



DEPARTMENT OF



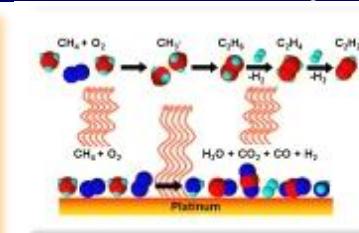
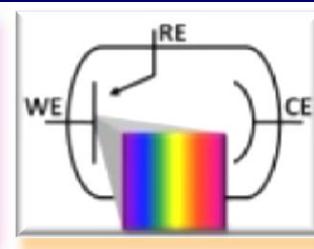
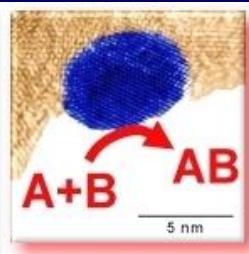
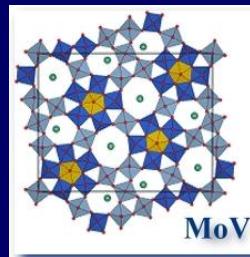
MAX-PLANCK-GESELLSCHAFT

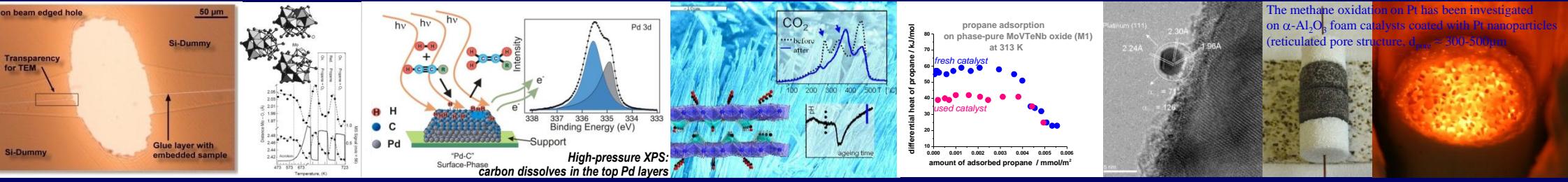
# INORGANIC CHEMISTRY



FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT

February 2013 / 8<sup>th</sup> Edition





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



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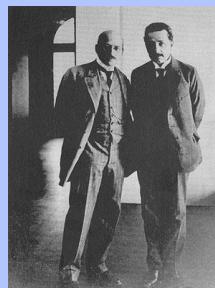


# History of the Fritz-Haber-Institut



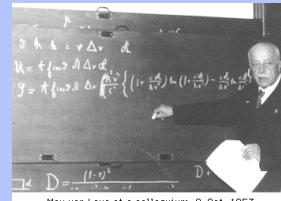
The Kaiser-Wilhelm Institutes for Chemistry (left) and for Physical Chemistry and Electrochemistry (right) --(1913).

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

## One Hundred Years at the Intersection of Chemistry and Physics

The Fritz Haber Institute of the Max Planck Society 1911 - 2011

James, Jeremiah / Steinhauser, Thomas / Hoffmann, Dieter / Friedrich, Bretislav  
DE GRUYTER 2011



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:

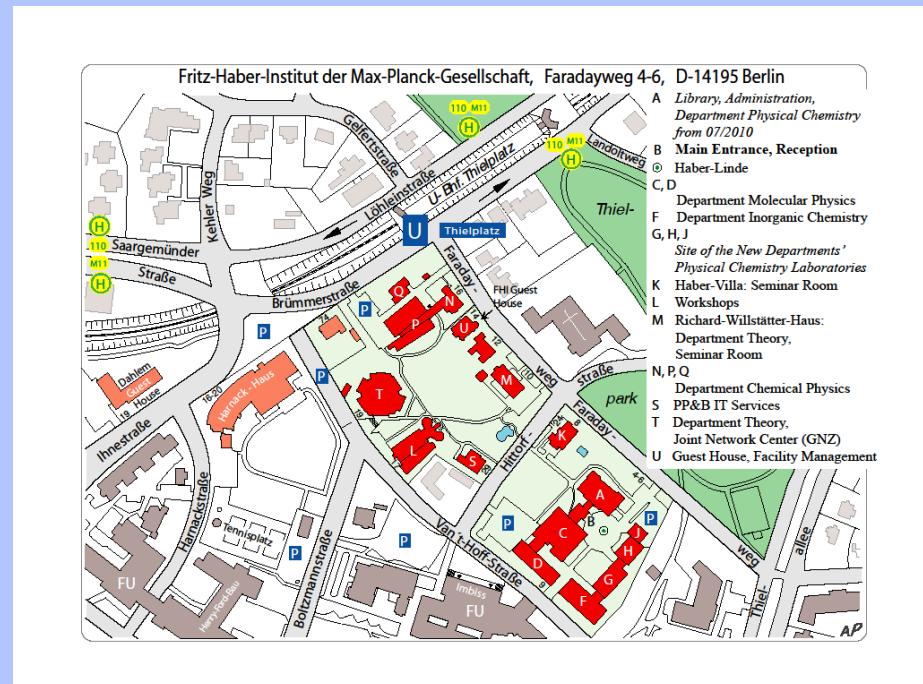
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs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



Fritz-Haber-Institut der Max-Planck-Gesellschaft

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Department of Inorganic Chemistry  
Prof. Dr. Robert Schlögl

# Preface



Director:

**Prof. Dr. Robert Schlögl**

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The department Inorganic Chemistry in the Fritz-Haber-Institut 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.

Kinetically demanding reactions of interest are selective oxidations of non-functionalized or weakly functionalized hydrocarbons, selective hydrogenations of various functionalities, dehydrogenations, skeletal rearrangements of small organic molecules and C1 chemistry. The discovery of experimental structure-function relationships requires quantitative kinetic and spectroscopic investigations including the investigation of molecular precursors, nucleation and growth during the inorganic synthesis of nano-structured catalysts. The materials of interest comprise metal nano-particles, complex transition metal oxides and carbon nano-structures. Aberration corrected high resolution electron microscopy (HR-TEM) combined with electron spectroscopy (EELS/ELNES) is used to analyze termination, defect nature, and local structure of the catalysts.



The *in-situ* analytical capabilities include electron spectroscopy in presence of gas phase molecules using synchrotron radiation, molecular spectroscopy (UV-vis, FTIR, and spatial resolved Raman spectroscopy), neutron and X-ray diffraction, and environmental scanning electron microscopy. Instrumentation development 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.

Nonetheless, the study of MgO in pure and in deliberately doped forms continued at present will give valuable insights into the mode of operation of the OCM reaction. A thorough statistical analysis of the about 2600 literature reports on OCM (with M. Baerns) yielded some insight into the nature of a possible catalyst that seems to operate successfully in a combination of surface reactions and gas-phase chemistry. Such a coupling is the ultimate example of the inadequacy of separating material and reaction in heterogeneous catalysis research.

Energy research strategy : The AC department with its initiating role for the MPG network enerchem started its respective engagement long before the general interest arose. The analysis of the greatest bottlenecks in turning away from the fossil fuel basis yielded the insight that chemical energy storage of regenerative primary energy (electricity in all foreseeable future) would be critical.



Thus an integrated approach towards basic energy science for chemical energy conversion was developed. The foundation of the Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, in 2011 has given energy research further momentum. Close collaboration and exchange of research personnel are enhancing research at both institutes. [www.cec.mpg.de](http://www.cec.mpg.de)

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. Academically the department focussed on a broad collaboration with the Technical University Berlin (TUB) through the collaborative research network SFB 546 and through the CoE UniCat (anchoring partner: R. Schomäcker). International major collaborations: the synthesis mechanism of nanocarbon is studied with the University of Cambridge (J. Robertson) partly supported by EU projects.

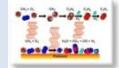
The biomass conversion activity partly initiated by the CoE UniCat is now conducted within the PIRE collaboration (coordinator: A. Datye, Univ. of Albuquerque). Numerous smaller collaborations are conducted within our BEESY group supporting the broad usage of the ambient pressure XPS facility which was upgraded by an instrument for ambient pressure (500 mbar) XAS spectroscopy as announced in the last report.

In collaboration with Uppsala university (J. Nordgren) and with the ALS we explore the potential of RIX as in-situ method using as example the silver-oxygen system in selective oxidation. Other collaborative projects are the “Pd project” encompassing groups in Austria (B. Klötzer, M. Rupprechter) and the US (D. Zemlianov), the “intermetallics” project conducted with the MPI CPFS (Dresden) (J. Grin, M. Armbrüster), the contribution to “Carboscale” (with M. Muhler and W. Wirth) and various other projects within the framework of the national competence network on nanocarbon “INNOCNT”. Industrial collaborations : With BASF our various collaborations will be focussed through a joint laboratory installed at TUB within the framework of UniCat. With BAYER we collaborate within the “INNOCNT” platform and together with the TU Berlin in a multi-national project on the chemo- and electro-catalytic oxidation of HCl to chlorine (“Deacon”). Further collaboration projects exist with VOLKSWAGEN and CLARIANT. The FHI-internal collaboration is continuing on multiple projects. With the CP department we collaborate on the issue of ultra-thin oxide over-layers and are deeply connected through the OCM issue. A visual element of the collaboration with the TH department is the continuation of the work of K. Hermann after his formal retirement in the AC department where he will strengthen our activities in evaluating X-ray absorption and EELS spectroscopy.

Ng



# Internal Structure

Reactivity		Electronic Structure	Nanostructures
GL: Dr. Annette Trunschke  	Tel: 49 30 8413 4457 E-mail: trunschke@fhi-berlin.mpg.de	Dr. Axel Knop-Gericke  	Dr. Malte Behrens  
Scientific Field: Nanostructured MoV catalysts in activation of light alkanes	49 30 8413 4422	49 30 8413 4408	
Instrumentation: Synthesis, Vibrational and UV-vis spectroscopy, Reactor technology and Catalytic testing	knop@fhi-berlin.mpg.de	behrens@fhi-berlin.mpg.de	
Members: 19	Metals in selective oxidation reactions	Copper and palladium catalysts in C1 chemistry	
	Ambient Pressure + UHV X-ray photoelectron spectroscopy, (ambient pressure) X-ray absorption spectroscopy, (ambient pressure) X-ray emission spectroscopy, BESSY II, TP desorption, TP reaction, calorimetry, BET	Synthesis, Elemental analysis, X-Ray and Neutron diffraction, TG, DSC, EXAFS	
	18	18	
High Temperature Catalysis		Electron Microscopy	Electrochemistry
GL: Dr. Raimund Horn  	Tel: 49 30 8413 4585 E-mail: horn_r@fhi-berlin.mpg.de	Dr. Marc Willinger  	Dr. Julian Tornow  
Scientific Field: High temperature catalysis research	49 30 8413 4643	49 30 8413 4640	tornow@fhi-berlin.mpg.de
Instrumentation: High temperature high pressure reactor for spatial profile measurements, Laser Spectroscopy (Raman, LIF), Molecular Beam Mass Spectrometry (MBMS)	Microstructural characterization, geometric and electronic structure	Li-ion batteries and water splitting	
Members: 5	SEMs: FEI Quanta 200 environmental FEG SEM; Hitachi S-4800 high resolution FEG SEM; TEMs: Philips CM200 LaB6, Philips CM200 FEG FEI Titan 80-200	Chemical vapor deposition, Metal evaporation, Potentiostats/Galvanostats, Gloveboxes	
	9	8	

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, research areas and main methodical activities.

# 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, RAMAN 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.

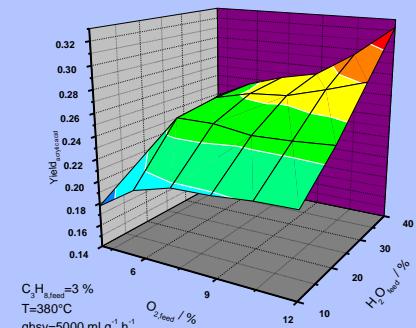
### Examples of the technical equipment:

- 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:  
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trunschke@fhi-berlin.mpg.de



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



Screening of reaction parameters in the Oxidation of propane to acrylic acid over crystalline MoVTeNb oxide



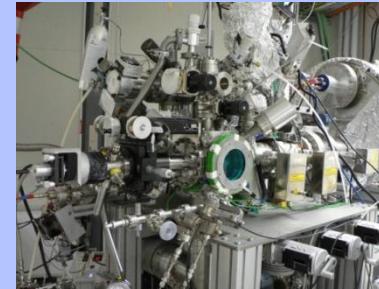
## ELECTRONIC STRUCTURE AND ADSORPTION

Dr. A. Knop-Gericke



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### ISISS: Soft X-ray station at BESSY :



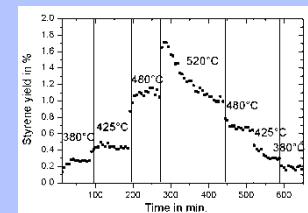
In situ XPS endstation at ISISS

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 < 700 C.) One aim of these investigation is the identification of correlation between the electronic surface structure of a working catalyst and its catalytic performance. Subsurface species were observed under reaction conditions by the help of photon energy variation (depth profile).

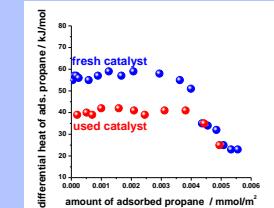
### Combined TDS, XPS and reactivity studies of low surface area (model) catalysts

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



### Measurement of isotherms & differential heats of adsorption by microcalorimetry

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 evolving 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 are of substantial value for comparing theoretical and experimental hypotheses about reaction pathways.



Differential heats of propane adsorption on fresh and used phase-pure MoVTeNb oxide catalyst ,313K.



# 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:  
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## ELECTRON MICROSCOPY Dr. M. Willinger

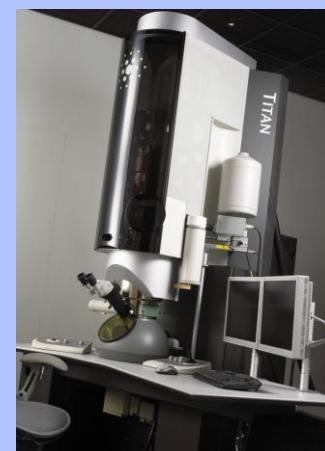


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Dr. M. Willinger,  
willinger@fhi-berlin.mpg.de

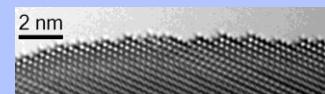
The Electron Microscopy group is equipped with a laboratory for sample preparation and the facilities for ex- and in-situ morphological, compositional and structural characterization of catalyst materials from the millimeter to the Sub-Ångström scale.

In-situ studies at variable temperatures under vacuum or at low pressures are carried out in a FEI Quanta 200 FEG environmental scanning electron microscope (E-SEM). The instrument is capable of operating at pressures of up to 4000Pa and is equipped with a heating stage and a feeding system with mass flow controllers for reaction gases. Routine morphological and compositional studies are performed with a high resolution Hitachi S-4800 FEG SEM microscope. The instrument provides a resolution of 1.4nm/0.8nm at 1kV/30kV and is equipped with various types of detectors.

Three transmission electron microscopes (TEM) are available. For fast screening and general morphological and compositional studies a Philips CM200 LaB6 with an information limit of 2Å is used. For more detailed studies, a Philips CM200 with a field emission gun is available. This microscope has an information limit of about 1.4Å. Finally, Sub-Ångström resolution is provided by the aberration-corrected FEI Titan 80-300. This microscope has an information limit of 0.8Å and is used to study the finest details in the atomic arrangement of catalysts. The CM200 FEG and the Titan are both equipped with a Gatan Tridiem energy filter (GIF) for acquiring energy-loss spectra (EELS) and energy-filtered images, with an energy resolution <1eV and <0.8eV respectively. All electron microscopes are equipped with EDAX Genesis energy-dispersive X-ray spectrometers (EDS) For the quantitative chemical analysis of macroscopic bulk materials, powders and fluids, wavelength dispersive X-ray fluorescence spectrometry (WDXRF) is used.



FEI Titan 80-300 aberration corrected TEM.



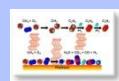
Surface of a silver particle imaged using an aberration corrected TEM.

# Instrumentation

## HIGH TEMPERATURE CATALYSIS

Dr. R. Horn

Catalytic reactions at high temperatures ( $T > 550^{\circ}\text{C}$ ) are characterized by rapid reactions at the catalyst surface, mass and heat transport limitations and in certain cases gas phase radical reactions. In consequence high temperature catalytic reactions cannot be decomposed into simple laboratory kinetic experiments but have to be studied under high temperature high pressure conditions requiring dedicated methods which are developed or adapted by the high temperature catalysis group.



Contact:  
Dr. R. Horn  
horn\_r@fhi-berlin.mpg.de

- **High Temperature High Pressure Spatial Profile Reactor** for measurement of spatially resolved species, temperature and spectroscopic profiles inside a catalyst bed at temperatures up to  $1000^{\circ}\text{C}$  and pressures up to 40 bar (in-house development). Species quantification by MS (Pfeiffer Balzers QME 200) and micro-GC (Varian 490).



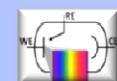
- **Triple Stage Spectrometer** (TriVista CRS) with **Confocal Upright Microscope** (Olympus BX51) for Raman and Fluorescence spectroscopy of catalyst and gas phase. The spectrometer can be coupled to the profile reactor for spatially resolved spectroscopy. The microscope is equipped with a catalytic cell reactor (Linkam CCR 1000) for micro Raman spectroscopy.

- **Various pulsed and CW lasers** are operated in the high temperature catalysis lab as excitation source for in-situ Fluorescence and Raman Spectroscopy (Spectra Physics Stabilite 2018 Ar+/Kr+, Spectra Physics Series 2000 Ar+, Coherent Verdi-V10 Nd:YVO<sub>4</sub>, Spectra Physics Wave Train, Quanta Ray Pro 230 30Hz Nd:YAG, Sirah Cobra Stretch Dye Laser).



## ELECTROCHEMISTRY

Dr. J. Tornow



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Understanding electrochemical reactions requires well defined sample material, profound electrochemical testing equipment, spectroscopic and microscopic instrumentation. Consequently we have the infrastructure for thin film deposition and electrochemical characterization. Microscopic and spectroscopic techniques are provided by the electronic structure and the electron microscopy groups.

### Gloveboxes

Battery cells are mounted before and disassembled after a cycling experiment in an argon purged and water free glovebox (mbraun). Furthermore FTIR-spectroscopy is performed under inert gas conditions.



### Potentiostats/Galvanostats

A bi-potentiostat/-galvanostat (biologic VSP) with a special low current module and a rotating disc electrode is used for water splitting experiments, while the battery test experiments are performed on a 12-channel multipotentistat/-galvanostat (ARBIN BT2143).



### Metal evaporation

Deposition of thin metallic films with only a few nanometers thickness by a metal evaporator (Edwards FL 400) is required for in-situ experiments as either electrical contact or the investigated electrode itself.



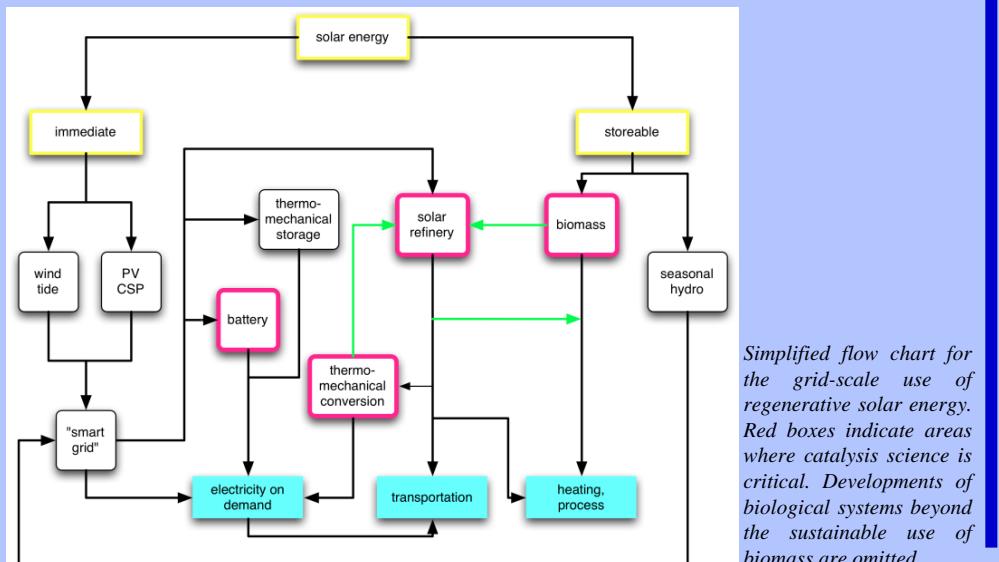
### Chemical Vapor Deposition

For the investigation of interface properties of silicon based anodes for lithium-ion batteries, we use an inductively heated AP/LPCVD-reactor. It allows for well defined deposition of silicon and carbon materials.

# Energy research strategy

The AC department with its initiating role for the MPG network enerchem started its respective engagement long before the general interest arose.

The analysis of the greatest bottlenecks in turning away from the fossil fuel basis yielded the insight that chemical energy storage of regenerative primary energy (electricity in all foreseeable future) would be critical. Thus an integrated approach towards basic energy science for chemical energy conversion was developed. Defining priority areas for basic catalysis science as outlined in Figure 2 led to the development of the concept of a solar refinery recently published. A research strategy resulted towards the fundamentals for such a refinery discriminating the MPG approach from multiple shorter-term oriented efforts going straight for the solution of phenomenological partial solutions.



These considerations were strongly encouraged by the MPG when it became clear that the capacities of a single department (AC) even when embedded in a research network (enerchem) would not be adequate to address such a challenge. A strategic approach of the MPG towards fundamental aspects of chemical energy conversion. Central element of the longterm path-finding approach of MPG is the new MPI for chemical energy conversion (MPI CEC) established in Muelheim. Restructuring the there existing MPI for "bioinorganic chemistry" and utilizing its resources, a new MPI with 4 departments and the adequate central infrastructure is being formed to address all relevant aspects of chemo-, electro- and photo-catalysis relevant in the areas indicated in the Figure. The substantial expertise in these areas existing within other MPI including the AC department at FHI are connected into a network structure following the (formalized) concept of a MAXNET initiative providing a long-term infrastructure for building a stable collaborative basis with dedicated personnel (partly concentrated in a joint laboratory at MPI CEC) without binding the participating MPI in their strategic developments on the topic of chemical energy conversion. The director of the AC department was charged with the implementation of this concept and in this capacity also with the honour to act as founding director of the MPI CEC. This is designed as a part-time activity that will be handed over to the collegium of the MPI CEC at latest upon its completion. The chemical energy conversion science will continue to form a central element of the research strategy of the AC department that will stay connected continuously through its participation in the MAXNET activity also after completion of the founding process of the MPI CEC.

# Scientific Progress

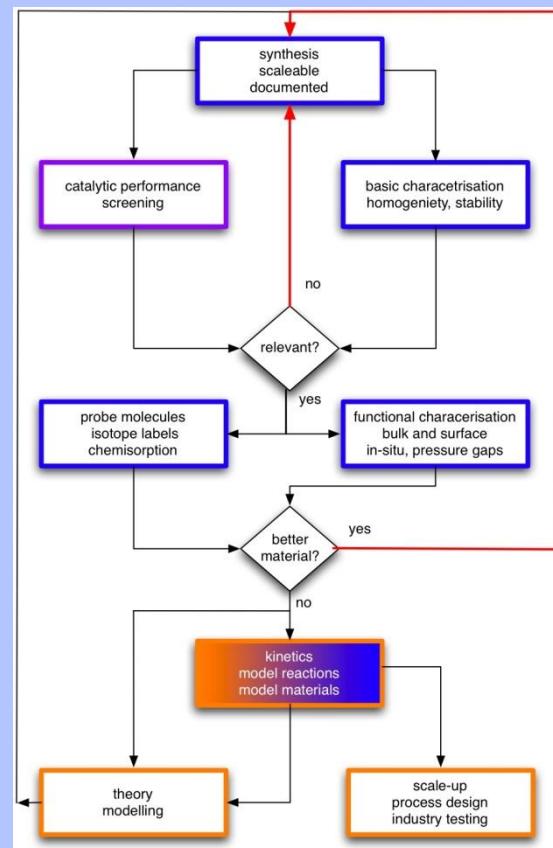
The Department AC is uniquely positioned at the crossroads of synthetic inorganic chemistry and metrology augmented by method development capabilities. Using these elements it seems possible to arrive at the development of truly rational synthesis procedures of nanostructured (defined in several dimensions 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 six of the research areas :

- Reactivity : “*Nanostructured MoV catalysts in activation of light alkanes*”
- Nanostructures: “*Copper and palladium catalysts in C1 chemistry*”
- Electronic Structure and Adsorption: “*Metals in selective oxidation reactions*”
- Electrochemistry: “*Li-ion batteries and water splitting*”
- High Temperature Catalysis: “*High temperature catalysis research*”
- Electron Microscopy: “*Microstructural characterization, geometric and electronic structure*”

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.

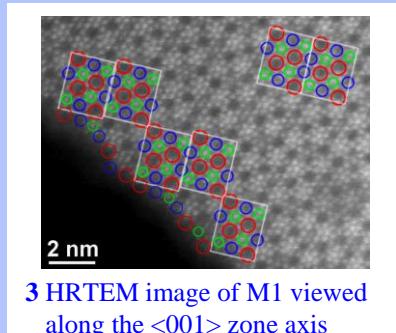
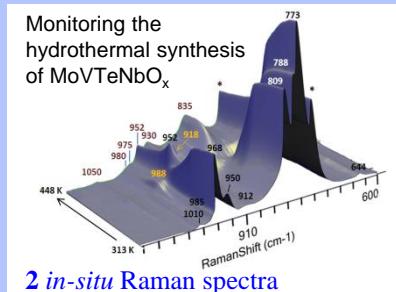
## Research concept



- 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

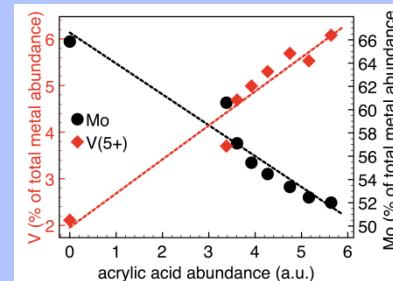
## Nanostructured MoV catalysts in activation of light alkanes



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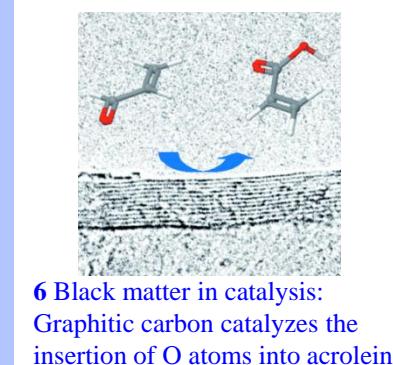
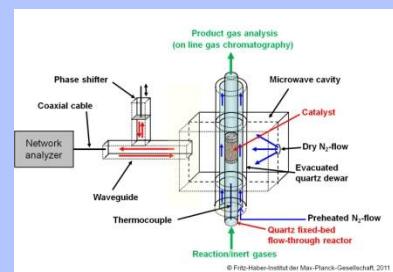
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External collaborations:  
Ruhr Universität Bochum (Prof. Dr. Muhler), Bayer Technology Services, Clariant Produkte



## Results

New approaches in hydrothermal synthesis of complex mixed metal oxides are pursued. Target structures are prepared by assembling secondary building units stepwise (**1**). The inorganic synthesis is guided by monitoring reaction intermediates using *in-situ* Raman spectroscopy (**2**). Correlations between structural characteristics, surface termination and catalytic properties in the selective oxidation of propane to acrylic acid have been studied over MoVTeNbO<sub>x</sub> model catalysts consisting of an orthorhombic phase called M1 (ICSD 55097, **3**). Acrylic acid formation correlates with surface depletion in Mo<sup>6+</sup> and enrichment in V<sup>5+</sup> sites in presence of steam in the feed (**4**). The rate of selective oxidation can be limited by electronic and/or ionic transport properties. We have developed a contactless method based on the microwave cavity perturbation technique (MWCPT) to probe the electrical conductivity of heterogeneous catalysts under reaction conditions (**5**). First results show remarkable sensitivity of this method towards gas-phase induced changes on the catalyst (VPO, M1) surface. Applying carbon nano-materials in oxidation catalysis, we have shown that the graphitic carbon has the potential to selectively mediate the insertion of an oxygen atom into an organic molecule (**6**).



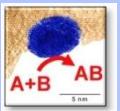
Financial support:  
BASF, Mitsubishi Chemicals  
BMBF 03X0204C, DFG



Department of Inorganic Chemistry  
Prof. Dr. Robert Schlögl

# Scientific Progress

## Copper and palladium catalysts in Cl chemistry



### 1. Methanol chemistry

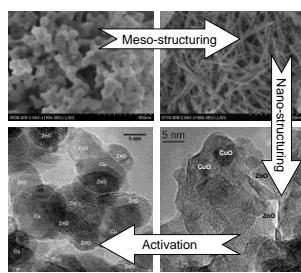
Methanol synthesis



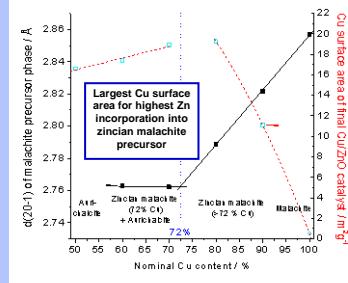
Methanol steam reforming



### 2. Preparation of Cu/ZnO



### 3. Precursor effects



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### Cu/ZnO/(Al<sub>2</sub>O<sub>3</sub>) for Hydrogenation of CO<sub>2</sub> to Methanol

Methanol is one of the most important basic chemicals in chemical industry. Furthermore, it has the potential to act as a sink for the greenhouse gas CO<sub>2</sub> 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/Al<sub>2</sub>O<sub>3</sub> 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 multi-step catalyst synthesis to establish a basis for further and more rational optimization. We also develop new methods of preparation using novel precursor systems. 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):

Stanford University, SUNCAT (J.K. Nørskov)

Technical University Berlin (T. Ressler, R. Schomäcker)

Ruhr-University Bochum (M. Muhler)

University Malaya, Kuala Lumpur (Sharifah Bee Abd Hamid)

Clariant, Bruckmühl

Examples of results from our recent work are the 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), in-situ neutron diffraction of a methanol synthesis catalyst under industrial higher pressure conditions (4), and elaboration of a model for the active site of methanol synthesis based on a defect-function-relationship (5).

### Novel Catalysts for CO<sub>2</sub>-Reforming of Methane

The catalytic conversion of anthropogenic CO<sub>2</sub> to useful chemicals is the goal of the BMBF-funded CO<sub>2</sub>RRECT project ("CO<sub>2</sub>-Reaction Using Regenerative Energies and Catalytic Technologies"). We have developed a novel Ni-based catalyst for the dry reforming of methane that converts CO<sub>2</sub> and CH<sub>4</sub> into useful synthesis gas (CO/H<sub>2</sub>). The material was prepared by a precursor route and consists of a Ni-nanoparticles embedded in a matrix of MgAl<sub>2</sub>O<sub>4</sub> (6). This composite catalyst shows an excellent thermal stability against sintering, thus allowing applications of high reaction temperatures that were found to suppress undesired coking of the catalyst.

#### External collaborations (CO<sub>2</sub>RRECT):

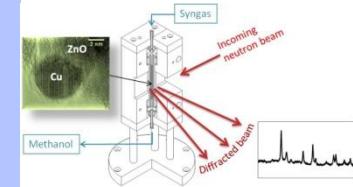
Ruhr-University Bochum (M. Muhler)

LIKAT Rostock (A. Brückner)

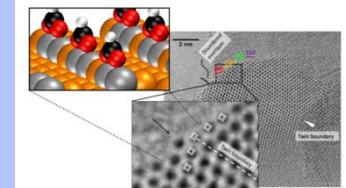
University Stuttgart (U. Nielen)

Bayer Materials Science

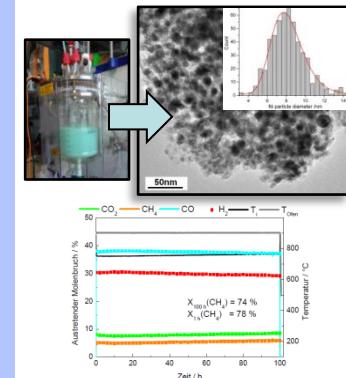
### 4. In-situ Neutron Diffraction



### 5. Active Site Model



### 6. CO<sub>2</sub> Conversion with CH<sub>4</sub>



# Scientific Progress

## Silver and alloys in ethylene epoxidation

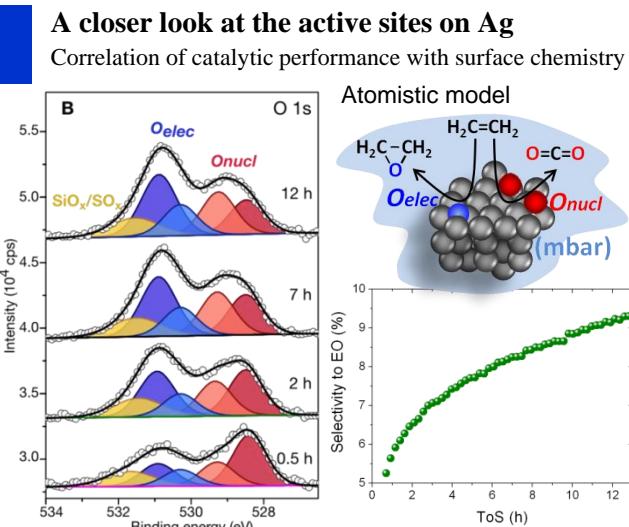


Many important feedstock chemicals used for polymer-synthesis are produced via partial oxidation of small hydrocarbons. While metal oxides catalyze many partial-oxidation reactions, there is one particularly valuable reaction for which oxides are ineffective-ethylene epoxidation. For this process, Ag is the only industrially used catalyst. Recent studies have indicated that one can increase the catalyst's selectivity for ethylene oxide by alloying Ag with other metals like Cu, Au and Re. Our ongoing work utilizes Near-Ambient-Pressure X-ray Photoemission Spectroscopy (NAP-XPS) to correlate the active oxygen species and oxide phases present on the surface of the metals and alloys with the catalytic performance during ethylene epoxidation. For instance, the figure below shows the dynamics of a Ag catalyst under ethylene epoxidation ( $C_2H_4:O_2 = 1:2$ ) at 0.3 mbar, 230 °C. The NAP-XPS data indicate that the increase in selectivity to the epoxide is related to changes in the balance between electrophilic and nucleophilic species that constitute the active sites for the selective and unselective oxidation pathways.

### Ethylene epoxidation

The O species on Ag are classified as electrophilic (*Oelec*) or nucleophilic (*Onucl*) according to their electronic properties.

*Oelec* reacts with the  $\pi$ -bonds in ethylene to yield the ethylene oxide (EO), while *Onucl* attacks C-H bonds that is the first step to total oxidation



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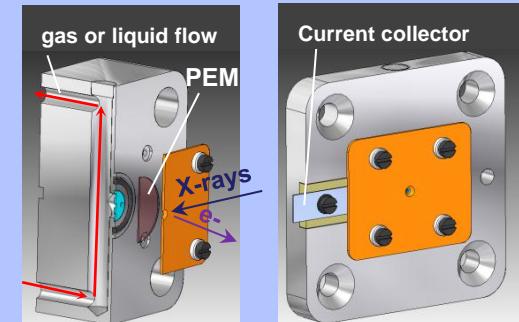
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# Scientific Progress

## Electrochemical O evolution/reduction

Electrochemical processes have a dominant role in the actual “sustainable” energy scenario. Energy conversion and storage technologies of interest such as Li-batteries, fuel cell and electrolyzers are electrocatalytic processes. Research in material science is challenged to develop cost-effective, high efficient and long term stable electrocatalyst. In-situ studies aimed to reveal mechanistic aspects of the electrocatalytic interfacial reaction are fundamental to enable nanoscale control of the catalytic properties. Our aim is the characterization of an electrode surface upon electrochemical activation by means of the near ambient pressure X-ray photoemission spectroscopy (NAP-XPS) end-station at the soft X-ray ISISS beamline (HZB/BESSY II). In particular, we focus on the study of the oxygen evolution reaction (OER) in the water electrolysis and the inverse oxygen reduction reaction (ORR) in fuel cell. For this purpose, we designed a electrochemical cell based on polymer electrolyte membrane (PEM) suitable to characterize the surface of the electrode upon polarization. The electro-active element is deposited on both sides of the PEM, functioning as cathode on one side and anode on the other side. A sketch of the designed cell is reported in the figure below. The cell presents a internal compartment into which liquid or gas can be continuously fed. The leak-tightness of the cell is realized through the coated membrane placed below the lid (in orange). The cell is then placed into the XPS chamber where another type of gas can be introduced. The orifice in the orange lid allows exposure of the electrocatalyst to the X-rays.

Electrochemical techniques such as cyclic voltammetry (CV) and chrono-amperometry (CA) under relevant polarization are applied and the electrode/gas interface of the exposed electrode is simultaneously characterized by means of photoemission Spectroscopy. Additionally the gas composition is continuously monitored by mass spectrometry (online MS).



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# Scientific Progress

## Electrochemistry

### Electrochemical processes in lithium-ion batteries

Among energy storage devices, lithium ion batteries exhibit a large gravimetric and volumetric energy density. Nonetheless substantial enhancements in energy storage capacities, charging times and long term stability are necessary to meet today's and future demands. New materials and concepts need to be developed. This requires a fundamental understanding of the electrochemical processes in current batteries. We reveal them at an atomistic level by a combination of electrochemical, spectroscopic and microscopic investigations.

We focus on a battery system with  $\text{LiFePO}_4$  as the cathode material and a silicon based battery anode. Electron energy loss spectroscopy for  $\text{LiFePO}_4$  indicates that lithium in the olivine structure is not purely ionically bonded. This would deduce a new understanding of the charge storage mechanism and it is currently under verification by a comparison with theoretical modeling performed in the electron microscopy group.

Silicon based battery anodes show an about 10 times higher charge storage capacity compared to conventional carbon based anodes, but they suffer from an insufficient cycling stability.

We are investigating the electrochemical processes responsible for this degradation. Here we observe that the standard electrolytes are not stable and a continuously growing interphase forms. Besides this, the silicon nanoparticles which are used to withstand the high volume changes during lithiation, always

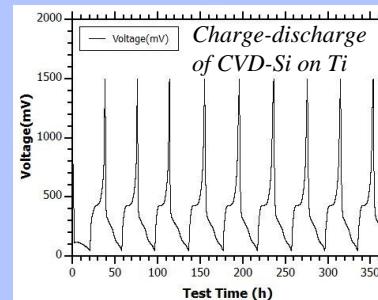
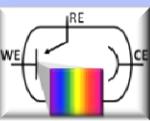
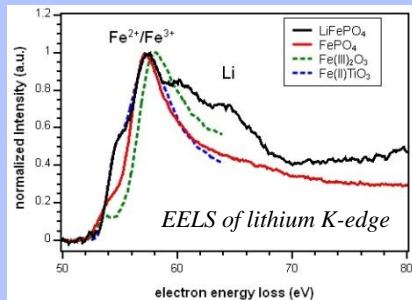
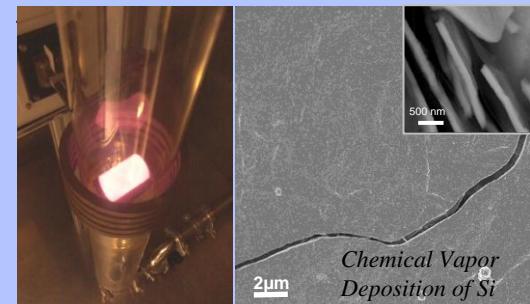
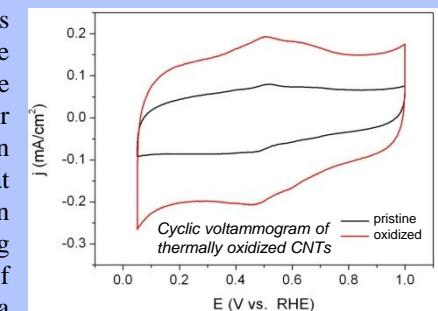


exhibit a not well defined native silicon oxide layer of up to several nanometers we therefore built up a CVD reactor for a rational design with well defined interfaces of the silicon anode on a carbon or metal support. The latter is of importance to study the electrochemical properties of the pure silicon without any side reactions from the carbon support which is also an active battery anode. Hereby we observe a significant influence of carbon especially during the first cycle, where the so called solid electrolyte interphase is formed from electrolyte decomposition.



### Carbon support for electrocatalytic water splitting

Another route for storing energy is electrochemical water splitting to generate separated hydrogen and oxygen gas. The challenge is the development of catalyst for especially the anodic reaction (oxygen evolution reaction - OER), which operate at a low overpotential and are stable even under alternating load. A promising pathway to increase the overall activity of the catalyst is to increase their surface area by dispersing it onto a reasonable support. Due to its high electrical conductivity and abundance, carbon is an interesting support material. Even though carbon is thermodynamically unstable under OER conditions, it might be kinetically stabilized. We therefore investigate the degradation mechanism of carbon nanotubes and do observe that this differs significantly from thermal oxidation.



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#### External collaborations:

MPI for Solid State Research (Prof. Antonietti, Dr. Samuelis)  
MPI for Colloids and Interfaces (Prof. Antonietti, Dr. Titirici)

Financial support:  
Volkswagen AG



# 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

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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, Laser Induced Fluorescence Spectroscopy and Molecular Beam Mass Spectrometry (MBMS, Fig.2) are developed and applied to provide insight into surface and gas phase chemistry under high temperature, high pressure reaction conditions. Experimental results are compared to microkinetic numerical simulations coupling detailed surface and gas phase reaction models with physical transport mechanisms of mass, heat and momentum.

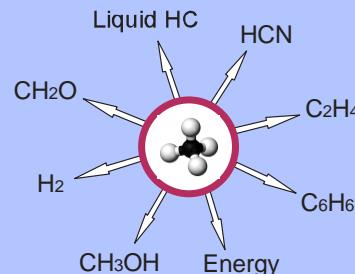


Fig. 1

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  $160\text{cm}^{-1}$  show  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{H}_2\text{O}$  and  $\text{CO}_2$  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.  $\text{CO}_2$  reforming is not observed.

Methane oxidation in a Pt tube with only  $\sim 7\text{cm}^{-1}$  surface to volume ratio leads at temperatures below 1100°C also to  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{H}_2\text{O}$  and  $\text{CO}_2$ . However, above 1100°C surface temperature, a sudden formation of C2 products ( $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_2$ ) is observed (Fig. 6). Quantitative measurements of gas phase  $\text{CH}_3\cdot$  radicals reveal the onset of gas phase chemistry at this point. C2 products are obviously formed by reaction of  $\text{CH}_3\cdot$  radicals with  $\text{CH}_4$  molecules in the gas phase and subsequent dehydrogenation.  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{H}_2\text{O}$  and  $\text{CO}_2$  are formed by surface oxidations supplying heat to drive the gas phase chemistry.

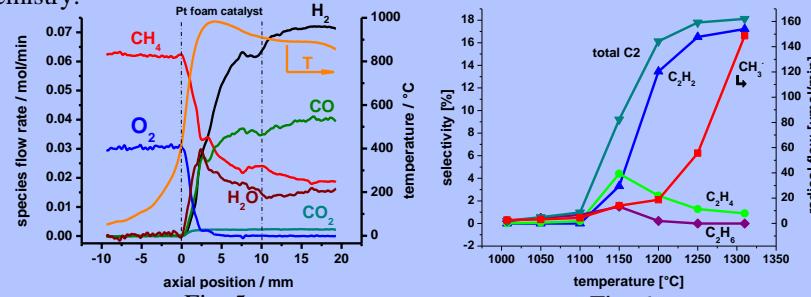


Fig. 5

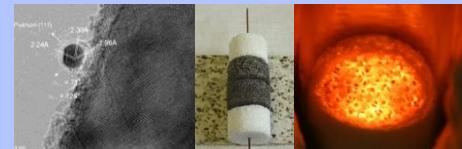


Fig. 3

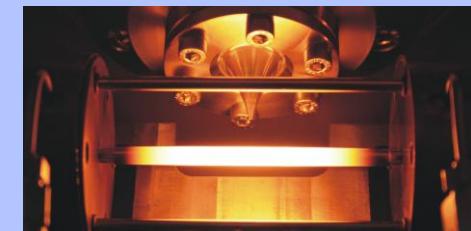


Fig. 4

Financial support:  
BMBF

German Research Foundation

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

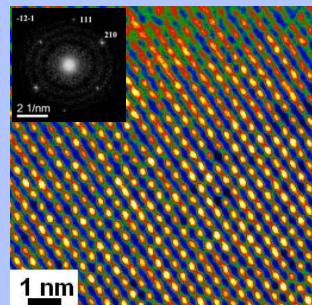
# Scientific Progress

## Analytical TEM for energy related materials

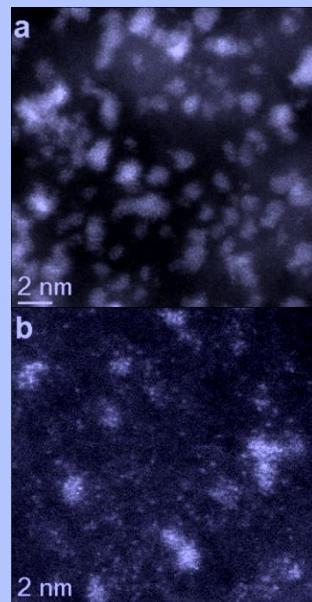


### Li Ion Battery materials

In a joined project with the Electrochemistry group, we investigate materials for Li ion batteries. The aim of the work is to understand Li ion transport and storage in the host materials and mechanisms involved in cycling induced aging. In the case of LiFePO<sub>4</sub> the cycling behavior of commercially available cathode materials was investigated by a combined approach based on high resolution TEM (HRTEM), electron energy loss spectroscopy (EELS) as a bulk sensitive local method and near edge X-ray absorption fine structure (NEXAFS) as non-local surface (bulk) sensitive method. It was possible to link cycling behavior with particle size and crystalline imperfection. Further research is aiming on improved cycling behavior of LiFePO<sub>4</sub>.



HRTEM of LiFePO<sub>4</sub>- contrast variations due to defects in the atomic arrangement

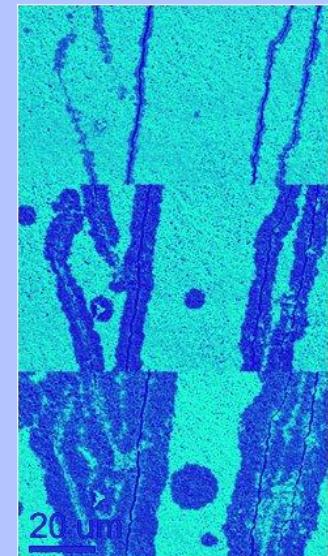


HAADF STEM images of Pt on carbon: (a) before and (b) after electrochemical cycling

### Electron microscopy of dynamic processes

#### In-situ studies by Environmental SEM

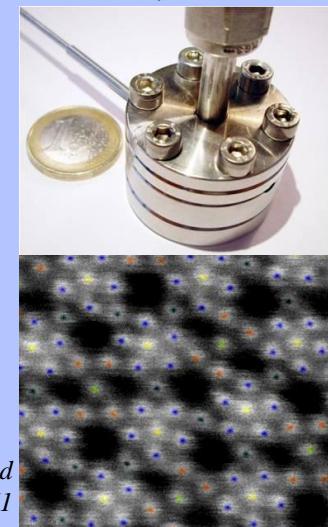
For in-situ studies of dynamic processes, we use a modified ESEM (Environmental Scanning Electron Microscope). The instrument is equipped with a heating stage, a gas feeding system with mass flow controllers and a mass spectrometer. The set-up allows direct observation of reaction induced morphological changes for example in the interaction of silver with oxygen at temperatures relevant for the ethylene epoxidation or methanol oxidation. It is also used to study the metal catalyzed chemical vapor deposition of thin carbon layers and graphene using copper and nickel catalysts. Surface reconstruction can be followed and linked to the evolution of relevant species that are recorded by complementary in-situ XPS experiments that are performed under the same conditions by the Electronic Structure group.



Carbon precipitation on Ni monitored by in-situ ESEM

#### The TEM grid micro-reactor

For the study of reaction induced modifications of catalysts we have developed a TEM grid micro-reactor. It was designed to allow a close coupling of analytical transmission electron microscopy with catalytic reactions. Microscopic amounts of catalyst on an inert TEM grid can be exposed to relevant catalytic conditions and subsequently transferred via glove box and vacuum transfer holder from the reactor into the TEM without contact to ambient air. A highly sensitive proton transfer-reaction mass spectrometer is used to monitor catalytic activity. Using this set-up we are able to monitor structural and compositional modifications of catalyst particles that are induced under well-defined and catalytically relevant conditions.



The TEM grid micro-reactor (top) and a HAADF STEM image of the M1 phase that is studied using this set-up

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# Scientific Progress

## Theory Support

### Core Electron Spectroscopy

In close collaboration with the experimental groups of the department which measure core electron spectra in systems of catalytic interest using the synchrotron radiation at BESSY II we evaluate theoretical spectra of corresponding model systems applying our DFT cluster code StoBe. The comparison allows us to interpret experimental results from X-ray absorption (XAS/NEXAFS) or X-ray photoemission (XPS) and can provide an understanding of structural detail on a microscopic scale. As examples we mention recent work on electronic and structural properties of different vanadia-, molybdena-, and titania-silica species which can form active centers in catalysts of industrial relevance. Differently binding oxygen, inside MeOx (Me = V, Mo, Ti) and SiO<sub>2</sub>, can be clearly distinguished in the theoretical spectra. A comparison with experimental O K-edge NEXAFS spectra for different vanadia species provides clear evidence that polymeric VOx exists at the catalyst surface. The evaluation for molybdena species indicates that tetrahedral dioxo MoO<sub>4</sub> units dominate the experimental spectrum. Further, the theoretical results suggest that monomeric titania species at low coverage on SBA-15 will form tetrahedral complexes where titanyl oxygen is saturated by hydrogen yielding OH groups at the Ti centers, see Figs. 1a, b.

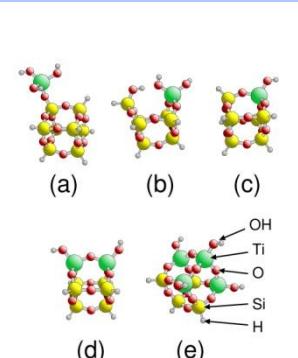


Fig. 1a

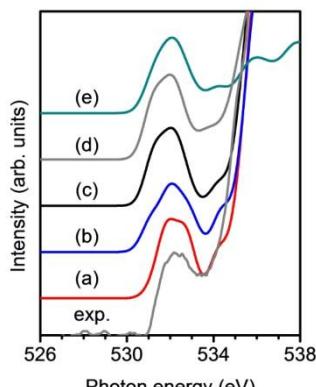


Fig. 1b

### Modeling Catalytic Reactions

Catalytic reactions can be modeled at an atomic level by their energetics, reaction paths, and corresponding reaction barriers obtained from quantum chemical calculations using our StoBe code. These simulations yield detailed information about possible reaction steps that can help the experimentalist to get deeper insight into properties of realistic catalysts.

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As an example, we have studied the selective catalytic reduction (SCR) of NO<sub>x</sub> with NH<sub>3</sub> over vanadium based metal-oxide catalysts (VOx) where details of the reaction mechanism are still under discussion. Here adsorption and (de)hydrogenation of NH<sub>3</sub>, diffusion of reactants, reactions with NO, and surface water formation at the VOx catalyst contribute elementary steps. These processes are examined in theoretical studies where the VOx substrate is modeled by clusters cut out from the ideal and reduced V<sub>2</sub>O<sub>5</sub>(010) surface. NH<sub>3</sub> is found to interact only with the V<sub>2</sub>O<sub>5</sub>(010) surface in the presence of OH groups (Brønsted acid sites) where it can form a rather strongly bound surface NH<sup>4+</sup> species, see Fig. 2, or with the reduced surface, adsorbing at vanadium centers of lower coordination (Lewis acid sites). This leads to two different SCR reaction scenarios where the evaluation of corresponding reaction paths reveals qualitative differences as to the formation of NH<sub>2</sub>NO intermediates.

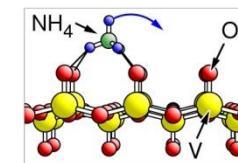


Fig. 2

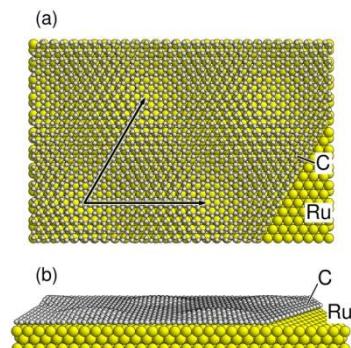


Fig. 3

### Crystallography for Bulk and Surfaces

The analysis of complex crystallographic details of model catalysts including their surfaces can be greatly facilitated by interactive visualization tools, such as Balsac or LEEDpat, developed locally, as well as by appropriate crystallographic methods. As examples we mention recent work on Moiré interference patterns of rotated and/or scaled overlayers at regular single crystal surfaces, such as graphene on hexagonal metal substrate or on graphene. These systems exhibit long-range order expressed by approximate 2-dimensional surface periodicity with very large lattice constants. The resulting patterns, consisting of similar local surface regions (moirons), can be examined by Fourier analysis and coincidence lattice theory. This yields algebraic expressions for all moiré lattice parameters characterizing moiron positions for (p1 x p2)Ra overlayers and explains the surprising behavior of moirons as well as their shapes, see Fig. 3.

### External collaborations / Financial support:

German Research Foundation (DFG), joint collaborative research center (Sfb) 658 "Elementary processes in molecular switches at surfaces", Coordinator F. von Oppen (FU Berlin), Project B3 "Magnetism and lateral ordering phenomena of switchable molecules on surfaces", PIs W. Kuch (FU Berlin), K. Hermann (FHI), 2005 – 2013.

# Photo of the department members



AC Department trip from 15. - 17. October 2012 to Dresden





## FHI Library

The library collects special literature covering the research fields of the institute. The library has about 15.500 monographs and several eBook collections (i.e. Springer eBook Collection 2005-2015). 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.

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## Move of the library

Following the trend to electronic information media while still maintaining a valuable collection of monographs the library was restructured on the occasion of its move into building A in 2010. It is planned to develop the library into a common room for the whole institute.

## 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 Association
- university libraries in Berlin and Brandenburg
- local bookshops and international publishers

## Max Planck Virtual Library (VLib)

Max Planck  
Virtual Library



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## Open Access

### Open Access

@ Max Planck Society

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 PubMan. Currently about 1950 open access documents from FHI scientists are available on PubMan.

The library has attended with some activities on the annual International Open Access Week since October 2009 (<http://www.openaccessweek.org/>). The head librarian is member of the workgroup for open access in the MPS.



## PubMan

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

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Xu, Z., Zhang, H., Zhong, H., Lu, Q., Wang, J., & Su, D. S. (2012). Effect of particle size on the activity and durability of the Pt/C electrocatalyst for proton exchange membrane fuel cells. *Applied Catalysis B: Environmental*, 111-112, 264-270. doi:10.1016/j.apcatb.2011.10.007.

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# Publications

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- Zhang, G.-R., Zhao, D. S., Feng, Y.-Y., Zhang, B. S., Su, D. S., Liu, G., & Xu, B.-Q. (2012). Catalytic Pt-on-Au Nanostructures: Why Pt Becomes More Active on Smaller Au Particles. *ACS Nano*, 6(3), 2226-2236. doi:10.1021/nn204378t.
- Zhang, J., Wang, R., Liu, E., Gao, X., Sun, Z., Xiao, F.-S., Girgsdies, F., & Su, D. S. (2012). Spherical Structures Composed of Multiwalled Carbon Nanotubes: Formation Mechanism and Catalytic Performance. *Angewandte Chemie International Edition: a journal of the Gesellschaft Deutscher Chemiker*, 51(30), 7581-7585. doi:10.1002/anie.201200969.
- Zhang, M., Guang, J., Zhang, B. S., Su, D. S., Williams, C. T., & Liang, C. (2012). Chemical Vapor Deposition of Pd(C<sub>3</sub>H<sub>5</sub>)(C<sub>5</sub>H<sub>5</sub>) to Synthesize Pd@MOF-5 Catalysts for Suzuki Coupling Reaction. *Catalysis Letters*, 142(3), 313-318. doi:10.1007/s10562-012-0767-7.
- Zhao, X.-C., Zhang, Q., Chen, C., Zhang, B. S., Reiche, S., Wang, A., Zhang, T., Schlögl, R., & Su, D. S. (2012). Aromatic sulfide, sulfoxide, and sulfone mediated mesoporous carbon monolith for use in supercapacitor. *Nano Energy*, 1(4), 624-630. doi:10.1016/j.nanoen.2012.04.003.
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- X. Shi, J. Wang, and K. Hermann (2010). Theoretical Cluster Studies on the Catalytic Sulfidation of MoO<sub>3</sub>. *J. Phys. Chem. C* 114, 6791.
- M.A. Van Hove, K. Hermann, P.R. Watson, D.P. Woodruff, S.Y. Tong, R.D. Diehl, K. Heinz, C. Minot, and H. Tochihara (2010). A standard format for reporting atomic positions: Further needs and options". *Surf. Science* 604, 1544.
- X. Shi, J. Wang, and K. Hermann (2010). CO and NO adsorption and dissociation at the β-Mo2C(0001) surface: A density-functional theory study, *J. Phys. Chem. C* 114, 13630 (2010).
- X. Shi, R.Q. Zhang, C. Minot, K. Hermann, M. A. Van Hove, W. Wang, and N. Lin (2010). Complex Molecules on a Flat Metal Surface: Large Distortions Induced by Chemisorption Can Make Physisorption Energetically More Favorable. *J. Phys. Chem. Letters* 1, 2974.
- K. Hermann (2011). Crystallography and Surface Structure, an introduction for surface scientists and nanoscientists, Wiley-VCH, Berlin 2011", ISBN 978-3-527-41012-5.
- C. Guo, K. Hermann, M. Hävecker, L. J. Gregoriades, J. Sauer, A. Trunschke, and R. Schlögl (2011). Structural Analysis of Silica-Supported Molybdena: combined theoretical and experimental studies, *J. Phys. Chem. C* 115, 15449.
- K. Diller, F. Klappenberger, M. Marschall, K. Hermann, A. Nefedov, Ch. Wöll, and J. V. Barth (2012). Self-metalation of 2H-Tetraphenylporphyrin on Cu(111): an X-ray spectroscopy study, *J. Chem. Phys.* 136, 014705.
- K. Hermann (2012). Periodic Overlays and Moiré Patterns: theoretical studies of geometric properties, *J. Phys.: Condensed Matter* 24, 314210.
- C. S. Guo, K. Hermann, M. Hävecker, A. Trunschke, and R. Schlögl (2012). Small Silica-Supported Titania Particles: Structural Analysis from Quantum Theory and X-ray Spectroscopy, *J. Phys. Chem. C* 116, 22449.
- C. S. Guo, K. Hermann, L. Sun, F. Hermanns, and W. Kuch (2012). X-ray Absorption from Large Molecules at Metal Surfaces: Theoretical and Experimental Results for Co-OEP on Ni(100), *J. Chem. Phys.* 137, 194703.
- M. Gruber and K. Hermann (2013). Elementary Steps of the Catalytic NO<sub>x</sub> Reduction with NH<sub>3</sub>: Cluster Studies on Reactant Adsorption at Vanadium Oxide Substrate , *J. Chem. Phys.* (2013) in print.



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“Metallfullerene intercalation compounds, process for their preparation and use as catalysts”

Inventors: R. Schloegl, H. Werner, M. Wohlers

DE4404329/PN February 11, 1994, EP0667180

“Process for the disposal of halogenated hydrocarbons”

Inventors: C. Scholz, W. Holzinger, R. Schloegl

DE19637205/PN, September, 12, 1996

„Ion molecule reaction mass spectroscopy method for gas analysis“

Inventors: H. Hertl, D. Bassi, I. Povo, R. Schloegl

EP925111/PN September 5, 1997

„Catalyst of process for its manufacture“

Inventors: R. Schloegl, M. Wohlers, Th. Belz, Th. Braun

DE 19843329/PN, April 08, 1999

„Preparation of methacrylic acid“

Inventors: F. Rosowski, H. Hibst, R. Schloegl, D. Herein, S. Berndt

DE 198 10 539, October 7, 1999/US No.6, 212,253 B1 April 3, 2001

„Apparatus and method for X-ray absorption spectroscopy“

Inventors, Th. Schedel-Niedrig, A. Knop-Gericke, M. Haevecker

PCT/EP2004/002765 March 17, 2004 based on EP03 005 953.9,

“Cu-CuO/ZrO<sub>2</sub> catalyst in Steam reforming of Methanol”

Inventors: R. Schlögl, 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. Schlögl

EP2005/008022, July 22, 2005

“Metal oxide catalyst and method for the preparation”

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

EP2005/007619, 2005

“Carbon nanotubes fixed on activated carbon”

Inventors: R.Schlägl, S.B. Abd Hamid

DE 102004 034 630.5, 2004, WO06008049A1, January 26,2006

“Catalyst comprising nanocarbon structures for the production of unsaturated hydrocarbons”

Inventors: R. Schlögl, G. Mestl

EP06005209.9, March 14, 2006

“Zirconium oxynitride catalysts for ammonia decomposition”

Inventors: R. Schlögl, T. Ressler, R. Jentoft

EP 06005310.5, March 15, 2006; WO2007104569, 2007; 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. Schlögl

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

“Nanocarbon-activated carbon composites”

Inventors: R. Schlögl, S.B. Abd Hamid

EP07018368, 2007

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

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

EP07021904.3 ., 2007; PCT/EP/2008/064668 7/2009

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

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

EP07019469.1, 2007; PCT/EP2008/008383;

US application 12/681,385 based on PCT/EP2008/008383 April 2010

“A new assembly of nanocarbon structure for energy storage”

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

PCT/EP2007/063523, 2007

“Novel synthetic route to mesostructured MoVTe mixed oxide”

Inventors: R. Schlögl, A. Trunschke

Application USA 2008

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

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

EP submission 08167109.1, 10/ 2008

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

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

EP submission 08167110.9, 10/ 2008

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

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

# Patents

1993 - 2011

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. Schlägl

Int. application based on EP07021904.3, 2008; PCT/EP/2008/064668 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. Schlägl

June 19, 2009, EP09157875.7

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

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

Invention registered Oct. 2009

"Hydrotalcite-precursor based composite catalyst: Palladium-Gallium intermetallic compound on oxide support for hydrogenation reactions", 2009, pending

Inventors: M. Behrens, A. Ota, R. Schlägl, M. Armbrüster, Y. Grin

34634-MPG-P-WO 2009

"Reactor Concept for In-Situ Measurements of Spatially Resolved Kinetic and Spectroscopic Data"

Inventor: R. Horn

EP 05770 735.8-2104 2010; US application No. 11/623,513, 2010

"Catalyst for the production of unsaturated hydrocarbons"

Inventors: R. Schlägl et. al.

Application EP 10 002419.9 March 9, 2010

"Palladium-modified hydrocalcites and their use as catalyst precursors"

Inventors: M. Behrens, A. Ota, R. Schlägl, M. Armbrüster, Y. Grin

Deutsche Patentanmeldung 102011076347.3. May 2011

"Microwave Cavity Perturbation Technique"

Inventors: M. Eichelbaum, A. Trunschke, R. Schlägl

Application 12157274.7, Feb. 2012

Nanostructured manganese oxide for electrocatalytic water splitting

Inventors: M. Behrens, A. Bergmann, K. Mette, J.-P. Tessonniere, R. Schlägl, P. Strasser

Application 11 186 177.9, 2012

Stabilization of carbon nanosstructures and hydrophobic organic molecules by copolymers

Inventors: R. Schlägl, Y. Grin, M. Armbrüster



# Guest - lectures

2010 - 2012

Date	Speaking Guest	Titel
17.02.2010	<b>Dr. Benoit Louis</b> LMSPC (Strasbourg, France)	Rational design of zeolite catalysts: toward a green organic chemistry
05.05.2010	<b>Prof. François Beguin</b> Centre de Recherche sur la Matière Divisée Centre National de la Recherche Scientifique and Orléans University Orléans, France	Carbon based electrochemical capacitors
02.06.2010	<b>Prof. Dr. Christian Limberg</b> Humboldt-Universität zu Berlin, Institut für Chemie	From surface-inspired oxovanadium models to active catalysts for the oxidation of alcohols with O <sub>2</sub>
14.06.2010	<b>Dr. Cornelia Jäger</b> Laborastrophysik- und Clusterphysikgruppe des Max-Planck-Institutes für Astronomie, am Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena	Formation and spectral properties of carbonaceous cosmic dust analogs
13.08.2010	<b>Prof. John Robertson</b> University of Cambridge, UK	Catalytic growth mechanism of Carbon Nanotubes
30.09.2010	<b>Dr. Tobias Rüffer</b> TU Chemnitz, Institut fuer Chemie	Verbrennen/Oxidieren dünner Filme von mehrkernigen Übergangsmetall-komplexen
17.11.2010	<b>Dr. Jong Hoon Joo</b> Max-Planck-Institut für Festförforschung	In-situ XPS of adsorbed oxygen and protonated species on mixed conducting perovskites cathode under close to SOFC operation condition
01.12.2010	<b>Dr. Ekatarina Skorb</b> MPI für Kolloid- und Grenzflächenforschung in Golm	Ultrasound Induced Formation of Mesoporous Multi Metal Catalysts
08.12.2010	<b>Dr. Oleksiy Khavryuchenko</b> Kiew National Taras Shevchenko University, Ukraine	Active carbon and spin catalysis: a quantum chemical insight
17.12.2010	<b>Prof. Dr. De Chen</b> Department of Chemical EngineeringNorwegian University of Science and Technology	Carbon nanotube based nanoelectrode array for energy storage

Date	Speaking Guest	Titel
12.01.2011	<b>Prof. Vera Bolis</b> Università del Piemonte Orientale "A. Avogadro" Faculty of Pharmacy - Dept. DiSCAFF	Joint use of microcalorimetry, spectroscopy and molecular modelling in surface studies of inorganic (bio)materials
09.02.2011	<b>Prof Wolfgang Bensch</b> Inst.f.Anorg.Chemie, Uni Kiel	Following chemical reactions with in-situ scattering techniques
16.02.2011	<b>Prof. Martin Schmal</b> COPPE Rio de Janeiro, Brazil	LaCoO <sub>3</sub> and LaCoMeO <sub>3</sub> Perovskite for Partial Oxidation of Methanol and Selox reaction
23.02.2011	<b>Prof. Thorsten Ressler</b> Technische Universität Berlin	Structure function relationships of molybdenum oxide based model systems for selective oxidation catalysts
09.03.2011	<b>Prof. Ronald Imbihl</b> Institut für Physikalische Chemie und Elektrochemie Leibniz-Universität Hannover	Facts and fiction in the electrochemical promotion of catalytic reactions
14.03.2011	<b>Prof. Markus Antonietti</b> MPI of Colloids and Interfaces, Dept. of Colloid Chemistry, Research Campus Golm	A Chimie Douce of metallic and semiconducting Carbon-nanostructures
23.03.2011	<b>Prof. Dr. Liu Hao Tjeng</b> Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden	Hard x-ray photoelectron spectroscopy: recent developments and new opportunities
11.04.2011	<b>Prof. Serena DeBeer</b> Cornell University, Chemistry and Chemical Biology	Valence to Core X-ray Emission as a Probe of Biological and Chemical Catalysis
15.04.2011	<b>Dr. Vladimir V. Roddatis</b> National Research Center "Kurchatov Institute" Moscow	High Resolution Scanning Transmission Electron Microscopy of Heterostructures
17.05.2011	<b>Prof. Reinhard Stößer</b> Humboldt University of Berlin, Institute of Chemistry, Dept. of Physical Chemistry	ESR application to selected solids and fluids using probes of different spin states

# Guest - lectures

## 2010- 2012

Date	Speaking Guest	Titel
27.05.2011	<b>Dr. Nicole Grobert</b> University of Oxford, Department of Materials	Tailoring Carbon-based nanomaterials
23.06.2011	<b>Prof. Christian Pettenkofer</b> Helmholtz Zentrum Berlin	Energy converting interfaces-surface science on semiconductor junctions
28.06.2011	<b>Prof. Gary L. Haller</b> Dept. of Chemistry Yale University	Aqueous Phase Reforming over Carbon Nanotube Supported Catalysts for Hydrogen Production
17.08.2011	<b>Prof. Dr. Christian Hess</b> Eduard-Zintl-Institut für Anorg. Chemie und Phys. Chemie Technische Universität Darmstadt	Probing catalysts, batteries and gas sensors at work
22.08.2011	<b>Dr. Karl J. J. Mayrhofer</b> Max-Planck-Institut für Eisenforschung, Düsseldorf	Catalysis in electrochemical reactors - fundamental investigations for real applications
07.10.2011	<b>Professor Wolfram Jaegermann</b> Technische Universität Darmstadt	Innovative photovoltaic energy converters: A challenge for materials science and thin film technology
12.10.2011	<b>PD Dr. Werner Lehnert</b> Institut für Energie- und Klimaforschung, Forschungszentrum Jülich GmbH	Investigation of HT-PEFC MEAs by means of electrochemical impedance spectroscopy and synchrotron X-ray radiography

Date	Speaking Guest	Titel
12.01.2012	<b>Dr. Karl Doblhofer</b> Fritz-Haber-Institut der MPG	Struktur einer zukunftsfähigen Energieversorgung
29.02.2012	<b>Dr. Dirk Niemeyer, Dr. Jörg Wölk</b> SASOL Germany GmbH Werk Brunsbüttel	Development of tailor made Catalyst Supports from an industrial perspective
11.04.2012	<b>Prof. Dr. Michael Smith</b> Department of Chemical Engineering Villanova University	Catalysis on Real Surfaces - Studies on the effect of surface roughness

Date	Speaking Guest	Titel
30.05.2012	<b>Dr. Dominik Samuelis</b> Max Planck Institute for Solid State Research, Stuttgart, Germany	Ionic / electronic wiring of lithium ion battery electrodes
13.06.2012	<b>Prof. Dr. Israel Wachs</b> Lehigh University Department of Chem. Engineering Bethlehem, PA, USA	Pervasiveness of Surface Metal Oxide Phases in Mixed Metal Oxide Catalysts
19.06.2012	<b>Prof. Dr. Dieter Vogt</b> Eindhoven Uni. of Technology Schuit Institute of Catalysis Laboratory of Homogeneous Catalysis	Catalytic Cascade Reactions Involving Hydroformylation
25.06.2012	<b>Prof. Dr. Israel Wachs</b> Lehigh University Department of Chem. Engineering Bethlehem, PA, USA	In situ and Operando Raman/IR/UV-vis/XAS/MS Spectroscopic Studies during Propylene Metathesis by Supported WO <sub>x</sub> /SiO <sub>2</sub> Catalysts
27.06.2012	<b>Prof. Dr. Israel Wachs</b> Lehigh University Department of Chem. Engineering Bethlehem, PA, USA	New Insights into the Water-Gas Shift Reaction over Bulk Cr <sub>2</sub> O <sub>3</sub> *Fe <sub>2</sub> O <sub>3</sub> Mixed Oxide Catalysts: A Combined Operando Raman-IR-XAS-MS Investigation
11.07.2012	<b>Prof. Dr. Lars C. Grabow</b> Assistant Professor of Chemical and Biomolecular Engineering University of Houston	Computational Catalysis Approaches for the Synthesis of Chemicals and Liquid Fuels
25.07.2012	<b>Prof. Dr. Jaeyoung Lee</b> Erl Center for Electrochemistry & Catalysis Gwangju Institute of Science and Technology (GIST), South Korea	Oxygen catalysts in electrochemical energy technologies
25.07.2012	<b>Prof. Dr. Jeffrey D. Rimer</b> Department of Chemical and Biomolecular Engineering Uni. of Houston, Texas, U.S.A	Rational Design of Zeolite Catalysts: New Platforms to Tailor Crystal Habit and Polymorphism
02.08.2012	<b>Prof. Dr. Anders Nilsson</b> SLAC National Accelerator Laboratory, Stanford University	In-situ X-ray Studies of Photo-and Electrocatalysis
29.08.2012	<b>Prof. Dr. Michael R. Buchmeiser</b> Lehrstuhl für Makromolekulare Stoffe und Faserchemie Institut für Polymerchemie, Universität Stuttgart	Oxidic and Non-Oxidic Ceramic Fibers: Synthesis, Structure and Applications
23.10.2012	<b>Prof. Dr. Elena R. Savinova</b> Professor of Physical Chemistry, CNRS-ECPM, University of Strasbourg, France	Shedding light on interfacial processes occurring in a membrane-electrode assembly of a fuel cell by applying ambient pressure XPS
01.11.2012	<b>Maya Kiskinova Ph.D. Sc.D.</b> Elettra Laboratory, Trieste, Italy	Microscopic insights on chemical state and morphology of key components in operating model fuel cells
06.11.2012	<b>Dr. Cristina Africh</b> CNR-IOM Laboratorio TASC, Trieste(Italy)	Graphene growth on Ni(111): STM movies under in-operando conditions

# External funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
International Partnership for Research and Education: “Molecular Engineering for Conversion of Biomass derived Reactants to Fuels, Chemicals and Materials”	PIRE			2012	Prof. R. Schlögl Dr. M. Behrens (host German site)	Prof. M. Antonietti Prof. M. Scheffler Prof. R. J. Davis Prof. J. A. Dumesic Prof. M. Neurock Prof. B. Shanks Prof. C. Christensen Prof. I. Chorkendorff Prof. J. K. Nørskov Prof. S. Hellweg	Prof. A.K.Datye (Univ.of New )
Partner group Dalian, Chinese Academy of Sciences. “Carbon-based challenging nanostructured materials for catalytic application”	Bao	MCHAFHI 00001	MPG	2000- 2011	Dr. D. S. Su		Prof. Dr. Xinhe Bao
Development of an ambient Pressure XES reaction cell	APXES		MPG	2010 continuing	Dr. A. Knop-Gericke	Dr. Laurent Duda Uppsala University	
In situ studies of oxygen species in the ethylene epoxidation over silver			MPG	1999 continuing	Dr. A. Knop-Gericke	Prof. V. L. Bukhtiyarov (, Russian)	Dr. A. Knop-Gericke
Development of high pressure hard X-ray photoelectron spectrometer			MPG	2011	Dr. A. Knop-Gericke	SPECS Surface Nano Analysis GmbH	Dr. A. Thissen
Pd model catalysts in oxidation reactions			MPG	2004 continuing	Dr. M. Behrens	Dr. B. Klötzer (Innsbruck, Austria) Dr. D. Zemlyanov (Limerick, Irland)	Dr. M. Behrens
Identification of local environment of transition metal promoter cations in heterogeneous catalysts.	MAX-PLANCK-GESELLSCHAFT		MPG	2004 continuing	Dr. A. Trunschke	Prof. Dr. S. Klokishner (, Acad. Sci. Moldova)	

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Cooperation Zagreb “TEM and Raman spectroscopy of nanostructured transition metal oxides”	DAAD		DAAD	2012 - 2015	Dr. M. Willinger	Dr. A. Gajović (Zagreb, Kroatiens)	Dr. A. Gajović

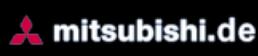
# External funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Oxidenitride des Zirconiums als Materialien und Modellverbindungen für die katalytische Aktivierung von Ammoniak	DFG	SCHL 332/9-2	DFG	continuing	Prof. R. Schlögl	Prof. M. Lerch Prof. R. Schomäcker	Prof. T. Ressler
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	DFG	2008 - 2013	Dr. R. Horn		
Novel Pd-based catalysts for non-oxidative methane activation	DFG	444 BRA-113/56/0-1	DFG	2009-2011 continuing	Dr. M. Behrens	Prof. Dr. M. Schmal (Centro de Technologia, COPPE, Rio de Janeiro, Brazil)	
Der Einfluss des Ladungstransports in Hochleistungsoxidationskatalysatoren auf Aktivität und Selektivität		PSFHI 711	DFG	2012 - 2015	Dr. M. Eichelbaum		
Nanostructured mixed metal oxides for the electrocatalytic oxidation of water	SPP 1613	PSFHI 712	DFG	2012 - 2015	Dr. A. Knop Dr. J. Tornow	Prof. P. Strasser (TU Berlin)	
Neue kostengünstige und nachhaltige Materialien für die PEM-Elektrolyse zur Herstellung von H <sub>2</sub> aus regenerativen Energien		PSFHI 111	DFG	2012 - 2015	Dr. J. Tornow		



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 Universities	starting 2007 continuing	Prof. R. Schlögl Dr. R. Horn Prof. H.J. Freund Prof. G. Meijer Prof. M. Scheffler	<a href="http://www.unicat.tu-berlin.de">http://www.unicat.tu-berlin.de</a>	Prof. M. Driess (TU Berlin)

# External funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Activation of C2-C4 hydrocarbons	BasCat 	PSFHI 771	BASF	2013 - 2017	Prof. Dr. R. Schlögl Dr. A. Trunschke	BASF TU Berlin	Prof. R. Schlögl Prof. M. Driess (TU Berlin) Dr. F. Rosowski (BASF)
Chemical vapor deposition of Si for battery anodes		PSFHI 990	VW	01.07.2011-30.06.2013	Prof. R. Schlögl Dr. J. Tornow	MPI f. Solid State Research, Stuttgart	Prof. R. Schlögl
Effect of Support Structure and Modifications on the Stability of Fuel Cell Catalysts		PSFHI 258	BASF	2011- 2013	Dr. M Willinger	Prof. R. Schlögl	
Mo-based catalysts in olefin metathesis		PSFHI 255	Mitsubishi Chemicals	2008-2012	Prof. R. Schlögl Dr. A. Trunschke		Prof. R. Schlögl

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Development of a long-term stable methanol synthesis catalyst	Cu IX	PSFHI 256	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 
Innovationsallianz CNT	CarboKat	PSFHI 110	BMBF FKZ 03X0204C	01.01.2011 – 31.12.2013	Prof. R. Schlögl Dr. A. Trunschke	Bayer Technology Services Prof. M. Muhler (Ruhr Universität Bochum) Südchemie AG	Bayer Technology Services 
Verwertung von CO <sub>2</sub> als Kohlenstoff-Baustein unter Verwendung überwiegend regenerativer Energie	CO <sub>2</sub> RRECT	PSFHI 109	BMBF	01.04.2011 - 31.03.2014	Dr. M. Behrens		
Construction of a photon energy beamline and several endstations @ BESSY	EMIL		BMBF HZB MPG	2010-2012	Dr. A. Knop-Gericke	HZB 	

# External funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Graphene chemical vapour deposition: roll to roll technology	Grafol	PS FHI 879	European Union	01.10.2011–30.09.2014	Dr. A. Knop-Gericke	Cambridge University, AIXTRON, Philips, AMO, Thales, Intel, Commissariat à l'Energie Atomique, TU Denmark, Ecole Polytechnique Federale Lausanne, Cambridge CMOS Sensors, CNRS, Graphena	Prof. J. Robertson Uni. of Cambridge  UNIVERSITY OF CAMBRIDGE



# Cluster of Excellence CoE

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



Unifying Concepts in Catalysis



## What is UniCat ?

UniCat is the acronym for a new initiative on the area of catalysis research in the Berlin-Brandenburg area (Germany). This initiative is being developed within the bounds of the Excellence Initiative started by the German Federal and State Governments, under the supervision of the German Research Foundation (Deutsche Forschungsgemeinschaft: DFG).

## 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>

K

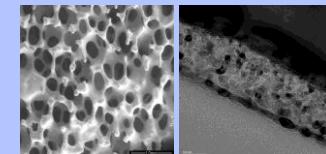
## The projects of FHI / Dept. of AC within UniCat

### Research area A: Bridging the materials gap in complex catalysis

#### 1. Oxidative coupling of methane to ethylene

(Dr. R. Horn, Sardor Mavlyankariev, Pierre Schwach, Heiner Schwarz, Dr. Annette Trunschke)

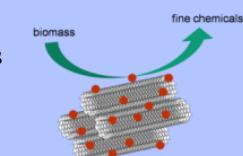
Goal: Understanding of mechanistic details of gas phase and catalytic methane oxidative coupling. Development of a microkinetic model for catalytic and non-catalytic reactions and their linkage by physical transport processes.



#### 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

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

University of New Mexico,  
USA

Iowa State University,  
USA

University of Wisconsin-Madison, USA

University of Virginia,  
USA

Technical University of Denmark

Haldor Topsoe A/S,  
Denmark

The Max Planck Institute of Colloids and Interface, Germany

Fritz Haber Institute of the Max Planck Society, Germany

Eindhoven University of Technology, Netherlands

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 12 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/>)

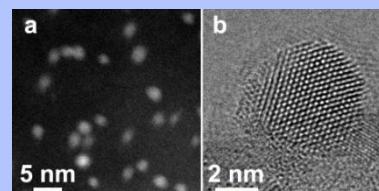
Contacts:  
Dr. Malte Behrens  
[behrens@fhi-berlin.mpg.de](mailto:behrens@fhi-berlin.mpg.de)

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

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.

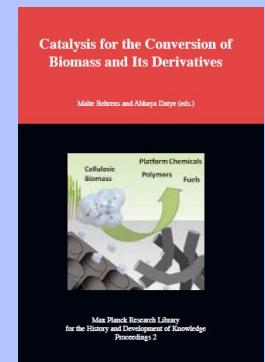


Pd nanoparticles on carbon

Utrecht University,  
Netherlands

Twente University,  
Netherlands

The University of Turku,  
Finland



The Open Access Book „Catalysis for the Conversion of Biomass and Its Derivatives“ evolved fro the FHI-organized PIRE summer-school.



# 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.



## Welcome to the International Max Planck Research School Complex Surfaces in Materials Science

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

Dr. Niklas Nilius; FHI; Dept. of Chemical Physics

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

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



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

## Tsinghua University Beijing, China

Instructor: D. S. Su

"Electron Microscopy and Its Application in Heterogeneous Catalysis: A basic lecture to understanding electron microscopy"

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

Instructors: A. Trunschke

"Reaction Mechanisms in Heterogeneous Catalysis"

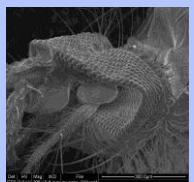
# Practical Courses



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

**Rodger Rausch (18) and Jakob Bader (18)** Sept. 2011

*During our stay between the 29th of august and the 9th of September we had the unique opportunity to work with the institute's instruments, such as infrared spectroscopy, X-ray photoelectron spectroscopy, thermal desorption spectroscopy, laser spectroscopy and many more. The research mainly focused on catalysis and surfaces. We accompanied the scientists for one or two days to get an idea of their working principles, their typical tasks, the technical equipment, and their aims. That way we become acquainted with the synthesis of catalysts, their classification and analysis with many different methods. Apart from a very interesting range of spectroscopical analysis we were most impressed by the imaging measuring techniques such as SEM, scanning tunneling microscopy (STM) and transmission electron microscopy (TEM). All things considered, we are very thankful to the FHI, especially to Dr. Sabine Wrabetz, who organized and coordinated this uniquely interesting and exciting placement.*



A mosquito head

## 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.*



## 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

## Pupil practical course



**Torsten Scholl (April 2009):**

*Mein Name ist Torsten Scholl und ich bin Auszubildender zum Chemielaboranten 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. VO<sub>x</sub>/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 Chemielaboranten anwenden kann. Für die schönen und interessanten drei Wochen möchte ich mich noch mal recht herzlich bedanken.*



Nina K.; January 2005



Anne T.; July 2006



Toni S.; July 2008



Paula W.; July 2009



Denis Z.; June 2011

# long Night of Science



## Hydrogen Technology

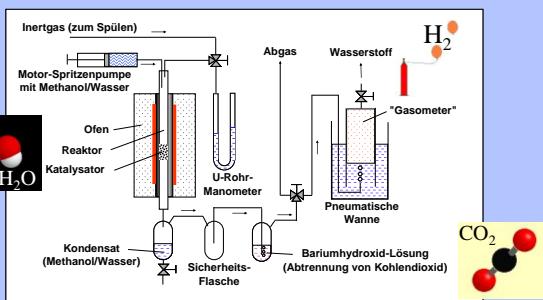
Ongoing discussions about power supply in future resulted in a general Public interest.

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

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

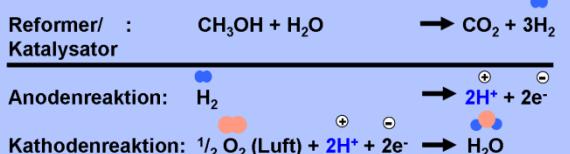
## Where does hydrogen come from?

z.B. aus Methanol  $\text{CH}_3\text{OH}$



## DMFC – Direct Methanol Fuel Cell

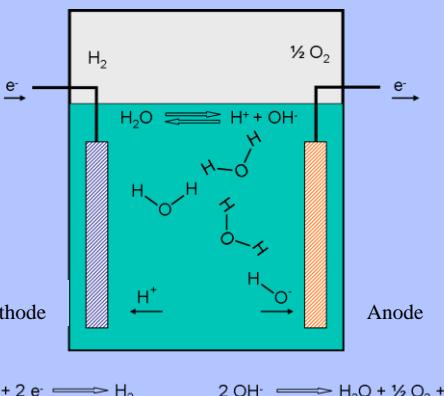
The DMFC converts methanol and oxygen electrochemically into electrical power, heat, carbon dioxide and water. At the anode (negative electrode), the methanol is first split into hydrogen and carbon dioxide before the same catalyst splits the hydrogen into protons and electrons. These reactions require 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.



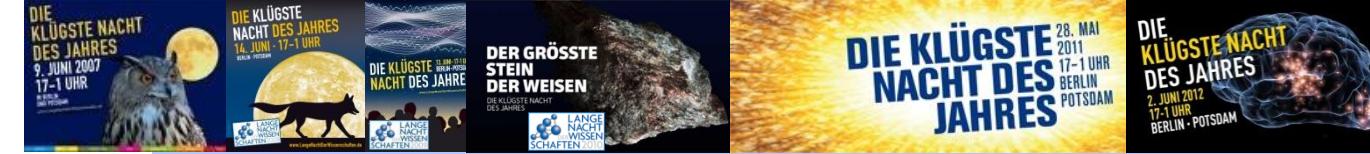
## Future Research and Perspective

Electrochemical conversions are a key issue of future energy storage to match the temporal fluctuations of sustainable sources with the demand of modern society. Herein the supply in mobile units is a special challenge.

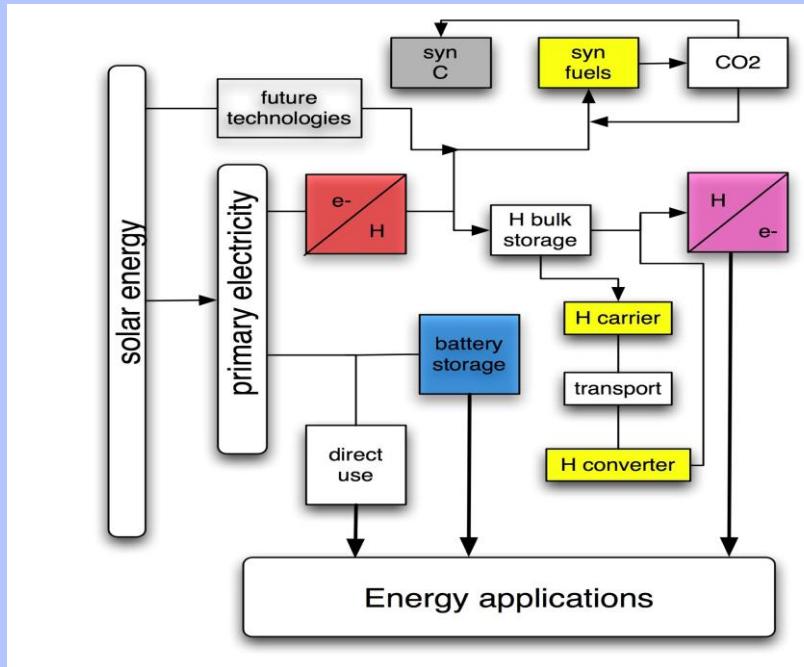
Fundamental insight and understanding of the dynamic phenomenon determining the performance of an (working) electrode is requested to design devices of higher energy efficiency and enhanced durability. The department entered in an integrated research field focussing on electrochemistry. The methodical core competences are combined into a complementary approach.



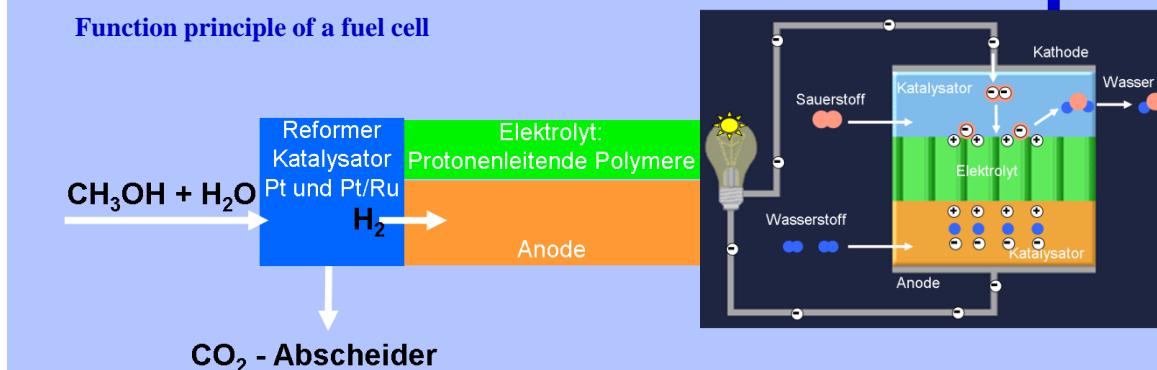
Additional energy makes water decompose into hydrogen and oxygen. Energy is saved in form of the generated hydrogen molecule and may be released again when water reforms.. Water decomposition is done best within an electrolysis cell (Hofmannscher Apparatus). Here energy is supplied in form of electric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



## A Global Energy Scenario



## Function principle of a fuel cell



## Exposition on the Long Night of Sciences

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.

Beuth Hochschule für Technik Berlin  
Fritz-Haber-Institut der Max-Planck-Gesellschaft  
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Geschäftsführender Direktor  
Faradayweg 4-6  
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University of Applied Sciences  
Der Präsident /  
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messen@beuth-hochschule.de  
Gesetzl. P. L. Urheb.

25.06.2010

*Feedback on the Long Night of Science*

## Lange Nacht der Wissenschaften

Sehr geehrter Herr Prof. Schlögl,

zu ihrem zehnten Jubiläum hat die Lange Nacht der Wissenschaften zwar erstmalig keinen neuen Besuchermarkt zu verzeichnen, mit 200.000 gezählten Besuchern stabilisiert sich die Besuchermeinung auf die Wissenschaftsnacht allerdings auf sehr hohem Niveau. Dieser Erfolg bestätigt uns darin, dass es der „Klugsten Nacht des Jahres“ in einzigartiger Weise gelingt, die Bedeutung von Wissenschaft und Forschung für unsere Region sichtbar zu machen und die Identifikation mit dem Wissenschaftsstandort zu stärken.

All dies wäre nicht möglich ohne das Engagement von tausenden von Wissenschaftlerinnen und Wissenschaftlern sowie Studierenden in den teilnehmenden Einrichtungen. Für diesen Einsatz möchte ich mich auch im Namen des Langlebigen der Wissenschaften e. V. ganz herzlich bei Ihnen bedanken. Bitte geben Sie den Dank auch an Ihre Mitarbeiterinnen und Mitarbeiter weiter. Sie gestalten alljährlich das spannende und vielfältige Programm und machen in der „Klugsten Nacht des Jahres“ Wissenschaft für ein breites Publikum zum Erlebnis!

Ein besonderes Jahr war 2010 für die Lange Nacht der Wissenschaften auch dadurch, dass aus dem bisherigen Kuratorium heraus ein gemeinnütziger eingetragener Verein (LNDW e.V.) gegründet wurde, der nun als Veranstalter für die Gesamtorganisation verantwortlich zeichnet. Es würde uns außerordentlich freuen, wenn sich der Kreis der Einrichtungen, die als Mitglieder des Vereins langfristig Verantwortung für die Wissenschaftsnacht übernehmen, noch erweitert und noch mehr Einrichtungen dem Verein beitreten würden. Weiterführende Informationen hierzu gibt Ihnen gerne Frau Dr. Buchholz in der Geschäftsstelle des LNDW e.V.

Mit freundlichen Grüßen

Prof. Dr.-Ing. Reinhard Thümer  
Lange Nacht der Wissenschaften e.V.  
Vorsitzender des Vorstands

■ ■ ■ ■ ■ [www.beuth-hochschule.de](http://www.beuth-hochschule.de)



## Application



# Early insight into the world of science



Schoolgirls visited the FHI (2005 ...2013).



24 preschoolers visited the FHI (2012).

The kids visited the library, workshops, and scientific laboratories of the institute. Taking part in basic experiments, the young children were encouraged to gain first hands-on experience with the purpose to awaken interest in science early.

Children in the workshop



Children examining each other with a magnifying lens



Visiting the library



The children used both stereo and optical microscopes to examine flies, moldy bread, leaves, and more



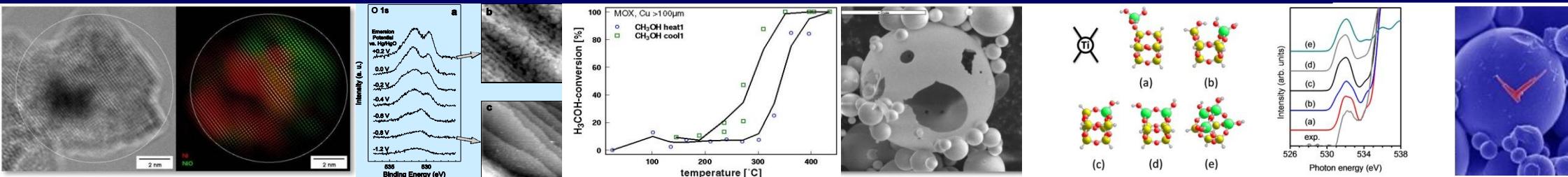
<http://www.fhi-berlin.mpg.de/acnew/department/pages/youngpeople.html>

# Notes

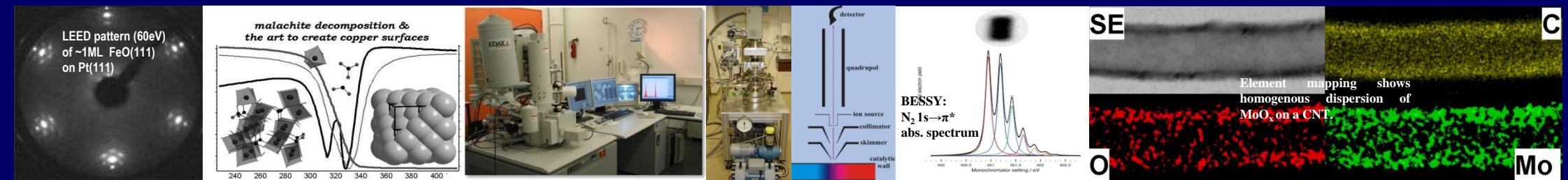


# Notes





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





## Scientific Art Gallery

Address           Fritz-Haber-Institut der Max-Planck-Gesellschaft  
                  Department of Inorganic Chemistry  
  
                  Faradayweg 4 – 6  
                  D-14195 Berlin  
                  Germany

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Fax             +49 (0) 30 8413 4401

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

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Press           February 2013