



DEPARTMENT OF



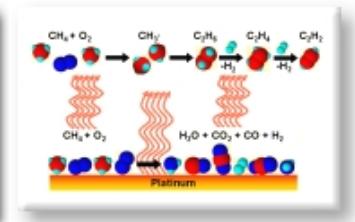
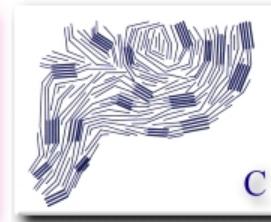
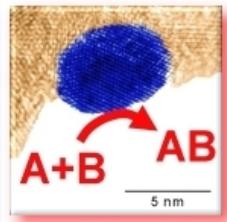
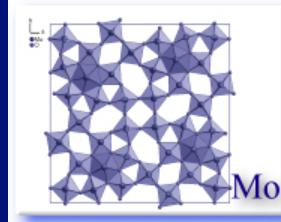
MAX-PLANCK-GESELLSCHAFT

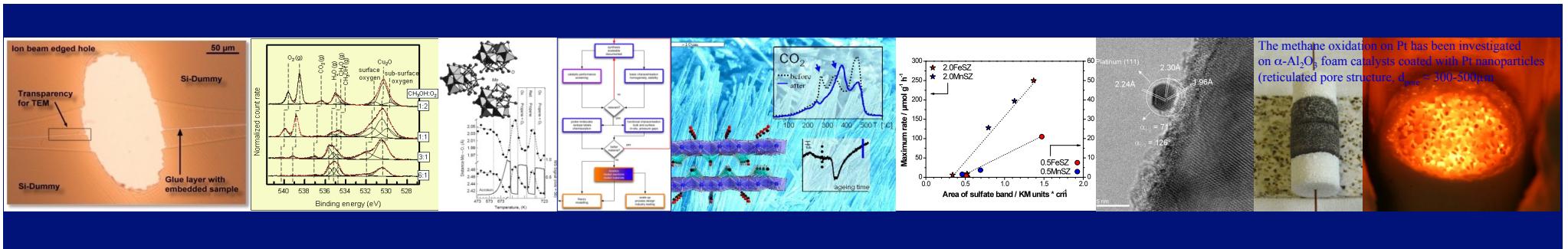
INORGANIC CHEMISTRY



FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT

November 2009 / 5th Edition





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



Table of Contents



- A History of the Fritz-Haber-Institut**
- B How to reach the Institute**
- C Preface**
- D Internal Structure**
- E Highlights**
- F Instrumentation**
- G Understanding Catalysis**
- H Scientific Progress**
 - Nanostructured MoV catalysts in activation of light alkanes
 - Copper and palladium catalysts in C1 chemistry
 - Silver in partial oxidation reactions
 - Oxygenated ruthenium in CO-oxidation
 - Carbon in catalysis
 - High temperature catalysis research

- I FHI Library / Publications**
- J Patents**
- K Guest-Lectures**
- L External Funds**
 - List of external funds
 - Cluster of Excellence: “Unifying Concepts in Catalysis”
 - European Union: Network of Excellence / NoE IDECAT
 - EnerChem: Nanochemical Concepts for a Sustainable Energy Supply
 - Collaborative Research Centers: SFBs, SFB 546, B2
 - PIRE: Partnership for International Research and Education
- M Teaching Activities**
- N Long Night of Science**
- O Practical Courses**
- P Notes**

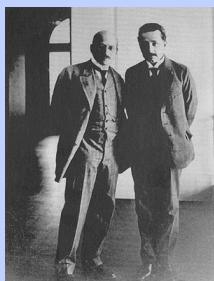


History of the Fritz-Haber-Institut



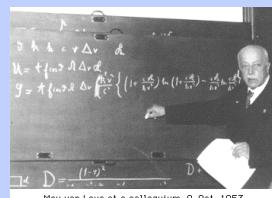
The Kaiser-Wilhelm Institutes for Chemistry (left) and for Physical Chemistry and Electrochemistry (right) --(1913).

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).

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



MAX-PLANCK-GESELLSCHAFT

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

- 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



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

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:

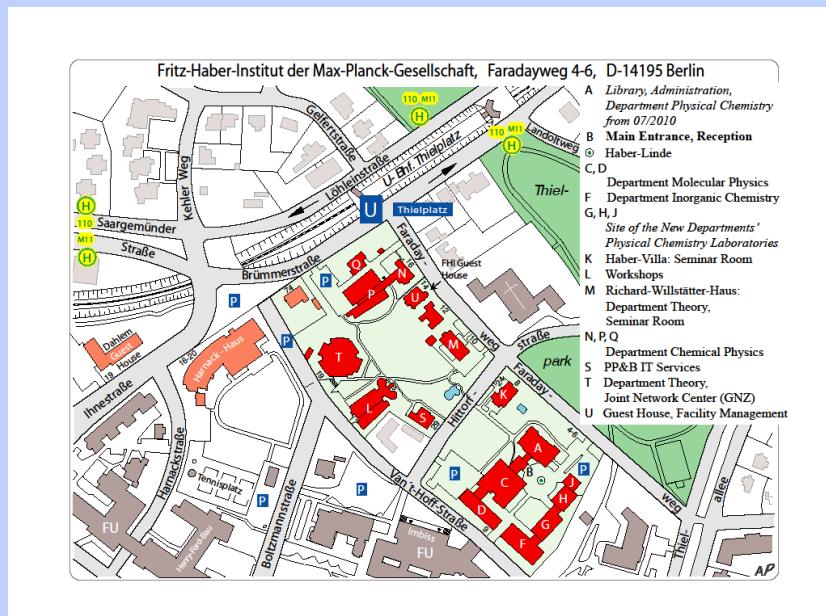
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs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



Fritz-Haber-Institut der Max-Planck-Gesellschaft

Faradayweg 4 – 6

14195 Berlin

Germany



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

B

Preface



Director:

Prof. Dr. Robert Schlögl

Tel: 49 30 8413 4400

Fax: 49 30 8413 4401

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

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



reaction steps with intermediates. The diversity is seen as important to achieve a generalized understanding. However, links between these reactions exist through common elementary steps.

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

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

The strategy of AC involves monitoring the synthesis of catalytically active materials by *in situ* techniques. Through understanding and ultimately controlling the processes of inorganic synthesis occurring during all unit operations of catalyst preparation an optimization is achieved resulting in reproducible and homogeneous active materials. The active centres are envisaged as unique configurations of one or more atoms at or near the surface whose existence is enabled by a surrounding matrix, which is ideally homogeneous.

For chemically and structurally complex systems simplified models are generated that exhibit the essential catalytic characteristics. Suitable specimens (e.g. polycrystalline thin films) are tailor-made for in-situ functional studies aiming at verifying the nature of the active ensemble and adsorbates.

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

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

A project is completed within the scope of the AC department when the scaling of chemical and structural complexity is defined and when a series of observable surface properties are described amenable to experimental and theoretical modelling.



An example for such a completed project is the dehydrogenation of ethylbenzene to styrene over iron oxide catalysts. Although the development of novel systems is not a primary goal, the department seeks to verify and implement its knowledge by the rational synthesis of improved catalysts (example Pd-Ga intermetallic compounds).

Co-operations are essential for the department. 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 and functional understanding are performed. A number of long-standing academic collaborations augment the research portfolio. The department actively contributes to the Berlin research networks within the SFB 546 (transition metal aggregates) and the COE UniCat. Within the MPG the department critically contributes to the research network enerchem and has close cooperations with MPI Mülheim (Schüth), Golm (Antonietti), Dresden (Grin), Mainz (Müllen), Stuttgart (Maier). Larger external projects are the “Pd project” encompassing groups in Austria (Klötzter, Rupprechter) and the US (Zemlianov), the “intermetallics” project conducted with the MPI CPFS (Dresden) (Grin), the contribution of carboscale (Muhler/Wirth) to the national competence network INNOCNT and a PIRE project on renewable energies conducted with a consortium from the US led by J. Dumesic and A. Datye. Within the framework of the EU-NOE IDECAT and our franco-italian (Centi, Garin) collaboration (ELCASS) the department pioneered together with the TU Berlin the awarding of 2 European Doctoral Diplomas emphasizing the multinational character of the degree. This year we started work in the 7. Framework EU Programm Technotubes.

NG



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 alkane activation
18 members

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



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
22 members

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

Group leader: GL Project leader: PL

NANOSTRUCTURES

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

Cu, Pd in C1 chemistry
15 members

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



MICRO- AND NANOSTRUCTURE

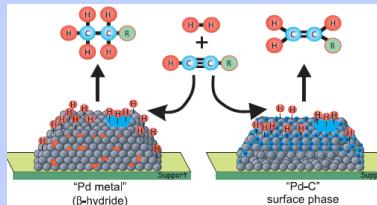
GL: Dr. D. S. Su
Tel: 49 30 8413 5406
E-mail: dangsheng@fhi-berlin.mpg.de

Nanocarbon in energy chemistry
C-OH chemistry / PL: J. P. Tessonnier
TEM service group: Dr. D. S. Su
21 members



Highlights

The Roles of Subsurface Carbon and Hydrogen in Palladium-Catalyzed Alkyne Hydrogenation (*Science* 320 (2008) 86-98)

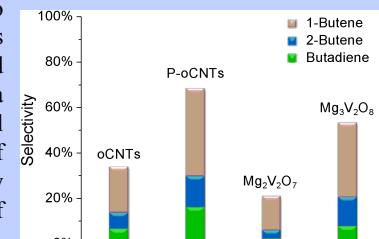


Alkenes can be selectively hydrogenated into alkenes on solid palladium catalysts. This process requires a strong modification of the near-surface region of palladium, in which carbon occupies interstitial lattice sites. In situ X-ray photoelectroscopic measurements under reaction

conditions indicated that much less carbon was dissolved in palladium during unselective, total hydrogenation. Additional studies of hydrogen content using in situ prompt gamma activation analysis, which allowed us to follow the hydrogen content of palladium during catalysis, indicated that unselective hydrogenation proceeds on hydrogen-saturated β -hydride, whereas selective hydrogenation was only possible after decoupling bulk properties from the surface events. Thus, the population of subsurface sites of palladium, by either hydrogen or carbon, governs the hydrogenation events on the surface.

Surface-modified Carbon Nanotubes Catalyze Oxidative Dehydrogenation of n-Butane (*Science* 322 (2008) 73)

Butenes and butadiene, which are useful intermediates for the synthesis of polymers and other compounds, are synthesized traditionally by oxidative dehydrogenation (ODH) of *n*-butane over complex metal oxides. Such catalysts require high O₂ to butane ratios to maintain the catalyst, which leads to unwanted product oxidation. We show that carbon nanotubes (CNTs) with modified surface functionality efficiently catalyze the ODH of *n*-butane to butenes, especially butadiene. (For low O₂ to butane ratios, a high selectivity to alkenes was achieved for periods as long as 100 hours. 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 hydrocarbon.



D/E



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Instrumentation

REACTIVITY

Dr. A. Trunschke



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.

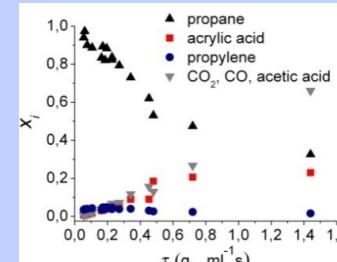
Examples of the technical equipment:

- 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)

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



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



Oxidation of propane to acrylic acid over crystalline MoVTNb oxide at $T = 400^\circ\text{C}$ and different residence times (3% C_3H_8 , 6% O_2 , 40% H_2O , 51% N_2)

ELECTRONIC STRUCTURE AND ADSORPTION

Dr. A. Knop-Gericke



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

ISISS: Soft X-ray station at BESSY :

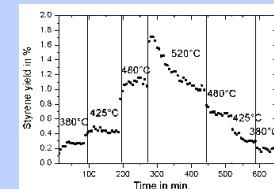


In situ XPS endstation of the ISISS beamline

BESSY and the FHI installed the facility ISISS (Innovative Station for In Situ Spectroscopy). ISISS consists of 3 main parts: a) the in situ XPS endstation, b) a state of the art soft X-ray beamline, and c) a permanent infrastructure on site for experiments with a chemical background. This facility allows measurements of XP and XA spectra in the soft energy range under reaction conditions (mbar pressure range, $T < 600^\circ\text{C}$.) 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).

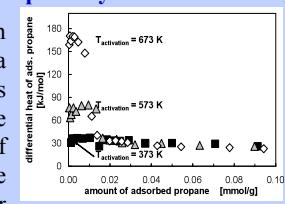
Combined TDS, XPS and reactivity studies of low surface area (model) catalysts

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 $\sim 0.03\text{mg}$ carbon nanotube on highly oriented pyrolytic graphite, HOPG.



Measurement of isotherms & differential heats of adsorption by microcalorimetry

This is a direct method to determine number, strength and energy distribution of the adsorption sites on a catalyst. It allows for measuring the differential heats evolved when known amounts of adsorbed gas probe molecules. The evolved heat is related to the energy of the bonds formed between the adsorbed species and the adsorbent. The data obtained of substantial value for comparing theoretical and experimental hypotheses about reaction pathways.



Differential heats of propane adsorption on differently dehydr. 10wt% $\text{V}_x\text{O}_y/\text{SBA15}$ at 313 K



Instrumentation

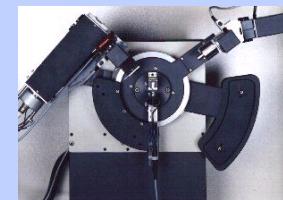
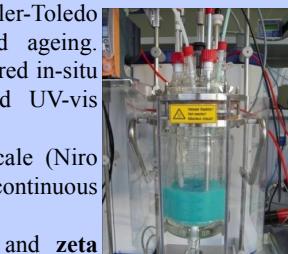
NANOSTRUCTURES

Dr. M. Behrens



Scalable 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 and ageing. 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 technical scale (Niro Minor Mobile, photo) **spray dryer** for rapid and continuous drying and solidification.
- Determination of **particle size distributions** and **zeta potentials** of suspensions (Malvern Zetasizer Nano).
 - **Gloveboxes** for handling of reactive 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)



Contact:

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

MICROSTRUCTURE

Dr. D. S. Su



Contact:

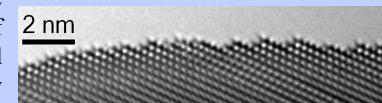
Dr. D. S. Su,
dangsheng@fhi-berlin.mpg.de

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.



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).

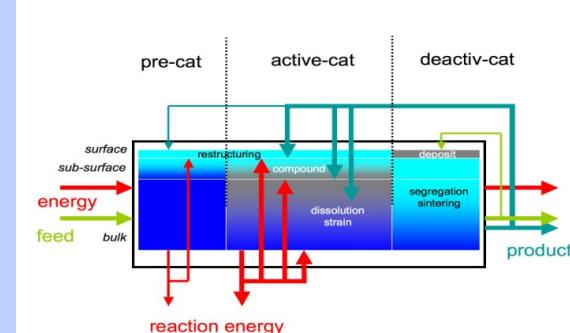
The key feature in the concept is the acknowledgement of the essential role of structural dynamics of an active catalyst (has been evidenced by numerous phenomena) under high performance operation conditions.

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*”

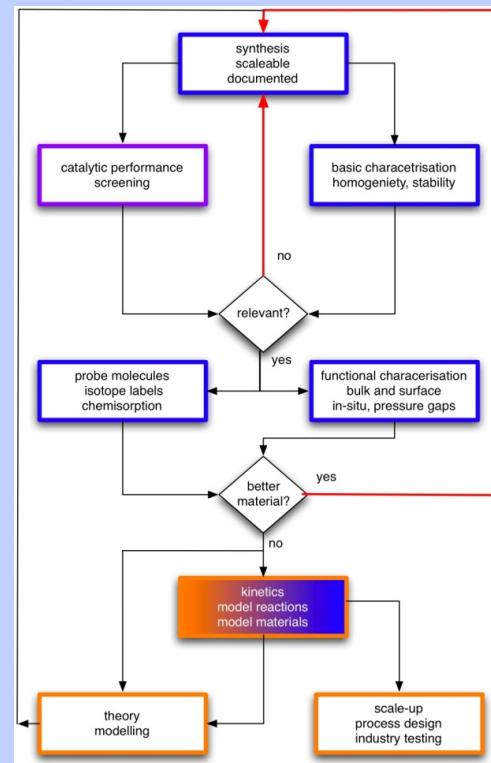
Electronic Structure and Adsorption / Metals: “*Metals in sel oxidation*”

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.

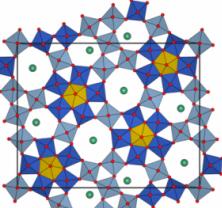
Research concept



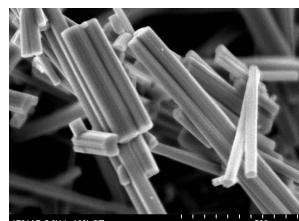
- We study non-equilibrium systems: kinetics is all-important:
 - optimize synthesis
 - document quantitatively the synthesis (in-situ observations)
 - thorough multi-method characterization including reactivity (probe molecule adsorption, thermal methods).
- We are interested in generic effects: always 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

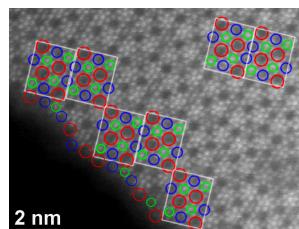
Nanstructured MoV catalysts in activation of light alkanes



1 Structural model of an orthorhombic MoVTeNbO_x phase



2 SEM image of phase-pure M1

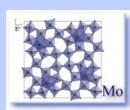


3 HRTEM image of M1 viewed along the $<001>$ zone axis

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

Background and objective

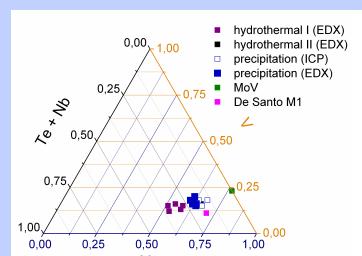
The project is aimed at understanding the factors that primarily determine the reactivity of MoV oxide based catalysts in oxidative dehydrogenation and selective oxidation of C2-C4 alkanes to valuable olefins, unsaturated aldehydes or acids. The research analyzes similarities and specifics of these reactions addressing the effects of (i) molecular structure of active ensembles on the catalyst surface, (ii) structural motives in the catalyst framework, (iii) chemical and structural complexity, (iv) oxidation state of the elements under reaction conditions, (v) the collective electronic properties of the solid, and (vi) the dynamics of the catalyst surface under varying operation conditions. The oxidative dehydrogenation of propane is studied on supported vanadium and molybdenum oxides. Vanadium in turn is an essential constituent of crystalline phases such as vanadium phosphates or molybdenum oxide based bronze structures, which are active in selective oxidation of propane to acrylic acid. Furthermore, the redox system of molybdenum and vanadium is approached from the side of low oxidation states by synthesis of model carbide catalysts and the study of their reactivity in alkane conversions.



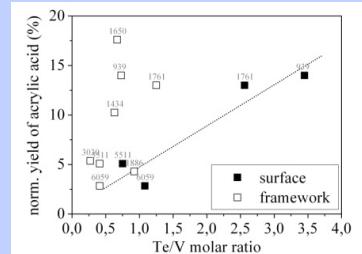
Results

Correlations between structural characteristics, surface termination and catalytic properties in selective oxidation of propane to acrylic acid have been studied over phase-pure MoVTeNbO_x model catalysts consisting of an orthorhombic bronze-like phase denominated as M1 (ICSD 55097, 1-3). The catalysts were prepared by hydrothermal synthesis. The chemical composition of M1 was varied resulting in homogeneous, isostructural materials within the phase width of the M1 structure (4). The yield of acrylic acid increases with decreasing percentage of Mo and increasing molar ratio of Te/V at the surface (5). In-situ XPS experiments revealed an enhanced mobility of Te especially in presence of water vapor. It is proposed that surface restructuring may provoke spatial isolation of vanadium containing active sites.

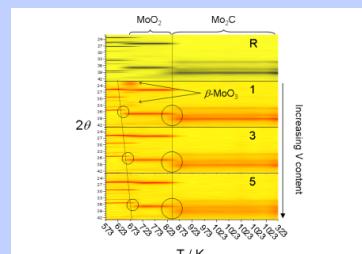
Starting from single phase mixed-metal oxide precursors such as $h\text{-}(\text{Mo},\text{V})\text{O}_3$ structures, M_5O_{14} -type oxides, ($\text{M}=\text{Mo,V,Nb}$), other oxidic bronzes and polyoxometallate species, a range of binary and ternary transition metal carbides with tunable compositions and nanostructures were synthesized by temperature-programmed reaction (6). The catalytic properties of the novel materials are explored in alkane conversions.



4 Phase width of M1



5 Yield of acrylic acid as function of the Te/V ratio in M1



6 Phase transformations during carburization monitored by in-situ XPS

Financial support:
Südchemie AG
BMBF 033R028B

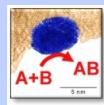


Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

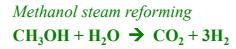
H

Scientific Progress

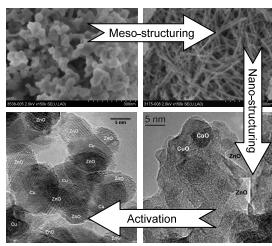
Copper and palladium catalysts in Cl chemistry



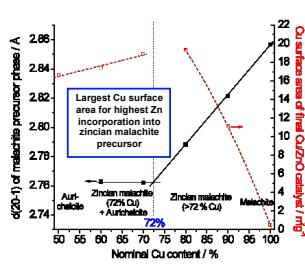
1 Methanol chemistry



2 Preparation of Cu/ZnO



3 Precursor effects



Cu/ZnO/(Al₂O₃) in methanol chemistry

Methanol is already one of the most important basic chemicals in chemical industry. Furthermore, it has the potential to act as a sink for the greenhouse gas CO₂ by chemical fixation. 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 Cu/ZnO/Al₂O₃ is active in both reactions, but increasing demand and variations in feed gas composition require further optimization.

Goal of our work is to understand the industrially applied complex multi-step catalyst synthesis to establish a basis for further more rational optimization. We also develop new methods of preparation using novel precursor systems. Moreover, we aim at finding (micro) structure-performance relations to better understand the nature of catalytically active "methanol copper". Our approach is to comprehensively characterize the nanostructured ensemble present in highly active "real" catalysts using a variety of complementary (in-situ) methods in order to identify relevant features for catalytic performance.

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

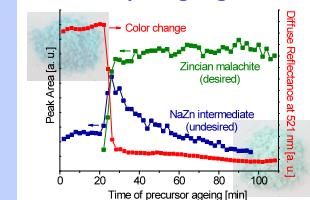
Contact:
Dr. Malte Behrens
behrens@fhi-berlin.mpg.de

Examples of results from our recent work are development of a hierarchical microstructure-directing model for catalyst preparation (2) based on a structure-property relationship found for the precursor phase of the catalyst (3), identification of a crystalline intermediate during precursor ageing by in-situ methods (4) and preparation of a novel catalyst material with very small Cu nano-particles and unique microstructure by application of the microemulsion technique for co-precipitation of CuZnAl hydrotalcite-like precursors (5).

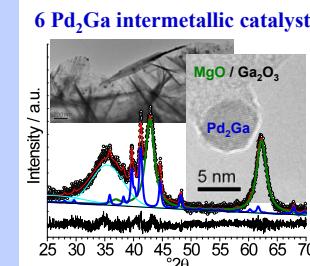
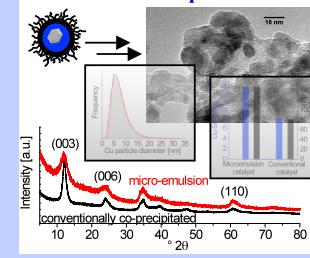
Intermetallic Pd/X catalysts (X=Ga, Zn, ...)

Pd/X model systems have been successfully investigated in our department for several years. In order to transfer the fundamental results obtained on model samples to high performance catalysts, the focus of the work in the Nanostructure group is on exploring co-precipitation methods as routes to Pd-based intermetallic catalysts by application of similar preparative concepts as for Cu/ZnO. As first results, a nanoparticulate Pd₂Ga catalyst supported on MgO/Ga₂O₃ has been developed (6). The average size of the intermetallic particles is below 20 nm, which is impossible to achieve by conventional melt synthesis.

4 Chemistry of ageing



5 Microemulsion precursors



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)

Federal University of Rio de Janeiro, COPPE (M. Schmal)



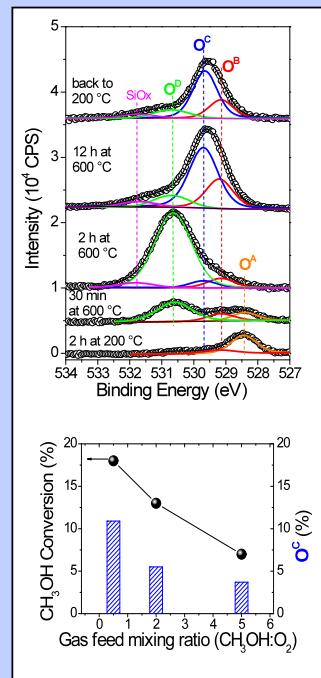
Department of Inorganic Chemistry

Prof. Dr. Robert Schlögl

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 processes 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 catalytic reactions is not clear and sometimes even controversial in the literature.



In order to shed some light on these questions, we have investigated Ag catalysts in equilibrium with gas phase under reaction conditions with pressures in the mbar range by *in situ* XPS.

The upper panel in the figure shows the oxygen 1s spectra of a Ag foil at different temperatures relevant for ethylene (200 °C) and methanol oxidation (600 °C) reactions. Briefly, four different oxygen species were identified with distinct binding energies, thermal stability and associated formation of ionic Ag.

The different thermal behavior and spectroscopic characteristics of these species arises from their dissimilar bonding with the Ag, which leads to different roles in oxidation reactions

For instance, under methanol oxidation reaction at 600 °C, the species named O^a is not present, O^b nearly vanishes, and O^d does not change. On the other hand, the species O^c, which appears only at high temperatures under pure O₂, present a good correlation with the methanol conversion, as can be seen in the lower panel, which suggests its role as a relevant site for this reaction.

Contact:

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

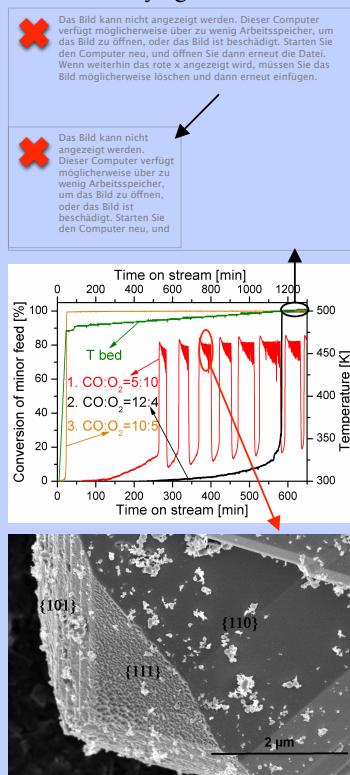


Scientific Progress

Oxygenated Ruthenium in oxidation reactions

CO-oxidation on oxygenated 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 calcined RuO₂ which exhibits an "octagonal" habit and is completely inactive in the CO-oxidation. Consecutive experiments with varying feed composition (100 Nml/min total flow) show long induction periods in net-oxidizing and net-reducing feed. After activation in net-oxidizing feed still a long induction period is necessary in net-reducing feed. Oscillations occur only in the net-oxidizing feed (figure 2). While roughening of apical facets occur in net-reducing feed the net-oxidizing feed leads to faceting of apical surfaces (SEM, figs. 1 and 3, respectively).

Chlorine is one of the essential basic chemicals of the chemical industry, because a large portion of processes require at certain steps chlorine. On the large scale, it is produced using electrolysis of NaCl (or HCl) solutions and very recently by the heterogeneous gas phase oxidation of HCl (Deacon Process). Interestingly both processes rely on RuO₂-based materials! Currently, we are involved in characterizing materials used in the above processes and find that the surface-near region of the samples undergoes strong modification (phase changes, segregation) during reaction. We will apply *in situ* methods to identify the active state of "RuO₂" and to suggest possible routes to enhance reactivity or substitute Ru with cheaper alternatives.



Contact:

Dr. D. Rosenthal, Dr. D. Teschner
dirkrose@fhi-berlin.mpg.de, teschner@fhi-berlin.mpg.de



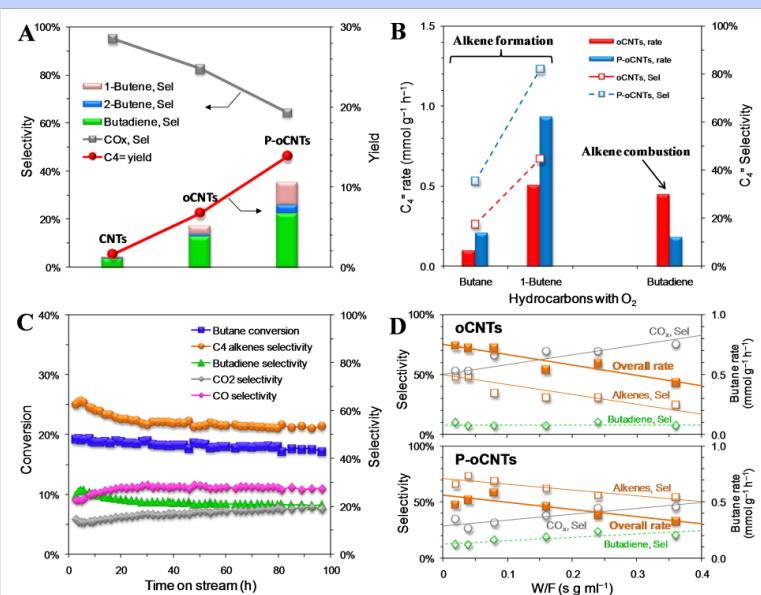
Scientific Progress

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))



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

H



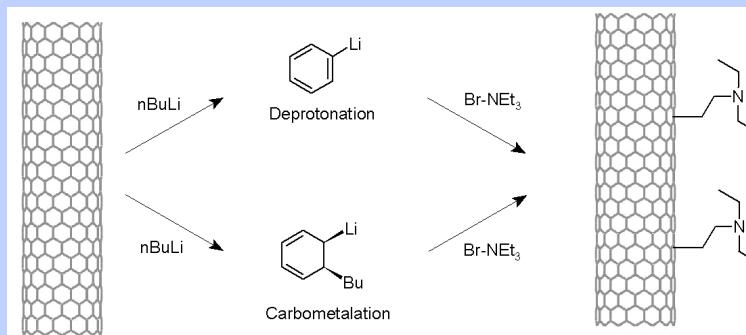
Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

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.

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. 2

Contact:
Dr. Raimund Horn
horn_r@fhi-berlin.mpg.de

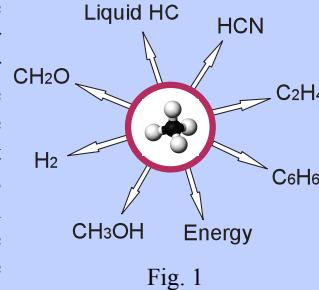
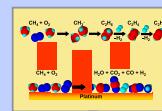


Fig. 1

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.



Results: The methane oxidation on Pt has been investigated both, on $\alpha\text{-Al}_2\text{O}_3$ foam catalysts coated with Pt nanoparticles (reticulated pore structure, $d_{\text{pore}} \approx 300\text{-}500\mu\text{m}$, 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 H_2 , CO , H_2O and CO_2 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. CO_2 reforming is not observed.



Fig. 3

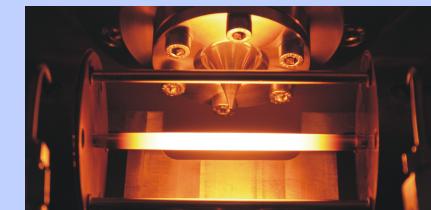
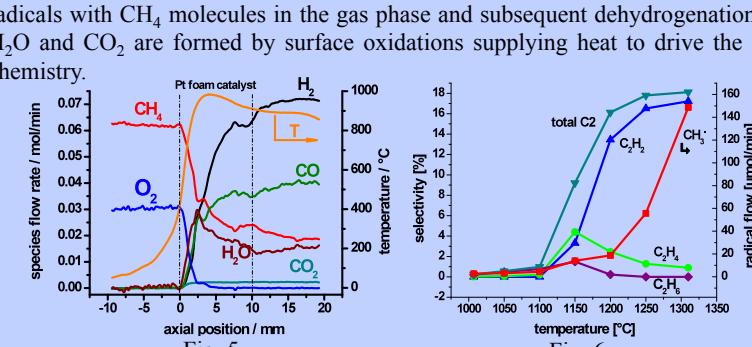


Fig. 4



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





FHI Library

collects special literature covering the research fields of the institute. The library has about 15.500 monographs and 32.000 journal volumes. In addition, the library offers about 30.000 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).



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.

External Collaborations

The library cooperates with various institutions, for example with:

- libraries of other Max Planck Institutes
- libraries of Fraunhofer Institutes and Institutes of the Helmholtz Society
- university libraries in Berlin and Brandenburg
- local bookshops and international publishers

Open Access

@ Max Planck Society

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 1400 open access documents from FHI scientists are available on the eDoc Server.

In July 2009 the library arranged a seminar on ‘Open Access and Author Rights’ (http://www.fhi-berlin.mpg.de/bib/news/oa_authorrights.epl).

The library attended with some activities on the International Open Access Week in October 2009 (<http://www.openaccessweek.org/>).



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.

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



Department of Inorganic Chemistry

Prof. Dr. Robert Schlägl

Publications

The following publication list 2007 – Nov. 2009
is generated by eDoc.
<http://edoc.mpg.de>

Max Planck Society
eDoc Server



2007

2007

- 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. Schlögl and M. Salmeron: In situ x-ray photoelectron spectroscopy studies of gas-solid interfaces at near-ambient conditions. In: Materials Research Society Bulletin **32**, 12, 1022-1030 (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. In: Catalysis Today **124**, 1-2, 71-79 (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. In: Physical Chemistry Chemical Physics **9**, 27, 3648-3657 (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. In: 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. In: 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. In: 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. In: 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. In: 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. In: 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. In: Advanced Functional Materials **17**, 16, 3159-3169, Seq. No.: 200601142 (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. In: 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/TiO_x catalysts - influence of the material gap. In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 110-112.

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. In: Jahresbericht 2007, Annual Report 1. (Eds.) Hasylab at Desy. Publisher Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Hamburg, Seq. No.: 1 (2007) 513-514.

Djerdj, I., G. Garnweimer, D. S. Su and M. Niederberger: Morphology-Controlled Nonaqueous Synthesis of Anisotropic Lanthanum Hydroxide Nanoparticles. In: 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. In: 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. In: Journal of Catalysis **246**, 1, 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. In: 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. In: Physical Chemistry Chemical Physics **9**, 4, 533-540 (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. In: Physical Chemistry Chemical Physics **9**, 533-540 (2007).

Gabasch, H., A. Knop-Gericke, R. Schlögl, W. Unterberger, K. Hayek and B. Klötzer: Ethene Oxidation on Pd(111): Kinetic Hysteresis Induced by Carbon Dissolution. In: Catalysis Letters **119**, 3-4, 191-198 (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. In: Journal of Power Sources **172**, 2, 666-675 (2007).



Publications

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

Hess, C., G. Tzolova-Müller and R. Herbert: Influence of water on the structure and dispersion of SBA-15 supported vanadia model catalysts studied by multi in situ spectroscopy. (Deutsche Zeolithtagung,, 2007-03, Leipzig [Germany]).

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

Imbihl, R., A. Scheibe, Y. F. Zeng, S. Günter, R. Krahnert, 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. In: *Physical Chemistry Chemical Physics* **9**, 27, 3522-3540, Seq. No.: 700866 (2007).

Janetzky, M., E. Rödel, C. Pietzonka, U. Müller, T. Ressler and B. Harbrecht: The valence problem of Pd/Br₂Te. In: *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. Adschari: Structural and morphological characterization of cerium oxide nanocrystals prepared by hydrothermal synthesis. In: *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. In: *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. In: *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. In: *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. In: *Applied Catalysis b: Environmental* **70**, 1-4, 111-118 (2007).

Max Planck Society
eDoc Server



2007

Kornelak, P., B. Borzęcka-Prokop, L. Lityńska-Dobrzańska, J. B. Wagner, D. S. Su, J. Camra and A. Weselucha-Birczyńska: The physicochemical properties of rutile-supported V-O-Mo catalyst. In: *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. In: *Science and Technology of Advanced Materials* **8**, 420-427 (2007).

Krahnert, R. and M. Baerns: Morphology changes of Pt-foil catalyst induced by temperature-controlled ammonia oxidation near atmospheric pressure. In: *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. In: *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. In: *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. In: *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. In: *Carbon* **45**, 8, 1622-1627 (2007).

Mastaler, A., A. Patzko, B. Frank, R. Schomäcker, T. Ressler and R. Schlögl: Steam reforming of methanol over Cu/ZnO/Al₂O₃ modified with hydrotalcites. In: *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. In: *Physical Chemistry Chemical Physics* **9**, 30, 4018-4025 (2007).

Paál, Z., N. Györffy, A. Woitsch, L. Tóth, I. Bakos, S. Szabó, U. Wild and R. Schlögl: Preparation, physical characterization and catalytic properties of unsupported Pt-Rh catalyst. In: *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. In: *European Physical Journal D* **43** (2007) 197-200.

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.

I



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Publications

2007

Max Planck Society
eDoc Server

- Perathoner, S., P. Lanzaflame, G. Centi, F. C. Jentoft, T. V. Venkov and R. Schlögl:* Nature of corona in TiO-SBA15-like mesoporous nanocomposite. In: From Zeolites to Porous MOF Materials - The 40th Anniversary of International Zeolite Conference, Proceedings of the 15th International Zeolite Conference. (Eds.) Xu, R.; Gao, Z.; Chen, J.; Yan, W. Studies in Surface Science and Catalysis **170 Part 2**. (2007) 1788-1795.
- 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. In: Catalysis Today **122**, 3-13 (2007).
- Pestryakov, A. N., N. Bogdanchikova, A. Simakov, I. Tuzovskaya, F. C. Jentoft, M. Farias and A. Díaz:* Catalytically active gold clusters and nanoparticles for CO oxidation. In: 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. In: Catalysis Today **119**, 187-193 (2007).
- Pozdnyakova-Tellinger, O., D. Teschner, J. Kröhnert, F. C. Jentoft, A. Knop-Gericke, R. Schlögl and A. Woitsch:* Surface water assisted preferential CO oxidation on Pt/CeO_x catalyst. In: 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. Winterlin, B. Kubias, B. Jacobi and R. Schlögl:* High-pressure STM of the interaction of oxygen with Ag(111). In: 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 H₂[PV_xMo_yO_z] partial oxidation catalyst. In: 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 Mo₆O₁₃-type structure. In: Catalysis Today **126**, 1-2, 112-118 (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)_xO_y selective oxidation catalysts. In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 83-85.

eDoc

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. In: 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. In: Journal of Porous Materials **14**, 3, 263-272 (2007).

Siebely, U.: Auf der Green Road to Open Access. Ein Praxisbericht aus dem Fritz-Haber-Institut der Max-Planck-Gesellschaft. In: Integrität wissenschaftlicher Publikationen in der Digitalen Bibliothek. (Eds.) Havemann, Frank; Parthey, Heinrich; Umstätter, Walther. Wissenschaftsforschung Jahrbuch **2007**. Gesellschaft für Wissenschaftsforschung, Berlin (2007) 121-135.

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. In: 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. In: 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. In: 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. In: Microporous and Mesoporous Materials **100**, 1-3, 356-360 (2007).

Teschner, D., E. Vass, S. Zafeiratos, P. Schnörch, M. Hävecker, A. Knop-Gericke, H. Sauer, J. Kröhnert, F. C. Jentoft, R. Schlögl, G. Hutchings, O. Pozdnyakova-Tellinger, K. Lázár and A. Woitsch: Preferential oxidation of CO over supported and alloy catalysts in H-rich gas for fuel cell application. In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 89-91.

Teschner, D., A. Woitsch, O. Pozdnyakova-Tellinger, J. Kröhnert, E. Vass, M. Hävecker, S. Zafeiratos, P. Schnörch, F. C. Jentoft, A. Knop-Gericke and R. Schlögl: Partial pressure dependent in-situ spectroscopic study on the preferential CO oxidation in hydrogen (PROX) over Pt/ceria catalysts. In: Journal of Catalysis **249**, 318-327 (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. In: Chemistry of Materials **19**, 17, 4205-4212 (2007).



Publications

2007

Max Planck Society
eDoc Server

- Vass, E. M., D. Teschner, M. Hävecker, S. Zafeiratos, P. Schnörrch, A. Knop-Gericke and R. Schlögl: Dehydrogenation and Oxidative Dehydrogenation of n-Butane using Vanadium Based Catalysts: an in situ XPS study. In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 94-96.
- Venkov, T. V., C. Hess and F. C. Jentoft: Redox Properties of Vanadium Ions in SBA-15 Supported Vanadium Oxide: an FTIR Spectroscopic Study. In: Langmuir **23**, 4, 1768-1777 (2007).
- Vernovskaja, 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 catalysts during ethane dehydrogenation experiments. In: Surface Science **601**, 1, 30-43 (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. In: Chemistry of Materials **19**, 11, 2894-2897 (2007).
- Wu, Y., H.-M. Liu, B.-Q. Xu, Z.-L. Zhang and D. S. Su: Single-Phase Titania Nanocrystallites and Nanofibers from Titanium Tetrachloride in Acetone and Other Ketones. In: Inorganic Chemistry **46**, 12, 5093-5099 (2007).
- Zafeiratos, S., V. I. Bukhtiyarov, M. Hävecker, D. Teschner, E. Vass, P. Schnörrch, G. Weinberg, A. Knop-Gericke and R. Schlögl: Ethylene epoxidation over copper-silver bimetallic catalyst: surface characterisation under reaction conditions. In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 71-73.
- Zemlyanov, D., H. Gabasch, B. Klötzer, A. Knop-Gericke and R. Schlögl: Kinetics of palladium oxidation and methane oxidation on Pd(111) and (110). In: BESSY Annual Report 2006. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2007) 121-123.
- Zenkovets, G. A., G. N. Kryukova, V. Y. Gavrilov, S. V. Tsibulya, V. A. Anufrienko, T. A. Larina, D. F. Khabibulin, O. B. Lapina, E. Rödel, A. Trunschke, T. Ressler and R. Schlögl: The structural genesis of a complex (MoVW)_xO_y oxide during thermal treatments and its redox behavior at elevated temperatures. In: Materials Chemistry and Physics **103**, 2-3, 295-304 (2007).
- Zhang, J., M. Comotti, F. Schütt, R. Schlögl and D. S. Su: Commercial Fe- or Co-Containing Carbon Nanotubes as Catalysts for NH₃ Decomposition. In: 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. In: Angewandte Chemie International Edition **46**, 38, 7319-7323 (2007).
- Zhang, Z.: Surface effects in the energy loss near edge structure of different cobalt oxides. In: Ultramicroscopy **107**, 8, 598-603 (2007).

eDoc

2008

- Akcakayiran, D., D. Mauder, C. Hess, T. K. Sievers, D. G. Kurth, I. Shenderovich, H. H. Limbach and G. H. Findenegg: Carboxylic Acid-Doped SBA-15 Silica as a Host for Metallo-supramolecular Coordination Polymers. In: Journal of Physical Chemistry B **112**, 46, 14637-14647 (2008).
- Ampli, C., R. Passalacqua, S. Perathoner, G. Centi, D. S. Su and G. Weinberg: Synthesis of TiO_x Thin Films: Relationship Between Preparation Conditions and Nanostructure. In: Topics in Catalysis **50**, 1-4, 133-144 (2008).
- Arrigo, R., M. Hävecker, R. Schlögl and D. S. Su: Dynamic surface rearrangement and thermal stability of nitrogen functional groups on carbon nanotubes. In: Chemical Communications, 40, 4891-4893 (2008).
- Baerns, M. and E. V. Kondratenko: Oxidative coupling of methane. In: Handbook of Heterogeneous Catalysis. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 3010-3023.
- Beato, P., R. Krahnert, S. Engelschalt, T. Frank and R. Schlögl: A micro-structured quartz reactor for kinetic and in situ spectroscopic studies in heterogeneous catalysis. In: Chemical Engineering Journal **135**, Suppl. 1, S247-S253 (2008).
- Behrens, M. and S. Kühl: Hydrotalcit-artige (Cu,Zn,Al)-Hydroxykarbonate als Vorstufen für Kupferkatalysatoren in der Methanolchemie. In: Zeitschrift für Anorganische und Allgemeine Chemie **634**, 11, 2014-2014 (2008).
- Behrens, M., J. Wontcheu, R. Kiebach and W. Bensch: Tuning the Magnetic Properties of Li_xCrTi_{1-x}Se_x (0.03≤x≤0.7) by Directed Deintercalation of Lithium. In: Chemistry - A European Journal **14**, 16, 5021-5029 (2008).
- Berthoud, R., A. Baudouin, B. Fenet, W. Lukens, K. Pelzer, J.-M. Basset, J.-P. Candy and C. Copéret: Mononuclear ruthenium hydride species versus ruthenium nanoparticles: the effect of silane functionalities on silica surfaces. In: Chemistry - A European Journal **14**, 12, 3523-3526 (2008).
- Berthoud, R., P. Delichere, D. Gajan, W. Lukens, K. Pelzer, J.-M. Basset, J.-P. Candy and C. Copéret: Hydrogen and oxygen adsorption stoichiometries on silica supported ruthenium nanoparticles. In: Journal of Catalysis **260**, 2, 387-391 (2008).
- Bojdys, M. J., J. O. Müller, M. Antonietti and A. Thomas: Ionothermal Synthesis of Crystalline, Condensed, Graphitic Carbon Nitride. In: Chemistry - A European Journal **14**, 27, 8177-8182 (2008).
- Bron, M., D. Teschner, U. Wild, B. Steinhauer, A. Knop-Gericke, C. Volckmar, A. Wootsch, R. Schlögl and P. Claus: Oxygen-induced activation of silica supported silver in acrolein hydrogenation. In: Applied Catalysis A **341**, 127-132 (2008).
- Cai, Y., T. L. Wong, S. K. Chan, I. K. Sou, D. S. Su and N. Wang: Growth behaviors of ultrathin ZnSe nanowires by Au-catalyzed molecular-beam epitaxy. In: Applied Physics Letters **93**, 23, 233107-1-233107-3 (2008).

Publications

2008

Max Planck Society
eDoc Server

- Celaya Sanfiz, A., T. W. Hansen, F. Girgdiess, O. Timpe, E. Rödel, T. Ressler, A. Trunschke and R. Schlögl: Preparation of phase-pure M1 MoVTeNb oxide catalysts by hydrothermal synthesis - Influence of reaction parameters on structure and morphology. In: *Topics in Catalysis* **50**, 1-4, 19-32 (2008).
- Celaya Sanfiz, A., T. W. Hansen, A. Sakthivel, A. Trunschke, R. Schlögl, A. Knoester, H. H. Brongersma, M. H. Looi and S. B. Abd Hamid: How important is the (001) plane of M1 for selective oxidation of propane to acrylic acid?. In: *Journal of Catalysis* **258**, 35-43 (2008).
- Clavel, G., M.-G. Willinger, D. Zitoun and N. Pinna: Manganese-Doped Zirconia Nanocrystals. In: *European Journal of Inorganic Chemistry*, 6, 863-868 (2008).
- Conant, T., A. M. Karim, V. Lebarbier, Y. Wang, F. Girgdiess, R. Schlögl and A. Datye: Stability of bimetallic Pd-Zn catalysts for the steam reforming of methanol. In: *Journal of Catalysis* **257**, 1, 64-70 (2008).
- Dinse, A., B. Frank, C. Hess, D. Habel and R. Schomäcker: Oxidative dehydrogenation of propane over low-loaded vanadia catalysts: Impact of the support material on kinetics and selectivity. In: *Journal of Molecular Catalysis A: Chemical* **289**, 1-2, 28-37 (2008).
- Dinse, A., A. Ozarowski, C. Hess, R. Schomäcker and K.-P. Dinse: Potential of High-Frequency EPR for Investigation of Supported Vanadium Oxide Catalysts. In: *Journal of Physical Chemistry C* **112**, 45, 17664-17671 (2008).
- Endo, M., K. Takeuchi, Y. A. Kim, K. C. Park, T. Ichiki, T. Hayashi, T. Fukuyo, S. Iinou, D. S. Su, M. Terrones and M. S. Dresselhaus: Simple Synthesis of Multiwalled Carbon Nanotubes from Natural Resources. In: *ChemSusChem* **1**, 10, 820-822 (2008).
- Fischer, A., P. Makowski, J. O. Müller, M. Antonietti, A. Thomas and F. Goettmann: High-surface-area TiO₂ and TiN as catalysts for the C-C coupling of alcohols and ketones. In: *ChemSusChem* **1**, 5, 444-449 (2008).
- url: <http://dx.doi.org/10.1002/cssc.200800019>
- Fischer, A., J. O. Müller, M. Antonietti and A. Thomas: Synthesis of Ternary Metal Nitride Nanoparticles Using Mesoporous Carbon Nitride as Reactive Template. In: *ACS Nano* **2**, 12, 2489-2496 (2008).
- Föttinger, K., R. Schlögl and G. Rupprechter: The mechanism of carbonate formation on Pd-Al₂O₃ catalysts. In: *Chemical Communications*, 3, 320-322 (2008).
- Fu, Q., G. Weinberg and D. S. Su: Selective filling of carbon nanotubes with metals by selective washing. In: *New Carbon Materials* **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. In: *Applied Surface Science* **254**, 2748-2754 (2008).

2008

eDoc

- Gajović, A., N. Tomašić, I. Djerdj, D. S. Su and K. Furić: Influence of mechanochemical processing to luminescence properties in Y₂O₃ powder. In: *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. In: *Physical Review B* **77**, 7, 075407-1-075407-2 (2008).
- Günther, S., A. Scheibe, H. Bluhm, M. Hävecker, E. Kleimenov, A. Knop-Gericke, R. Schlögl and R. Imbihl: In Situ X-ray Photoelectron Spectroscopy of Catalytic Ammonia Oxidation over a Pt(533) Surface. In: *Journal of Physical Chemistry C* **112**, 39, 15382-15393 (2008).
- Holena, M. and M. Baerns: Computer-Aided Design of Solid 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) 66-81.
- 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. In: *Journal of Catalysis* **255**, 2, 144-152 (2008).
- Huc, V. and K. Pelzer: A new specifically designed calix[8]arene for the synthesis of functionalized, nanometric and subnanometric Pd, Pt and Ru nanoparticles. In: *Journal of Colloid and Interface Science* **318**, 1, 1-4 (2008).
- Hu, Y.-S., R. Demir-Cakan, M.-M. Titirici, J.-O. Müller, R. Schlögl, M. Antonietti and J. Maier: Superior Storage Performance of a Si@SiO_x/C Nanocomposite as Anode Material for Lithium-Ion Batteries. In: *Angewandte Chemie International Edition* **47**, 9, 1645-1649 (2008).
- Jentoft, F. C.: Oxo-Anion Modified Oxides. In: *Handbook of Heterogeneous Catalysis*. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 262-278.
- Kaluza, S., M. K. Schröter, R. Naumann d'Alnoncourt, T. Reinecke and M. Muhler: High Surface Area ZnO Nanoparticles via a Novel Continuous Precipitation Route. In: *Advanced Functional Materials* **18**, 22, 3670-3677 (2008).
- Karge, H. G.: Acidity and Basicity. In: *Handbook of Heterogeneous Catalysis*. 2nd Edition. (Eds.) Ertl, Gerhard; Knözinger, Helmut; Schüth, Ferdi; Weitkamp, Jens. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008) 1069-1122.
- 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. In: *Applied Catalysis B: Environmental* **84**, 3-4, 497-504 (2008).



Publications

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. In: *Catalysis Today* **137**, 2-4, 273-277 (2008).

Kovnir, K., D. Teschner, M. Armbrüster, P. Schnörrch, M. Hävecker, A. Knop-Gericke, Y. Grin and R. Schlögl: Pinning the catalytic centre: A new concept for catalysts development. In: BESSY Highlights 2007. (Eds.) Kai Godehusen. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2008) 22-23.

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

Kurr, P., I. Kasatkin, F. Girgsdies, A. Trunschke, R. Schlögl and T. Ressler: Microstructural characterization of Cu/ZnO/Al₂O₃ catalysts for methanol steam reforming—A comparative study. In: *Applied Catalysis A: General* **348**, 2, 153-164 (2008).

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

Liu, X., D. S. Su and R. Schlögl: Oxidative dehydrogenation of 1-butene to butadiene over carbon nanotube catalysts. In: *Carbon* **46**, 547-549 (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. In: *Materials Letters* **62**, 8-9, 1297-1301 (2008).

Mattevi, C., C. T. Wirth, S. Hofmann, R. Blume, M. Cantoro, C. Ducati, C. Cepek, A. Knop-Gericke, S. Milne, C. Castellarin-Cudia, S. Dolafi, A. Goldoni, R. Schlögl and J. Robertson: In-situ X-ray Photoelectron Spectroscopy Study of Catalyst-Support Interactions and Growth of Carbon Nanotube Forests. In: *Journal of Physical Chemistry C* **112**, 32, 12207-12213 (2008).

Moehmel, S., N. Steinfeldt, S. Engelschalt, M. Holena, S. Kolf, M. Baerns, U. Dingerdissen, 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. In: *Applied Catalysis A: General* **334**, 1-2, 73-83 (2008).

Muhamad, E. N., R. Irmawati, Y. H. Tautiq-Yap, A. H. Abdullah, B. Kniep, F. Girgsdies and T. Ressler: Comparative study of Cu/ZnO catalysts derived from different precursors as a function of aging. In: *Catalysis Today* **131**, 1-4 (2008) 118-124.

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. In: *Journal of Catalysis* **258**, 1, 210-218 (2008).

Max Planck Society
eDoc Server



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. In: *Journal of Catalysis* **258**, 1, 219-227 (2008).

Rauwel, E., G. Clavel, M.-G. Willinger, P. Rauwel and N. Pinna: Non-Aqueous Routes to Metal Oxide Thin Films by Atomic Layer Deposition. In: *Angewandte Chemie International Edition* **47**, 19, 3592-3595 (2008).

Revay, Z., T. Belgya, L. Szentmiklosi, Z. Kis, A. Woitsch, D. Teschner, M. Swoboda, R. Schlögl, J. Borsodi and R. Zepernick: In Situ Determination of Hydrogen Inside a Catalytic Reactor Using Prompt γ [Gamma] Activation Analysis. In: *Analytical Chemistry* **80**, 15, 6066-6071 (2008).

Rinaldi, A., J. Zhang, J. Mizera, F. Girgsdies, N. Wang, S. B. Abd Hamid, R. Schlögl and D. S. Su: Facile synthesis of carbon nanotube/natural bentonite composites as a stable catalyst for styrene synthesis. In: *Chemical Communications*, 48, 6528-6530 (2008).

Salmeron, M. and R. Schlögl: Ambient Pressure Photoelectron Spectroscopy: A new tool for surface science and nanotechnology. In: *Surface Science Reports* **63**, 4, 169-199 (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.: Energy: Fuel for thought. In: *Nature Materials* **7**, 10, 772-774 (2008).

Schlögl, R.: Wie man Moleküle auf Trab bringt. Das Fritz-Haber-Institut der MPG. In: *Europa Report* **118**, (2008).

Schlögl, R. and F. Schüth: Transport- und Speicherformen für Energie. In: *Die Zukunft der Energie: Die Antwort der Wissenschaft*. Ein Report der Max-Planck-Gesellschaft. Gruss, P.; Schüth, F. C.H.Beck oHG, Munich [Germany] (2008) 246-281.

Schnörrch, P., E. Vass, S. Zafeiratos, D. Teschner, M. Hävecker, A. Knop-Gericke and R. Schlögl: In situ XPS study on Mo-based oxides under conditions of selective oxidation of C3 hydrocarbons. In: *BESSY Annual Report 2007*. (Eds.) Godehusen, Kai. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2008) 90-91.

Schwarz, O., B. Frank, C. Hess and R. Schomäcker: Characterisation and catalytic testing of VO/Al₂O₃ catalysts for microstructured reactors. In: *Catalysis Communications* **9**, 2, 229-233 (2008).

Publications

2008

Max Planck Society
eDoc Server

- Schwarz, O., D. Habel, O. Ovsitsser, E. V. Kondratenko, C. Hess, R. Schomäcker and H. Schubert: Impact of preparation method on physico-chemical and catalytic properties of VO_x/γ-Al₂O₃ materials. In: Journal of Molecular Catalysis A: Chemical **293**, 1-2, 45-52 (2008).
- Subbotina, I. R., V. B. Kazansky, F. C. Jentoft and R. Schlögl: IR extinction coefficients as a criterion for chemical activation upon adsorption: propene interaction with cationic forms of γ zeolite. In: Studies in Surface Science and Catalysis **174**, Part 2, 849-852 (2008).
- Su, D. S., X. Chen, X. Liu, J. J. Delgado, R. Schlögl and A. Gajović: Mount-Etna-Lava-Supported Nanocarbons for Oxidative Dehydrogenation Reactions. In: 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. In: Angewandte Chemie International Edition **47**, 27, 5005-5008 (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. In: 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. In: Environmental Science and Technology **42**, 5, 1761-1765 (2008).
- Teschner, D., J. Borsodi, E. Vass, S. Zafeiratos, P. Schnörch, M. Hävecker, A. Knop-Gericke, Z. Révay, A. Wootsch and R. Schlögl: The role of subsurface chemistry in Palladium catalyzed hydrogenation. In: BESSY Annual Report 2007. (Eds.) Godehusen, Kai. Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Berlin (2008) 60-62.
- 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. In: Science **320**, 5872, 86-89 (2008).
- Teschner, D., Z. Revay, J. Borsodi, M. Hävecker, A. Knop-Gericke, R. Schlögl, D. Milroy, S. D. Jackson, D. Torres and P. Sautet: Understanding Palladium Hydrogenation Catalysts: When the Nature of the Reactive Molecule Controls the Nature of the Catalyst Active Phase. In: Angewandte Chemie **120**, 48, 9414-9418 (2008).
- Thomas, A., A. Fischer, F. Goettmann, M. Antonietti, J. O. Müller, R. Schlögl and J. M. Carlsson: Graphitic carbon nitride materials: variation of structure and morphology and their use as metal-free catalysts. In: Journal of Materials Chemistry **18**, 41, 4893-4908 (2008).
- Vass, E. M., M. Hävecker, S. Zafeiratos, D. Teschner, A. Knop-Gericke and R. Schlögl: The role of carbon species in heterogeneous catalytic processes: an in situ soft x-ray photoelectron spectroscopy study. In: Journal of Physics: Condensed Matter **20**, 18, 184016 1-184016 13 (2008).

2008

eDoc

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

Widi, R. K., S. B. Abd Hamid and R. Schlögl: Effect of diluent and reaction parameter on selective oxidation of propane over MoVTeNb catalyst using nanoflow catalytic reactor. In: Journal of Natural Gas Chemistry **17**, 2, 130-134 (2008).

Willinger, M.-G., G. Neri, E. Rauwel, A. Bonavita, G. Micali and N. Pinna: Vanadium Oxide Sensing Layer Grown on Carbon Nanotubes by a New Atomic Layer Deposition Process. In: Nano Letters **8**, 12, 4201-4204 (2008).

Xu, Y.-J., G. Weinberg, X. Liu, O. Timpe, R. Schlögl and D. S. Su: Nanoarchitecturing of Activated Carbon: New Facile Strategy for Chemical Functionalization of the Surface of Activated Carbon. In: Advanced Functional Materials **18**, 22, 3613-3619 (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. In: 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. In: 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. In: Nano Letters **8**, 9, 2738-2743 (2008).

2009

Arrigo, R., M. Hävecker, S. Wrabetz, R. Blume, M. Lerch, A. Knop-Gericke, R. Schlögl and D. S. Su: Tuning the acid/base properties of nanocarbon by functionalization via amination. In: Journal of the American Chemical Society, submitted (2009).

Baerns, M. and M. Holena: COMBINATORIAL DEVELOPMENT OF SOLID CATALYTIC MATERIALS Design of High-Throughput Experiments, Data Analysis, Data Mining. Catalytic Science Series 7. ICP Imperial College Press, London [UK] (2009) 180 pages p.

Bégin, D., G. Ulrich, J. Amadou, D. S. Su, C. Pham-Huu and R. Ziessl: Oxidative dehydrogenation of 9,10-dihydroanthracene using multi-walled carbon nanotubes. In: Journal of Molecular Catalysis A: Chemical **302**, 119-123 (2009).

Behrens, M.: Meso- and nano-structuring of industrial Cu/ZnO/(Al₂O₃) catalysts. In: Journal of Catalysis **267**, 1, 24-29 (2009).

Behrens, M., F. Girgsdies, A. Trunschke and R. Schlögl: Minerals as model compounds for Cu/ZnO catalyst precursors: Structural and thermal properties and IR spectra of mineral and synthetic (zincian) malachite, rosasite and aurichalcite and a catalyst precursor mixture. In: European Journal of Inorganic Chemistry, 1347-1357 (2009).



Publications

2009

Max Planck Society
eDoc Server

Behrens, M., I. Kasatkin, S. Kühl and G. Weinberg: Phase-pure Cu_xZn_yAl Hydrotalcites-like Materials as Precursors for Copper-rich Cu/ZnO/Al₂O₃ Catalysts. In: Chemical Materials, submitted (2009).

Cavalleri, M., K. Hermann, A. Knop-Gericke, M. Hävecker, R. Herbert, C. Hess, A. Oestereich, J. Döbler and R. Schlögl: Analysis of silica-supported vanadia by X-ray absorption spectroscopy: Combined theoretical and experimental studies. In: Journal of Catalysis **262**, 2, 215-223 (2009).

Centi, G., M. Gangeri, M. Fiorello, S. Perathoner, J. Amadou, D. Bégin, M. J. Ledoux, C. Pham-Huu, M. E. Schuster, D. S. Su, J.-P. Tessonniere and R. Schlögl: The role of mechanically induced defects in carbon nanotubes to modify the properties of electrodes for PEM fuel cell. In: Catalysis Today **147**, 287-299 (2009).

Chan Thaw, C., F. Garin, R. Schlögl and F. C. Jentoft: Sulfated Zirconia Deactivation During n-Butane Isomerization: The Role of Monoenoic Allylic Species. In: Journal of Catalysis, submitted (2009).

Chen, X., O. Timpe, S. B. Abd Hamid, R. Schlögl and D. S. Su: Direct synthesis of carbon nanofibers on modified biomass-derived activated carbon. In: Carbon **47**, 1, 340-343 (2009).

Delgado, J. J., X. Chen, J.-P. Tessonniere, M. E. Schuster, E. Del Rio, R. Schlögl and D. S. Su: Influence of the microstructure of carbon nanotubes on the oxidative dehydrogenation of ethylbenzene to styrene. In: Catalysis Today, accepted (2009).

Dinse, A., S. Khennache, B. Frank, C. Hess, R. Herbert, S. Wrabetz, R. Schlögl and R. Schomäcker: Oxidative dehydrogenation of propane on silica (SBA-15) supported vanadia catalysts: A kinetic investigation. In: Journal of Molecular Catalysis A: Chemical **307**, 1-2, 43-50 (2009).

Frank, B., R. Fortrie, C. Hess, R. Schlögl and R. Schomäcker: Reoxidation dynamics of highly dispersed VO_x species supported on γ-alumina. In: Applied Catalysis A: General **353**, 2, 288-295 (2009).

Frank, B., J. Zhang, R. Blume, R. Schlögl and D. S. Su: Heteroatoms Increase the Selectivity in Oxidative Dehydrogenation Reactions on Nanocarbons. In: Angewandte Chemie International Edition **48**, 37, 6913-6917 (2009).

Frank, B., J. Zhang, R. Blume, R. Schlögl and D. S. Su: Heteroatoms steigern die Selektivität der oxidativen Dehydrierung an Nanokohlenstoff. In: Angewandte Chemie **121**, 37, 7046-7051 (2009).

Frank, B., J. Zhang, X. Liu, M. Morassutto, R. Schomäcker, R. Schlögl and D. S. Su: ODH @ CNTs – Metal-free Catalytic Alkane Activation. , accepted (2009).

Gajović, A., A. Šantić, I. Djerdj, N. Tomašić, A. Moguš-Milanković and D. S. Su: Structure and electrical conductivity of porous zirconium titanate ceramics produced by mechanochemical treatment and sintering. In: Journal of Alloys and Compounds **479**, 1-2, 525-531 (2009).

Gangeri, M., S. Perathoner, S. Cauda, G. Centi, J. Amadou, D. Bégin, C. Pham-Huu, M. J. Ledoux, J.-P. Tessonniere, D. S. Su and R. Schlögl: Fe and Pt carbon nanotubes for the electrocatalytic conversion of carbon dioxide to oxygenates. In: Catalysis Today **143**, 1-2, 57-63 (2009).

eDoc

2009

Geske, M., K. Pelzer, R. Horn, F. C. Jentoft and R. Schlögl: In-Situ Investigation of Gas Phase Radical Chemistry in the Catalytic Partial Oxidation of Methane on Pt. In: Catalysis Today **142**, 1-2, 61-69 (2009).

Girgsdies, F., M. Schneider, A. Brückner, T. Ressler and R. Schlögl: The crystal structure of δ-VOPO₄ and its relationship to α-VOPO₄. In: Solid State Sciences **11**, 1258-1264 (2009).

Győrffy, N., I. Bakos, S. Szabó, L. Tóth, U. Wild, R. Schlögl and Z. Paál: Preparation, characterization and catalytic testing of GePt catalysts. In: Journal of Catalysis **263**, 372-379 (2009).

Hävecker, M., M. Cavalleri, R. Herbert, R. Follath, A. Knop-Gericke, C. Hess, K. Hermann and R. Schlögl: Methodology for the structural characterisation of V₂O₅ species supported on silica under reaction conditions by means of in situ O K-edge X-ray absorption spectroscopy. In: Physica Status Solidi B **246**, 7, 1459-1469 (2009).

Hofmann, S., R. Blume, C. T. Wirth, M. Cantoro, R. Sharma, C. Ducati, M. Hävecker, S. Zafeiratos, P. Schnörch, A. Oestereich, D. Teschner, M. Albrecht, A. Knop-Gericke, R. Schlögl and J. Robertson: State of Transition Metal Catalysts During Carbon Nanotube Growth. In: Journal of Physical Chemistry C **113**, 5, 1648-1656 (2009).

Hohmeyer, J., E. Kondratenko, M. Bron, J. Kröhnert, B. Steinhauer, C. Volckmar, F. C. Jentoft, R. Schlögl and P. Claus: Activation of Dihydrogen on Supported and Unsupported Silver Catalysts. In: Journal of Catalysis, submitted (2009).

Hu, Y.-S., X. Liu, J.-O. Müller, R. Schlögl, J. Maier and D. S. Su: Synthesis and Electrode Performance of Nanostructured V₂O₅ by Using a Carbon Tube-in-Tube as a Nanoreactor and an Efficient Mixed-Conducting Network. In: Angewandte Chemie International Edition **48**, 1, 210-214 (2009).

Jentoft, F. C.: Ultraviolet–Visible–Near Infrared Spectroscopy in Catalysis: Theory, Experiment, Analysis, and Application under Reaction Conditions. In: Advances in Catalysis **52**, 129-211 (2009).

Knauer, M., M. E. Schuster, D. S. Su, R. Schlögl, R. Niessner and N. P. Ivleva: Soot Structure and Reactivity Analysis by Raman Microspectroscopy, Temperature Programmed Oxidation and High Resolution Transmission Electron Microscopy. In: Journal of Physical Chemistry, submitted (2009).

Knop-Gericke, A., E. V. Kleimenov, M. Hävecker, R. Blume, D. Teschner, S. Zafeiratos, R. Schlögl, V. I. Bukhtiyarov, V. V. Kachev, I. P. Prosvirin, A. I. Nizovskii, H. Bluhm, A. Barinov, P. Dudin and M. Kiskinova: X-Ray Photoelectron Spectroscopy for investigation of Heterogeneous Catalytic Processes. In: Advances in Catalysis **52**, 213-272 (2009).

Kovnir, K., M. Armbrüster, D. Teschner, T. Venkov, S. Szentmiklósi, F. C. Jentoft, A. Knop-Gericke, Y. Grin and R. Schlögl: In situ Surface Characterization of the Intermetallic Compound PdGa – A Highly Selective Hydrogenation Catalyst. In: Surface Science **603**, 10-12, 1784-1792 (2009).

Kovnir, K., J. Osswald, M. Armbrüster, D. Teschner, G. Weinberg, U. Wild, A. Knop-Gericke, T. Ressler, Y. Grin and R. Schlögl: Etching of the Intermetallic Compounds PdGa and Pd₂Ga: An Effective Way to Increase Catalytic Activity?. In: Journal of Catalysis **264**, 2, 93-103 (2009).

Publications

2009

Max Planck Society
eDoc Server

Liang, C., Z. Ma, H. Lin, L. Ding, J. Qiu, W. Frandsen and D. S. Su: Template preparation of nanoscale Ce_xFe_{3-x}O₄ solid solutions and their catalytic properties for ethanol steam reforming. In: *Journal of Materials Chemistry* **19**, 1417-1424 (2009).

Liu, Q., T. Wang, H. Guo, C. Liang, S. Liu, Z. Zhang, Y. Cao, D. S. Su and J. Qiu: Controlled synthesis of high performance carbon/zeolite T composite membrane materials for gas separation. In: *Microporous and Mesoporous Materials* **120**, 3, 460-466 (2009).

Liu, X., A. Wang, X. Yang, T. Zhang, C.-Y. Mou, D. S. Su and J. Li: Synthesis of Thermally Stable and Highly Active Bimetallic Au-Ag Nanoparticles on Inert Supports. In: *Chemistry of Materials* **21**, 2, 410-418 (2009).

Liu, X., Y.-S. Hu, J.-O. Müller, J. Maier, R. Schlögl and D. S. Su: Composites of molecular-anchored graphene and nanotubes with multi-tubular structure: a new type of carbon electrodes. In: *ChemSusChem*, submitted (2009).

Lorenz, H., S. Penner, W. Jochum, C. Rameshan and B. Klötzer: Pd/Ga₂O₃ methanol steam reforming catalysts: Part II. Catalytic selectivity. In: *Applied Catalysis A: General* **358**, 2, 203-210 (2009).

Miao, S., R. Naumann d'Alnoncourt, T. Reinecke, I. Kasatkin, M. Behrens, R. Schlögl and M. Muhler: A Study of the Influence of Composition on the Microstructural Properties of ZnO/Al₂O₃ Mixed Oxides. In: *European Journal of Inorganic Chemistry*, 7, 910-921 (2009).

Ocampo, F., H.-S. Yun, M. M. Pereira, J.-P. Tessonnier and B. Louis: Design of MFI zeolite-based composites with hierarchical pore structure: a new generation of structured catalysts. In: *Crystal Growth & Design*, accepted (2009).

Paál, Z. and R. Schlögl: Investigation of a traditional catalyst by contemporary methods: Parallel electron spectroscopic and catalytic studies on Pt black. In: *Surface Science* **603**, 10-12, 1793-1801 (2009).

Paraknowitsch, J. P., J. Zhang, D. S. Su, A. Thomas and M. Antonietti: Ionic Liquids as Precursors for Nitrogen-Doped Graphitic Carbon. In: *Advanced Materials* **21**, accepted (2009).

Parrott, E. P., J. A. Zeitler, J. McGregor, S.-P. Oei, S.-C. Tan, W. I. Milne, J.-P. Tessonnier, D. S. Su, R. Schlögl and L. F. Gladden: The use of terahertz spectroscopy as a sensitive probe in discriminating the electronic properties of structurally similar multi-walled carbon nanotubes. In: *Advanced Materials*, accepted (2009).

Parrott, E., J. A. Zeitler, J. McGregor, S.-P. Oei, H. Unalan, S.-C. Tan, W. Milne, J.-P. Tessonnier, R. Schlögl and L. Gladden: Understanding the Dielectric Properties of Heat-Treated Carbon Nanofibers at Terahertz Frequencies: a New Perspective on the Catalytic Activity of Structured Carbonaceous Materials. In: *The Journal of Physical Chemistry C* **113**, 24, 10554-10559 (2009).

Penner, S., H. Lorenz, W. Jochum, M. Stöger-Pollach, D. Wang, C. Rameshan and B. Klötzer: Pd/Ga₂O₃ methanol steam reforming catalysts: Part I. Morphology, composition and structural aspects. In: *Applied Catalysis A: General* **358**, 2, 193-202 (2009).

eDoc

2009

Plomp, A. J., D. S. Su, K. P. De Jong and J. H. Bitter: On the Nature of Oxygen-Containing Surface Groups on Carbon Nanofibers and Their Role for Platinum Deposition—An XPS and Titration Study. In: *Journal of Physical Chemistry C* **113**, 22, 9865-9869 (2009).

Rabin, I., O. Hahn, T. Wolff, A. Masic and G. Weinberg: On the origin of the ink of the Thanksgiving scroll (1QHodayot). In: *Dead Sea Discoveries* **16**, 1, 97-106 (2009).

Rinaldi, A., N. Abdullah, M. Ali, A. Furche, S. B. Abd Hamid, D. S. Su and R. Schlögl: Controlling the yield and structure of carbon nanofibers grown on a nickel/activated carbon catalyst. In: *Carbon* **47**, 13, 3023-3033 (2009).

Rinaldi, A., J. Zhang, B. Frank, D. S. Su, S. B. Abd Hamid and R. Schlögl: Oxidative purification of carbon nanotubes and its impact on catalytic performance in ODH reactions. In: *ChemSusChem*, accepted (2009).

Rosenthal, D., F. Girgsdies, O. Timpe, R. Blume, G. Weinberg, D. Teschner and R. Schlögl: On the CO-Oxidation over Oxygenated Ruthenium. In: *Zeitschrift für Physikalische Chemie* **223**, 1-2, 183-207 (2009).

Rosenthal, D., F. Girgsdies, O. Timpe, G. Weinberg and R. Schlögl: Oscillatory behavior in the CO-oxidation over bulk ruthenium dioxide – the effect of the CO/O₂ ratio. In: *Zeitschrift für Physikalische Chemie*, submitted (2009).

Rosenthal, D., M. Ruta, R. Schlögl and L. Kiwi-Minsker: Combined XPS and TPD study of oxygen-functionalized carbon nanofibers grown on sintered metal fibers. In: *Carbon*, submitted (2009).

Schlögl, R.: Concepts in selective oxidation of small alkane molecules. In: *Modern heterogeneous oxidation catalysis : design, reactions and characterization*. Mizuno, Noritaka. Wiley-VCH, Weinheim (2009) 1-42.

Schlögl, R.: Chapter 5 X-ray Diffraction: A Basic Tool for Characterization of Solid Catalysts in the Working State. In: *Advances in Catalysis* **52**, 273-338 (2009).

Schlögl, R.: The role of chemistry in the energy challenge. In: *ChemSusChem*, submitted (2009).

Schlögl, R. and S. Wrabetz: Department of Inorganic Chemistry - Fritz-Haber-Institut der Max-Planck-Gesellschaft. 4th Edition Department of Inorganic Chemistry / FHI, Berlin (2009) Total Numbers of Pages 48 p.

Steiner, S. A., T. F. Baumann, B. C. Bayer, R. Blume, M. A. Worsley, W. J. Moberly Chan, E. L. Shaw, R. Schlögl, J. A. Hart, S. Hofmann and B. L. Wardle: Nanoscale Zirconia as a Nonmetallic Catalyst for Graphitization of Carbon and Growth of Single- and Multiwall Carbon Nanotubes. In: *Journal of the American Chemical Society* **131**, 34, 12144-12154 (2009).

Subbotina, I. R., V. B. Kazansky, J. Kröhnert and F. C. Jentoft: Integral Absorption Coefficients of C-H Stretching Bands in IR Spectra of Ethane Adsorbed by Cationic Forms of Y Zeolite. In: *Journal of Physical Chemistry A* **113**, 5, 839-844 (2009).



Patents

2009

Max Planck Society
eDoc Server

- Su, D. S.: The Use of Natural Materials in Nanocarbon Synthesis.* In: ChemSusChem, accepted (2009).
- Su, D. S., J. J. Delgado, X. Liu, D. Wang, R. Schlögl, L. Wang, Z. Zhang, Z. Shan and F.-S. Xiao:* Highly Ordered Mesoporous Carbon as Catalyst for Oxidative Dehydrogenation of Ethylbenzene to Styrene. In: Chemistry- an Asian Journal **4**, 1108-1113 (2009).
- Su, D. S. and R. Schlögl:* Nanostructured Carbon Materials for Electrochemical Energy Storage Applications. In: ChemSusChem, submitted (2009).
- Su, D. S., J. Zhang, A. Thomas, X. Wang, J. Paraknowitsch and R. Schlögl:* Metal-free Heterogeneous Catalysis for a Sustainable Chemistry. In: ChemSusChem, accepted (2009).
- Teschner, D., E. M. Vass and R. Schlögl:* Photoelectron spectroscopy of catalytic oxide materials. In: Metal Oxide Catalysis. (Eds.) Jackson, S. Davis; Hargreaves Justin S. J. Wiley-VCH, Weinheim (2009) 243-298.
- Tessonniere, J.-P., O. Ersen, G. Weinberg, C. Pham-Huu, D. S. Su and R. Schlögl:* Selective Deposition of Metal Nanoparticles Inside or Outside Multiwalled Carbon Nanotubes. In: ACS Nano **3**, 8, 2081-2089 (2009).
- Tessonniere, J.-P., D. Rosenthal, T. W. Hansen, C. Hess, M. E. Schuster, R. Blume, F. Girgsdies, N. Pfänder, O. Timpe, D. S. Su and R. Schlögl:* Analysis of the structure and chemical properties of some commercial carbon nanostructures. In: Carbon **47**, 7, 1779-1798 (2009).
- Tessonniere, J.-P., A. Villa, O. Majoulet, D. S. Su and R. Schlögl:* Defect-Mediated Functionalization of Carbon Nanotubes as a Route to Design Single-Site Basic Heterogeneous Catalysts for Biomass Conversion. In: Angewandte Chemie International Edition **48**, 35, 6543-6546 (2009).
- Tessonniere, J.-P., A. Villa, O. Majoulet, D. S. Su and R. Schlögl:* Defect-Mediated Functionalization of Carbon Nanotubes as a Route to Design Single-Site Basic Heterogeneous Catalysts for Biomass Conversion. In: Angewandte Chemie **121**, 35, 6665-6668 (2009).
- Thurnherr, T., D. S. Su, L. Diener, G. Weinberg, P. Manser, N. Pfänder, R. Arrigo, M. E. Schuster, P. Wick and H. F. Krug:* New challenges for the immune defense? Effects of industrially relevant multiwalled carbon nanotubes on human Jurkat T cells in vitro. In: Environmental Health Perspectives, accepted (2009).
- Villa, A., N. Janjic, P. Spontoni, D. Wang, D. S. Su and L. Prati:* Au-Pd/AC as catalysts for alcohol oxidation: effect of reaction parameters on catalytic activity and selectivity. In: Applied Catalysis A: General **364**, 1-2, 221-228 (2009).
- Villa, A., J.-P. Tessonniere, O. Majoulet, D. S. Su and R. Schlögl:* Amino-functionalized carbon nanotubes as solid basic catalysts for the transesterification of triglycerides. In: Chemical Communication, 29, 4405-4407 (2009).
- Villa, A., J.-P. Tessonniere, O. Majoulet, D. S. Su and R. Schlögl:* Transesterification of triglycerides using N-functionalized CNTs: effect of reactions parameters. In: ChemSusChem, submitted (2009).

eDoc

2009

Villa, A., D. Wang, N. Dimitratos, D. S. Su, V. Trevisan and L. Prati: Pd on carbon nanotubes for liquid phase alcohol oxidation. In: Catalysis Today, accepted (2009).

Villa, A., D. Wang, D. S. Su and L. Prati: Gold sols as catalyst in the glycerol oxidation: the role of stabilizer. In: ChemCatChem, submitted (2009).

Wang, D., F. Ammari, R. Touroude, D. S. Su and R. Schlögl: Promotion effect in Pt-ZnO catalysts for selective hydrogenation of crotonaldehyde to crotyl alcohol: A structural investigation. In: Catalysis Today **147**, 224-230 (2009).

Wrabetz, S., X. Yang, G. Tzolova-Müller, R. Schlögl and F. C. Jentoft: Characterization of Catalysts in Their Active State by Adsorption Microcalorimetry: Experimental Design and Application to Sulfated Zirconia. In: Journal of Catalysis, submitted (2009).

Wuttke, S., S. M. Coman, J. Kröhnert, F. C. Jentoft and E. Kemnnitz: Sol-Gel Prepared Nanoscopic Metal Fluorides - a New Class of Tunable Acid-Base Catalysts. In: Catalysis Today, submitted (2009).

Xia, W., J. H. Bitter, D. S. Su, J. Quian and M. Muhler: Iron impregnation on the amorphous shell of vapor grown carbon fibers and the catalytic growth of secondary nanofibers. In: Diamond & Related Materials **18**, 1, 13-19 (2009).

Zafeiratos, S., T. Dintzler, D. Teschner, M. Hävecker, R. Blume, A. Knop-Gericke and R. Schlögl: On the surface reactivity of cobalt oxides for methanol oxidation. In: Journal of Catalysis, submitted (2009).

Zavyalova, U., F. Girgsdies, O. Korup, R. Horn and R. Schlögl: Microwave-Assisted Self-Propagating Combustion Synthesis for Uniform Deposition of Metal Nanoparticles on Ceramic Monoliths. In: Journal of Physical Chemistry C, accepted (2009).

Zhang, J., X. Wang, Q. Su, L. Zhi, A. Thomas, X. Feng, D. S. Su, R. Schlögl and K. Müllen: Metal-Free Phenanthrenequinone Cyclotrimer as an Effective Heterogeneous Catalyst. In: Journal of the American Chemical Society **131**, 32, 11296-11297 (2009).

Zhang, Y., S. Wei, W. Zhang, Y.-J. Xu, S. Liu, D. S. Su and F.-S. Xiao: Titania Nanocrystals and Adsorptive Nanoporous Polymer Composites: An Enrichment and Degradation System. In: ChemSusChem, accepted (2009).

Zhang, Z. and D. S. Su: Behaviour of TEM metal-grids during in-situ heating experiments. In: Ultramicroscopy **109**, 6, 766-774 (2009).

J



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Patents

1993 - 2008

EP635515/PN, July 23, 1993

"Metalfullerene 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-CuO/ZrO₂ catalyst in Steam reforming of Methanol”

Inventors: R. Schloegl, Th. Ressler, F. Giersdies, H. Purnama, R. Schomaecker, M. Antonietti, J.H. Schattka, Y. Wang, R. Caruso

EP04009874, April 26, 2004

“Assembly of carbon tube-in-tube nanostructures“
Inventors: Z. Zhu, D. Su, R. Schloegl

EP2005/008022, July 22, 2005

“Metal oxide catalyst and method for the preparation“
Inventors: R. Schloegl, O. Timpe, S.B. Abd Hamid

EP2005/007619, 2005

“Carbon nanotubes fixed on activated carbon“
Inventors: R. Schloegl, 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. Schloegl, G. Mestl

EP06005209.9, March 14, 2006

“Zirconium oxynitride catalysts for ammonia decomposition“
Inventors: R. Schloegl, T. Ressler, R. Jentoft

Max Planck Society
eDoc Server



EP 06005310.5, March 15, 2006; WO2007104569, 2007; Application in USA 12/282,920

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

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

Inventors: J. Osswald, R. Giedigkeit, M. Armbrüster, K. Kovnir, R.E. Jentoft, T. Ressler, Yu. Grin, R. Schloegl

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

“Nanocarbon-activated carbon composites“

Inventors: R. Schloegl, 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. Schloegl

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. Schloegl

EP07019469.1, 2007; PCT/EP2008/008383

“A new assembly of nanocarbon structure for energy storage“

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

PCT/EP2007/063523, 2007

“Novel synthetic route to mesostructured MoVTe mixed oxide“

Inventors: R. Schloegl, A. Trunschke

Application USA, 2008

“Phase-enriched MoVTeNb mixed oxide catalyst and methods for the preparation“

Inventors: O. Timpe, S. Ayyamperumal, A. Trunschke, R. Schloegl

EP submission 08167109.1, 10/ 2008

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

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

EP submission 08167110.9, 10/ 2008

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

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

PCT/EP2008/062424 , 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. Schloegl

Int. application based on EP07021904.3, 2008; PCT/EP2008/064668 Juni 2009

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

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

14.04.2009; EP09157875.7

“Ordered cobalt-aluminium and iron-aluminium intermetallic compounds as hydrogenation catalysts“

Inventors: M. Armbrüster, K. Kovnir, Yu. Grin, R. Schloegl, P. Gille, M. Heggen, M. Feuerbacher



Guest - lectures

2004 - 2009

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

K



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Guest - lectures

2004 – 2009

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

2004 - 2009

Date	Speaking Guest	Titel
22.11.2006	Prof. Feng-shou Xiao Jilin University, Changchun, China	Hydrothermally Stable Mesoporous Materials and Functionality of Catalytically Active Species in Mesoporous Materials
29.11.2006	Prof. Krijn P. de Jong Inorganic Chemistry and Catalysis, Department of Chemistry, Utrecht University, The Netherlands	Fundamental Studies on the Preparation of Supported Catalysts 
Date	Speaking Guest	Titel
10.01.2007	Dr. Xiaoming Ren Acta S.p.A., Crespina (PI) - Italy	Non-Pt catalysts for advanced direct alcohol fuel cells
17.01.2007	Prof. Claus Hviid Christensen Technical University of Denmark, Center for Sustainable and Green Chemistry, Department of Chemistry	Rational Approaches to Catalyst Design and Discovery
23.01.2007	Prof. Zhenping Zhu Institute for Coal Research, Chinese Academy of Science, Taiyuan, China	Construction, mechanism and properties of nanostructures
24.01.2007	Dr. Vincent Huc Université Paris – ORSAY 	Beyond the C60: from Calixarenes to metallic nanoparticules
07.02.2007	Prof. Jürgen Behm Abt. Oberflächenchemie und Katalyse, Universität Ulm	Electrocatalysis in Polymerelectrolyte Fuel Cell: Problems, Challenges and New Developments
15.02.2007	Dr. Frank de Groot Department of Chemistry, Utrecht University , Netherlands	New X-ray spectro-microscopic techniques for the in-situ study of heterogeneous catalysts
28.02.2007	Dr. Susana Valencia Instituto de Tecnología Química (UPV-CSIC), Valencia	New trends in the synthesis of zeolites 
25.04.2007	Dr. Xinyu Xia Industrial Chemistry, Ruhr-University Bochum, Germany	Temperature-Programmed Desorption from Porous Materials in a Flow Set-up: Experiments and Simulation
08.05.2007	Prof. Tao Zhang Dalian Institute of Chemical Physics, Dalian, China	Catalysis for aerospace applications

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

K



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl

Guest - lectures

2004 - 2009

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- / Bioingenieurwiss., ETH Zürich, Schweiz	Modified Metal-Organic Frameworks - Synthesis, Properties and Potential in Catalysis
09.07.2008	Prof. Michael Smith Villanova Univ., 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 Labelled 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?
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

Date	Speaking Guest	Titel
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
Date	Speaking Guest	Titel
21.01.2009	Prof. Douglas J. Buttrey Center for Catalytic Science and Technology, Department of Chemical Engineering, Univ. of Delaware/USA	Using Aberration-Corrected STEM Imaging to Explore Chemical and Structural Variations in the MoVNbTeO and Related Systems
13.05.2009	Prof. Claude F. Goldsmith Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge MA, USA	Predicting Combustion Properties of Hydrocarbon Fuel Mixtures
03.07.2009	Dr. E. Emilio Bunel Director Chemical Sciences and Engineering Division Argonne, National Laboratory Argonne/USA	Applications of Homogenous Catalysis to the Pharmaceutical Industry
14.07.2009	Prof. Alberto Morgante Laboratorio Nazionale TASC-CNR-INFN, Trieste Italy and Physics Department Trieste University, Italy	Resonant photoemission spectroscopy in organic thin films
21.08.2009	Prof. Dan V. Goia Clarkson University/Center for Advanced Materials Processing, Potsdam, NY/USA	Highly dispersed uniform metallic particles: Preparation and Applications
21.08.2009	Prof. Brent H. Shanks NSF Engineering Research Center for Biorenewable Chemicals, Iowa State University/USA	Biorenewable Chemicals: Creating a Generalized Production Paradigm



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 ERIC provides services to improve effectiveness of research	IDECAT / ERIC European Research Institute on Catalysis (ERIC)	PSFHI 805	European Union 	2005 – 2010 ERIC -Nov. 2008	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 continuing	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.I.F.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
Oxidenitride 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 - 2010	Prof. Dr. R. Schlögl Dr. A. Trunschke	Südchemie AG	Prof. Dr. S. B. Abd Hamid
Joint project with Bayer AG Teilprojekt API: "Aufklärung, Reaktionsmechanismus und Optimierung des bestehenden Katalysatoren"	CarboScale	PSFHI 105	BMBF Fkz: 03X0040H 	2007 - 2012	Prof. Dr. R. Schlögl Dr. D.S. Su Dr. J. P. Tessonnier	TU Berlin Ruhr-Uni. Bochum Univ. Erlangen Univ. Clausthal Future Carbon GmbH Bayer Ehrlfeld Mikrotechnik - BTS GmbH Leibnitz-Inst, Dresden TU Ilmenau Frauenhofer-Gesellschaft München H. C. Starck GmbH	Bayer

L



External Funds

Project Name	Akronym	Referenz No.	Funds' Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
“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	MPG		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 continuing	Prof. R. Schlögl	Prof. R. Schlögl (FHI der MPG) Prof. R. Schomäcker (TU Berlin)	
Struktur, Dynamik und Reaktivität von Übergangsmetallocid- Aggregaten	Sfb	Sfb 546	Sonderforschungsbereich	2000 - 2010	Prof. Dr. R. Schlögl	Prof. H.J. Freund Prof. R. Schomäcker Prof. Schubert	Prof. Dr. J. Sauer
Nanocarbon – Nanocarbon related materials in heterogeneous catalysis	ELCASS II	M.AP.AFHI 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)Design and characterisation of supported metal particles as selective oxidation catalysts 3)Synthesis, characterization and catalytic properties of mesoporous materials 4)Synthesis, characterization, and catalytic properties of ordered mesoporous silica and carbon materials 5)Characterization of the geometric and electronic structure of CNT supported vanadium oxides at the nanometer scale 6)Study of atomic structures at defects and interfaces in one-dimensional nanostructures by ultra high resolution transmission electron microscopy	DAAD	PS 963	Deutscher Akademischer Austauschdienst DAAD 	1) 2004 - 2005 2) 2007-2008 3) 2007 – 2009 4) 2008 5) 2008 – 2009 6) 2008-2009 continuing	Dr. D. S. Su	1) Prof. N. Wang 2) Prof. L. Prati 3) Prof. Feng-Shou Xiao (Changchun, China) 4) Prof. F. Xiao 5) Dr. M. Willinger 6) Prof. N. Wang	DAAD

External funds

Project Name	Akronym	Referenz No.	Funds' Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Partner group Dalian, Chinese Academy of Sciences. "Carbon-based challenging nanostructured materials for catalytic application"	Bao	MCHAFHI 00001	MPG	1.10.2000 – 2009 (2011)	Dr. D. S. Su		Prof. Dr. Xinhe Bao
Nonstructural catalysts for environment protection and green chemistry	Krakow		MPG	2002 – 2009 continuing	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, Kroatiens)	Dr. D. S. Su
In situ studies of oxygen species in the ethylene epoxidation over silver			MPG	1999 – 2010	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 – 2010	Dr. A. Knop-Gericke	Prof. Dr. M. Salmeron	Prof. Dr. M. Salmeron
Pd model catalysts in oxidation reactions			MPG	2004 - 2010	Dr. A. Knop-Gericke	Dr. B. Klötzer (Innsbruck, Austria) Dr. D. Zemlyanov (Limerick, Irland)	Dr. A. Knop-Gericke
Functional analysis of noble metal catalysts in selective hydrogenation	Partner Group	M.PG.A.FHI00 002	MPG and Inst. of Isotopes (Budapest, Hungary)	2006 – 2009 (2011)	Prof. 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	
Technology for Wafer-Scale Carbon Nanotube Applications	Technotubes		EU NMP-2008 4.0.3. CP-IP 228579-1	2009-2012	Dr. Axel Knop-Gericke	Univ. of Cambridge, AIXTRON, AG, Philips GmbH, IMEC, Thales Research and Technology, Thales Electron Devices, Cambridge CMOS sensors, Technical Uni. Berlin, Technical Uni. Denmark, ETH Zürich, CNR-Trieste	Prof. Dr. J. Robertson



L



External funds

Project Name	Akronym	Referenz No.	Funds' Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Ambient-XAS	EFRE		EU	2009	Dr. A. Knop-Gericke	Techical University Berlin	Prof. Dr. R. Schomäcker
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		
Identification of local environment of transition metal promoter cations in heterogeneous catalysts.	DFG	436 MOL	Deutsche Forschungsgemeinschaft	2004 – 2006 continuing	Dr. A. Trunschke	Prof. Dr. S. Klokishner (Kishinev, Acad. Sci. Moldova)	
Ressourceneffiziente AlkanSelektiveOxidation an neuen kristallinen Festkörperphasen. TP2: High-end In-situ-Analytik unter realistischen Bedingungen- Ermittlung verbessertswürdiger Strukturmotive	ReAlSelOx	FHI 107	BMBF Fkz : 033R028B 	1.7.2009-30.6.2012	Prof. R. Schlögl Dr. A. Trunschke	Prof. Dr. Glaum (Uni. Bonn), Prof. Dr. Kniep (MPI CPfS) BASF hte	BASF
Development of a long-term stable methanol synthesis catalyst	Cu IX	PSFHI 255	Bayerisches Staatsministerium für Wirtschaft, Infrastruktur, Verkehr u. Technologie 	Starting 2010	Prof. Dr. R. Schlögl Dr. M. Behrens	Südchemie, Prof. M. Muhler (Ruhr-Uni. Bochum), Prof. Hinrichsen (TU München)	Südchemie
Novel Pd-based catalysts for non-oxidative methane activation	DFG	444 BRA-113/56/0-1	Deutsche Forschungsgemeinschaft	2009-2010	Dr. M. Behrens	Prof. Dr. M. Schmal (Centro de Tecnologia, COPPE, Rio de Janeiro, Brazil)	

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



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

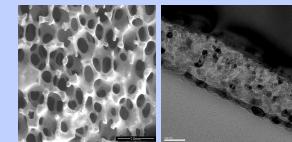
L

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 catalysts

(Dr. U. Zavyalova, S. Mavlyankariev, Dr. I. Oprea, Dr. R. Horn)

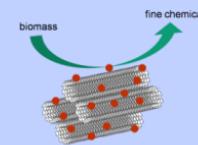
Goal: Understanding of mechanistic details of the methane activation towards design of tailored basic oxide catalysts. Comprehensive study of the heterogeneous-homogeneous reaction mechanism on Li/MgO catalysts with various surface-to-volume ratios.



2. 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>



Department of Inorganic Chemistry
Prof. Dr. Robert Schlögl



European Union - Network of Excellence / NoE

What is the SIXTH FRAMEWORK PROGRAMME (FP6) - PRIORITY 3 ?

Nanotechnology and nanosciences, knowledge based multifunctional materials, new production processes and devices –NMP



<http://idecat.org>

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>

NoE IDECAT: "Integrated Design of Catalytic Nanomaterials for a Sustainable Production"

NMP3-CT-2005-011730

What is a Network of Excellence

- An instrument to mobilize transnational research collaborations between partners sharing a commitment to long-term integration
- A series of common initiatives on integration, research, spreading of excellence and transfer to companies with the final goal to create a self-sustaining **Durable Integration Structure (DIS)**
- The DIS of IDECAT is the **European Research Institute on Catalysis** (ERIC) which started operations in Nov. 2008
- ERIC , with headquarter in Belgium, operates in close partnership with industry to create a long-term scientific, institutional, industrial and societal awareness on catalysis
- ERIC provides services to improve effectiveness of research



Courtesy: Prof. G. Centi; Coordinator
Contact: Dr. Sabine Wrabetz or Dorothea Damm
wrabetz@fhi-berlin.mpg.de, damm@fhi-berlin.mpg.de

<http://idecat.org>

Scientific vision of IDECAT

- Synthesis and mastering of nano-objects, to develop next-generation knowledge-based catalysts
- Bridging the gaps in catalysis and integrate homogeneous, heterogeneous and bio-catalysis
- A multi-disciplinary approach which synergistically integrates competencies from surface science and modeling to catalyst and reactor engineering

IDECAT: numbers

- 37 labs from 17 institutions, over 500 researchers
- 5 years project ending on Sep. 2010; 9.5 M€ budget
- 33 companies associated in the Industrial Council

IDECAT: activities

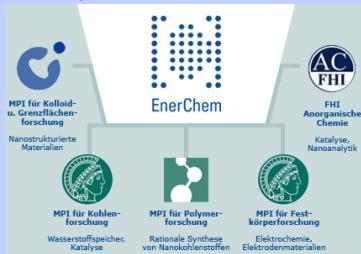
- 5 books resulting from the specific activity; many common publications and high-level reviews
- over 60 running research collaborative projects
- annual high-profile IDECAT Conference on Catalysis
- organization of many events (school, scientific meetings, promotion of science and catalysis, courses, etc.)
- 22 joint PhD, mobility and young researchers training
- start of various projects externally financed





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.



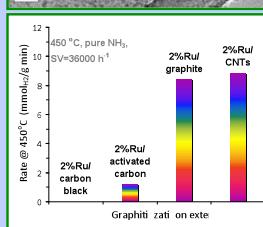
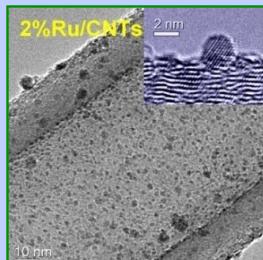
The world energy consumption is at present based nearly to 90% on fossil sources of energy (coal, oil, natural gas). Low efficiency of energy utilization has speeded up the depletion of fossil fuels and global warming. With the establishment of "nano-chemical concepts of lasting power supplies – EnerChem",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

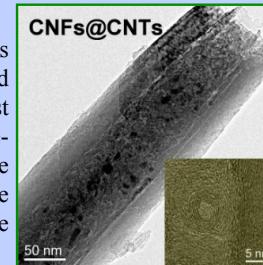
External collaborations:

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

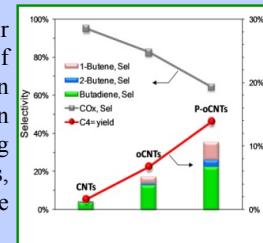
Li-ion rechargeable batteries are not only consumer electronics but, most importantly, green carrier of electricity in hybrid electric vehicles. Carbon as a richly available and low-cost resource is a promising electrode material. Carbon nanotube-encapsulated nanofibers (CNFs@CNTs) as a superior electrode 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

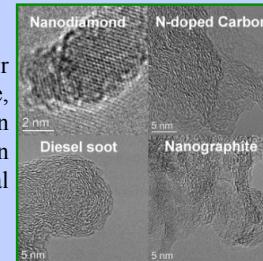
Traditional metal catalysts are deeply involved in their chemical complexity, such as lattice oxygen, various forms of polyvalent metals, parallel coke formation, etc. We use carbon with nanostructure to catalyze oxidative dehydrogenation reactions of propane, butane and ethylbenzene, producing important 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.



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:



Contact:

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

Spokesperson:

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

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

SFB 546: Structure, Dynamics and Reactivity of Aggregates of Transition Metal Oxides

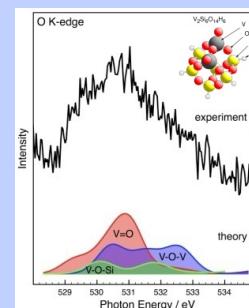
Sub-project B2: Partial oxidation of small hydrocarbon molecules with microscopic amounts of vanadia catalysts

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 V₂Si₆O₁₄H₆ 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.



**Molecular Engineering for the Conversion of Biomass Derived
Reactants into Fuels, Chemicals and Materials**

Prof. Abhaya K. Datye
(Principal Investigator)
University of New Mexico
Albuquerque, NM, USA

Prof. Robert J. Davis
(co-Principal Investigator)
University of Virginia
Charlottesville, VA, USA

Prof. James A. Dumesic
(co-Principal Investigator)
University of Wisconsin-Madison
Madison, WI, USA

Prof. Matthew Neurock
(co-Principal Investigator)
University of Virginia,
Charlottesville, VA, USA

Assoc. Prof. Brent Shanks
(co-Principal Investigator)
Iowa State University
Ames, IA, USA

Prof. Dr. Robert Schlögl
(Host: Germany site)
Fritz Haber Institute
Berlin, Germany

Prof. Claus Hviid Christensen
(Host: Denmark site)
Technical University of Denmark
Lyngby, Denmark

Environmental problems created by our dependence on fossil fuels, such as global climate change, are driving the search for renewable sources of energy, chemicals, and materials. While petroleum resources are highly concentrated in a few countries, biomass constitutes a more globally distributed resource. The PIRE research program serves to investigate critical steps in the chemical transformations of biomass-derived reactants into clean burnings fuels and other useful products.

The PIRE: Molecular Engineering for the Conversion of Biomass Derived Reactants to Fuels, Chemicals, and Materials program provides international research internship opportunities for graduate and undergraduate students.

The NSF PIRE program based out of the University of New Mexico is a collaborative partnership between educators and researchers at 8 institutions, spanning both the United States and Europe, and is also the international component of the NSF Engineering Research Center (ERC) for Biorenewable Chemicals based out of Iowa State University.

The UNM PIRE Program is funded by NSF grant OISE 0730277.

(Text and graphic: <http://www.unm.edu/~pire/>)

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

In the framework of the PIRE program, the Department of Inorganic Chemistry at FHI acts as a German host for student from the US sites. It offers its infrastructure and expertise to resolve scientific questions in a collaborative manner ideally within short-term projects of several months.

Moreover, the department contributes to the program by sending staff to research stays abroad, which are integrated into PhD or post-doctoral studies.

Issues related to the conversion of biomass currently studied at FHI include the application of functionalized carbon nanotubes as catalysts and the conversion of glucose using noble metal/carbon systems (see ??).

Prof. Dr. Matthias Scheffler
Fritz Haber Institute
Berlin, Germany

Prof. Dr. Markus Antonietti
Max Planck Institute of Colloids
and Interfaces
Potsdam, Germany

Prof. Ib Chorkendorff
Technical University of Denmark
Lyngby, Denmark

Prof. Jens K. Nørskov
Technical University of Denmark
Lyngby, Denmark

Dr. Stig Helveg
Haldor Topsøe A/S
Lyngby, Denmark



<http://www.unm.edu/~pire/>



Department of Inorganic Chemistry

Prof. Dr. Robert Schlögl

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://www.fhi-berlin.mpg.de/acnew/department/pages/lectures.html>

"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.

Annual forum for technology, science and economy organized by the HUMBOLDT secondary school to Berlin

Instructor: O. Timpe

"Concentration Ranges in Solution - Trace Analysis"



Department of Inorganic Chemistry

Prof. Dr. Robert Schlögl



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.

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

Instructor: D. S. Su

"Basics Course on Electron Microscopy and Its Applications"

Freie Universität Berlin (SoSe 2009)

Instructors: M. Behrens

Vorlesung AC III "Festkörperchemie", Bachelor-Studiengang Chemie

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

Instructors: A. Trunschke

"Reaction Mechanisms in Heterogeneous Catalysis"

lange Nacht der Wissenschaften



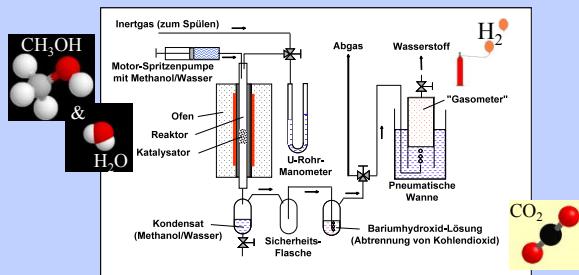
Wasserstofftechnologie

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

Fundamentale Prozesse der heterogen katalysierten Stoffumwandlung sind Gegenstand der Forschung in der Abteilung AC am Frith-Haber-Institut. Vielfältige Eigenschaften von katalytisch relevanten Materialien werden untersucht. Dabei kommen Methoden zur Anwendung, die Einblicke in Mechanismen des katalytischen Prozesses selbst auf atomarer Ebene gewähren. Mitarbeiter der Abteilung arbeiten seit längerem an der Aufklärung der Wirkungsweise von Katalysatoren für die Methanol-Reformierung wie auch der Wassergas-Shift-Reaktion. Beides Reaktionen, die im Rahmen der Wasserstofftechnologie eine Rolle spielen.

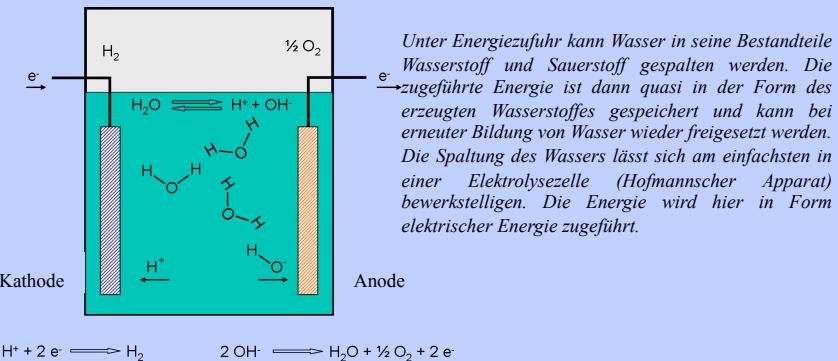
Woher kommt der Wasserstoff / Where does hydrogen come from?

z.B. aus Methanol CH_3OH



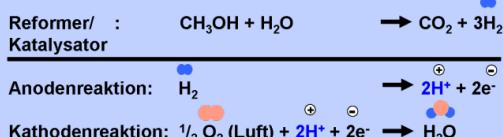
Anlässlich der Langen Nacht der Wissenschaften hat die Abteilung Anorg. Chemie einen generellen Überblick der physikalischen und chemischen Grundlagen zur Nutzung von Wasserstoff als Energieträger dargeboten. Mit einigen Exponaten und Versuchen wurden dem Besucher Entwicklungen und Techniken der Wasserstoffwirtschaft 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>)



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.





long Night of Science

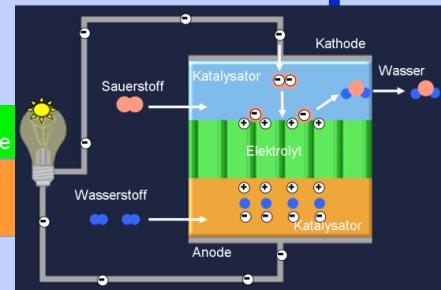
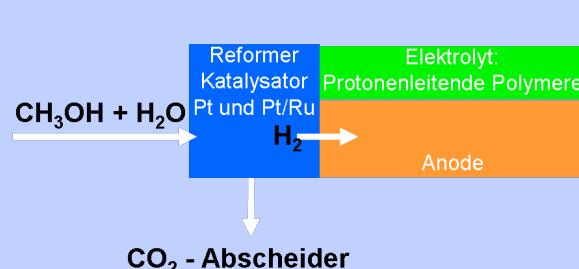


Hydrogen Technology

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

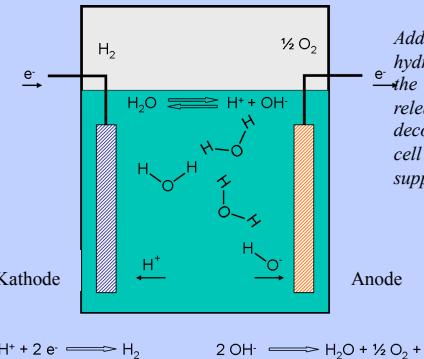
The Department of Inorganic Chemistry (IC) at the Fritz-Haber-Institut of the MPG is doing research related to basic processes of heterogeneously catalysed transformation of materials. We are studying for example properties of catalyst materials applying methods to allow insights into the mechanism of 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, 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



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 Mikrokalorimetrie. 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.



LetteVerein

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.

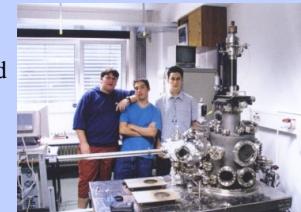


O



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

Torsten Scholl (April 2009):

Mein Name ist Törsten Scholl und ich bin Auszubildender zum Chemicelaboranten am MPI für Kohlenforschung in Mülheim. In meinem 3. Ausbildungsjahr konnte ich ein dreiwöchiges Praktikum in der Abt. für Anorganische Chemie des FHI absolvieren. Mein Praktikum wurde in drei Schwerpunkte gegliedert: Der erste war die Mikrokalorimetrie und deren Anwendung an Nb_2O_5 mit Hilfe von Gasen wie Propan. Der zweite Schwerpunkt war die UV-vis Spektroskopie. Anfangs wurde ich in diesem Abteilungsbereich in die Probenvorbereitung durch Verdünnen mit UV inaktiven Substanzen eingewiesen. Neben eigenen Probenvorbereitungen erlernte ich die Durchführung von Backgroundkorrekturen, die Kalibrierung von Gasströmen und das Messen von Proben (z.B. VOx/SBA-15) bei tiefen (flüssiger Stickstoff) und höheren Temperaturen. Die FTIR - Spektroskopie war meine dritte und letzte Station. Neben Probenvorbereitungen in KBr - Pressling und selbsttragender Presslingsform, untersuchte ich zunächst Karbonatgruppen auf LiMgO und anschließend Brönsted/Lewis - Säuren von Zirkonoxidkatalysatoren unter Zuhilfenahme von CO Adsorption. In allen Bereichen erhielt ich - neben der praktischen Arbeit - Einblicke in die Auswertungsarbeit über Excel und Origin. Durch die teils auch selbstständige Auswertungsdarstellung bekam ich insgesamt ein besseres Verständnis von Untersuchungen mit spektroskopischen Methoden. Während meines Aufenthalts fühlte ich mich, durch die herzliche Aufnahme in den Arbeitskreis, sehr wohl. Ich hoffe, dass ich das erlernte Wissen bei meiner Abschlussprüfung zum Chemicelaboranten anwenden kann. Für die schönen und interessanten drei Wochen möchte ich mich noch mal recht herzlich bedanken.



Nina K.; Januar 2005



Anne T.; July 2006



Toni S.; Juli 2008



Paula W.; Juli 2009



Department of Inorganic Chemistry

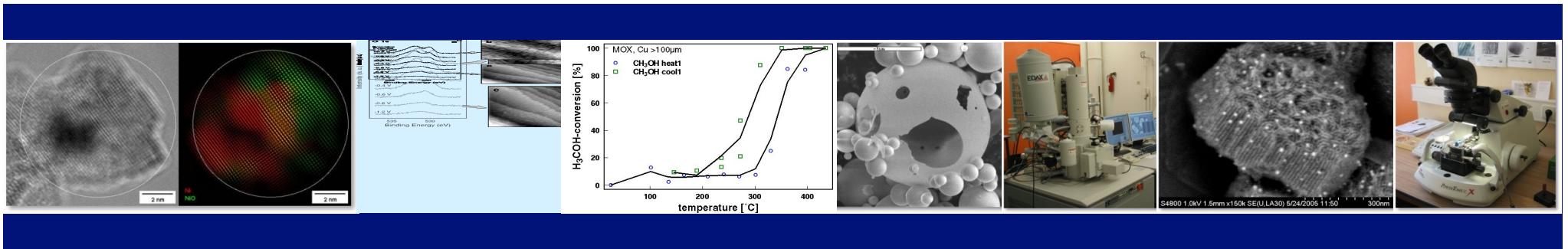
Prof. Dr. Robert Schlögl

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)
+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

November 2009

