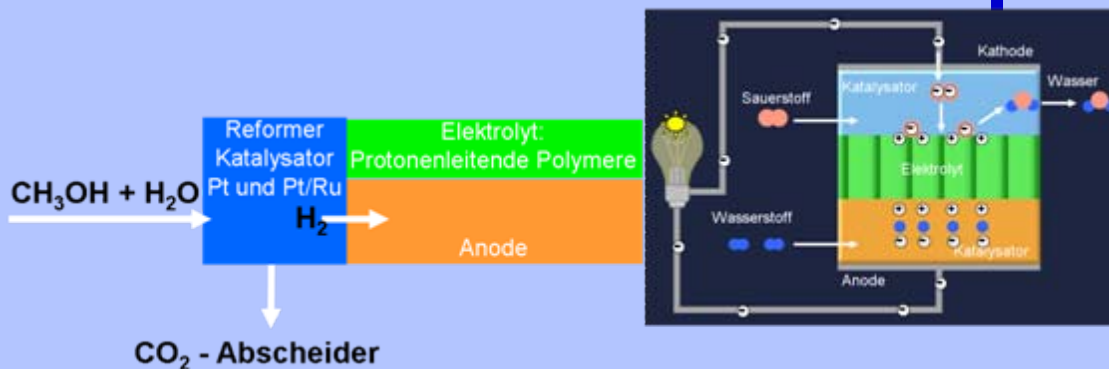
Hydrogen Technology

Ongoing discussions about power supply in future resulted in a general Public interest.

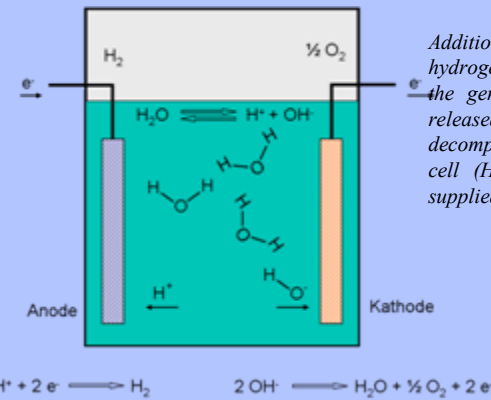
Innovative approaches comprise the processes well-known as hydrogen technology. Among these fuel cells are of special importance.

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.

Funktionsweise einer BZ / Function principle of a fuel cell



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.

Anwendung / Application



Practical Courses



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.

Johannes Kohlmann und Yosri Hassanein (Oktober 2008, 3. Semester, Chemiestudenten) *Noch in unserer Schulzeit nahmen wir an „Jugend forscht“ teil und gewannen ein zweiwöchiges Praktikum im Fritz-Haber-Institut der MPG. Während der 2 Wochen durchliefen wir verschiedene Forschungsgruppen der Abt. AC, welche sich mit heterogener Katalyse befassen. Zu den besuchten AG's gehören unter anderem TEM, SEM, IR- & UV-vis-Spektroskopie und Mikrokolorimetrie. Dort bekamen wir eine ausführliche und interessante theoretische Einweisung in die Arbeitsweise der Geräte und deren praktische Anwendung. Auch fehlte es niemals am entsprechenden chemisch-theoretischen Background. Durch das Praktikum haben wir viele neue fachliche Kenntnisse gewonnen und es gewährte uns einen Blick auf eine mögliche Zukunft als Forscher. Auch führten wir erste wissenschaftliche Gespräche in Englisch.*



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.

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



Toni Siewert (Juli 2008):

Mein Name ist Toni Siewert und ich besuche zurzeit die 13. Jahrgangsstufe des Sartre-Gymnasiums in Berlin. Ich bin naturwissenschaftlich sehr interessiert und befinde mich momentan in der Orientierungsphase für mein zukünftiges Studium. Um Einblicke in die wissenschaftliche Forschungsarbeit zu erhalten, nutzte ich die Chance, ein zweiwöchiges Praktikum in der Abteilung Anorganische Chemie am Fritz-Haber-Institut zu absolvieren.

Das Hauptthema war der Forschungsbereich heterogene Katalyse. Dabei wurde ich unter anderem in die verschiedensten Analysemethoden wie zum Beispiel BET, IR-Spektroskopie, UV-vis Spektroskopie, Adsorptions-Mikrokolorimetrie und Transmissionselektronenmikroskopie eingewiesen. Für mich war besonders das Kennen lernen der einzelnen Arbeitsabläufe und Arbeitsgeräte sehr informativ.

Positiv beeindruckt war ich von der freundlichen Arbeitsatmosphäre und der Hilfsbereitschaft der Mitarbeiter. Mir hat sehr gefallen, dass ich schon nach kurzer Einarbeitungszeit selbstständig und eigenverantwortlich arbeiten durfte. Faszinierend fand ich meinen Ausflug in die TU-Berlin, wo ich einiges über die Herstellung von Katalysatoren erfahren habe.

Das Praktikum am FHI hat mich in meinem Wunsch nach einem naturwissenschaftlichen Studium bestärkt.



*Nina K.
Januar 2005*



*Anne T.
July 2006*



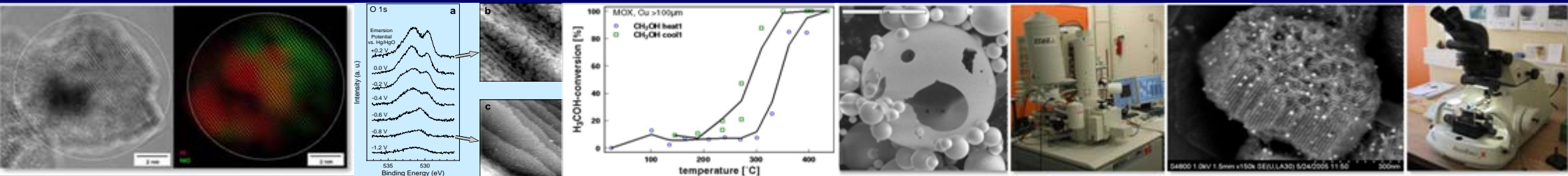
*Swantje P.
Sept. 2006*

Notes

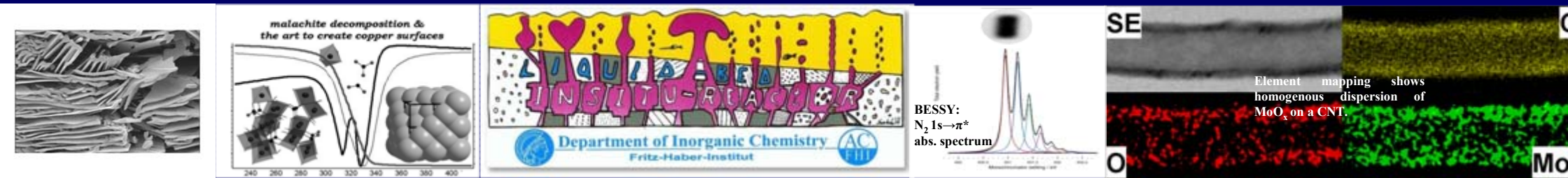


Notes





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



Address Fritz-Haber-Institut der Max-Planck-Gesellschaft
Department of Inorganic Chemistry

Faradayweg 4 – 6
D-14195 Berlin
Germany

Phone +49 (0) 30 8413 4404 (Prof. Dr. R. Schlögl)

+49 (0) 30 8413 4468 (Dr. S. Wrabetz)

Fax +49 (0) 30 8413 4401

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

Editor Prof. Dr. Robert Schlögl
acsek@fhi-berlin.mpg.de
Dr. Sabine Wrabetz
wrabetz@fhi-berlin.mpg.de

Press December 2008