Department of

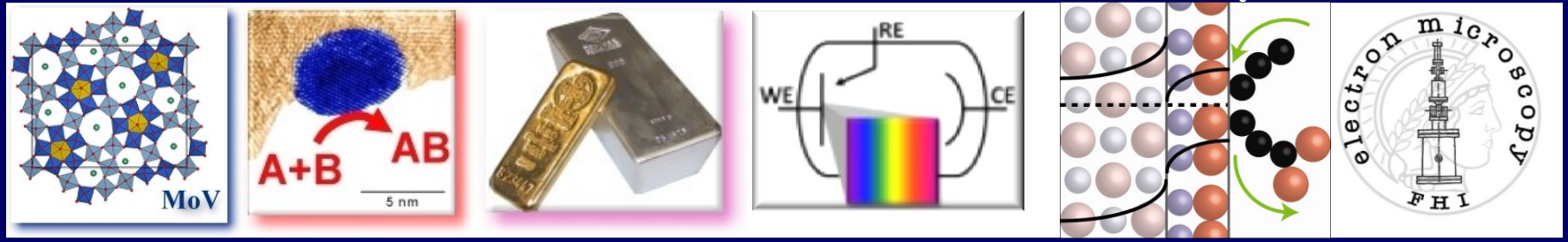
MAX-PLANCK-GESELLSCHAFT

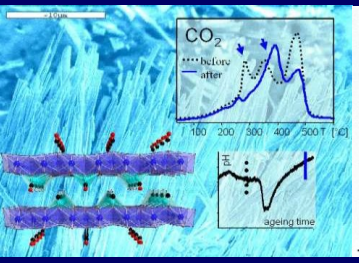
Inorganic Chemistry

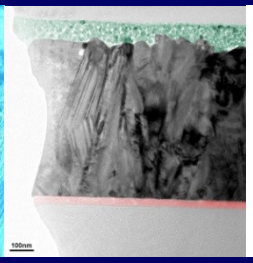
AC FHI

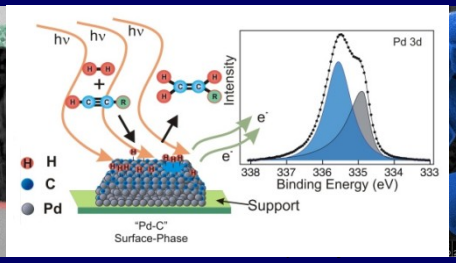
Fritz-Haber-Institut der Max-Planck-Gesellschaft

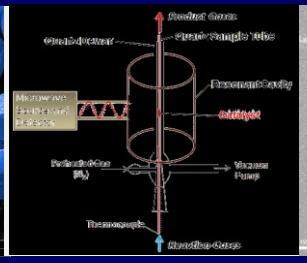
February 2014 / 9th Edition

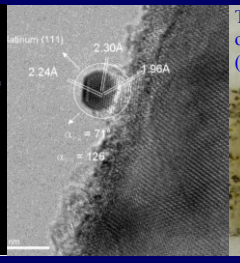




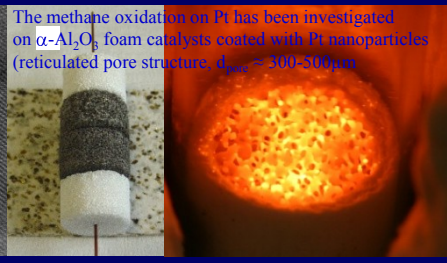




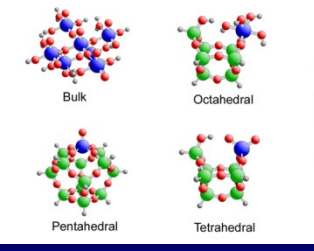


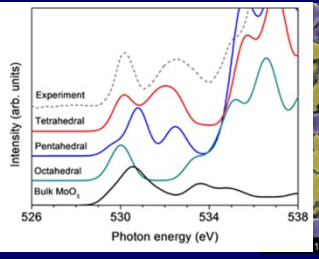


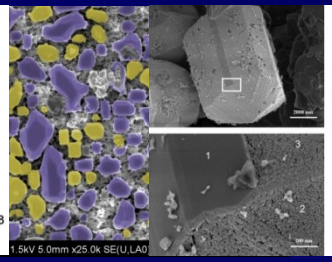
The methane oxidation on Pt has been investigated on α-Al_2O_3 foam catalysts coated with Pt nanoparticles (reticulated pore structure, d_{pore} = 300-500µm

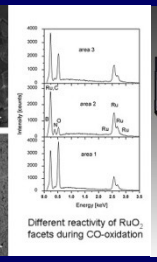


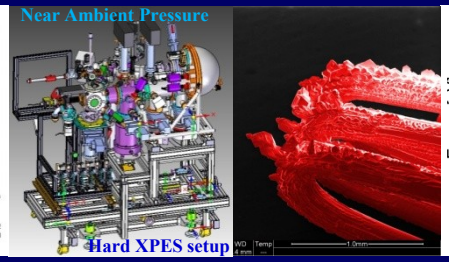
http://www.fhi-berlin.mpg.de

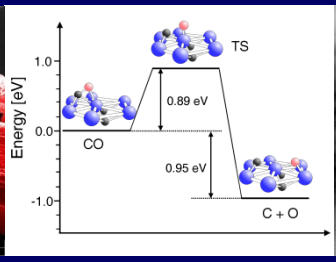


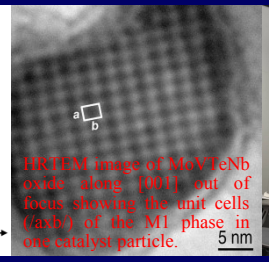












HRTEM image of MoVTeNb oxide along [001] out of focus showing the unit cells (/axb/) of the M1 phase in one catalyst particle. 5 nm

Titan 80-300

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History of the Fritz-Haber-Institut

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

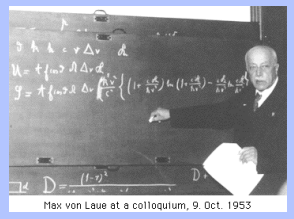
The Kaiser-Wilhelm Institutes for Chemistry (left) and for Physical Chemistry and Electrochemistry (right) --(1913).

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

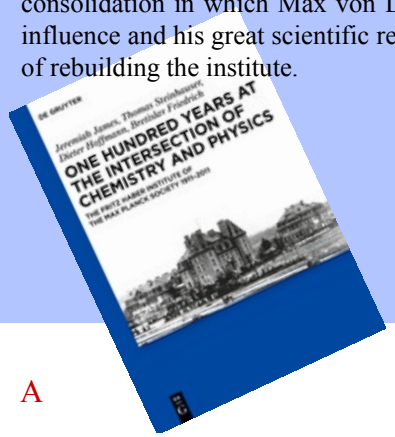
Fritz Haber was appointed director of the institute following the recommendation of the famous Swedish physical chemist Svante Arrhenius. Haber's personality and his previous scientific achievements were considered particularly appropriate for a leader of this new institute, focusing on basic research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

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

1955 **Max von Laue**, director of the institute
1953 Rename in Fritz-Haber-Institut of the Max-Planck-Gesellschaft
1954 **Ernst Ruska**, Scientific Fellow of the institute
1957 "Institute for Electron Microscopy of the Fritz-Haber-Institut".
1959 **Rudolf Brill**, director of the institute, *catalytic properties for heterogeneous reactions, XRD, kinetic measurements*
1969 **Heinz Gerischer**, Dept. of Physical Chemistry, *studies of solid surfaces under ultra-high vacuum conditions and their interaction with gases*
1969 **Jochen H. Block**, *kinetic processes on metal surfaces were studied using field electron and field ion microscopies*
1974 The institute was restructured to consist of three sections which were to combine their collaborative efforts: Physical Chemistry (directors: J. H. Block, H. Gerischer, K. Molière), Structure Research (directors: R. Hosemann, Kurt Ueberreiter), and Electron Microscopy (director: E. Ruska until 1974).
1976 **Elmar Zeitler**, Electron Microscopy
1980 Second reorganization introduced a collaborative structure for the institute with stronger emphasis on surface and interface science.
1980 **Alexander Bradshaw**, Dep. of Surface Physics, *spectroscopy of solid surfaces and the study of chemisorbed molecules*
1981 A. Bradshaw, Scientific Director of BESSY I, 1999 BESSY II, 1997 IPP
1985 **Gerhard Ertl**, Dept. of Physical Chemistry, *structure and chemical reactions on solid surfaces*
1986 Ernst Ruska was awarded the Nobel Prize in Physics
1988 **Matthias Scheffler**, Theory Dept., *surface theory, solid state research, quantum chemistry, computational physics*
1994 **Robert Schlögl**, Dept. of Inorganic Chemistry, *heterogeneous reactions on inorganic surfaces*
1995 **Hans-Joachim Freund**, Dept. of Chemical Physics, *adsorption and reaction on solids, in particular, on oxide surfaces*
2002 **Gerard Meijer**, Dept. of Molecular Physics, *molecular physics using the free-electron-laser*
2007 Gerhard Ertl was awarded the Nobel Prize in Chemistry
2008 **Martin Wolf**, appointed director of Dept. of Physical Chemistry

How to reach the Institute

By Train from Zoologischer Garten station:

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 Tegel Airport:

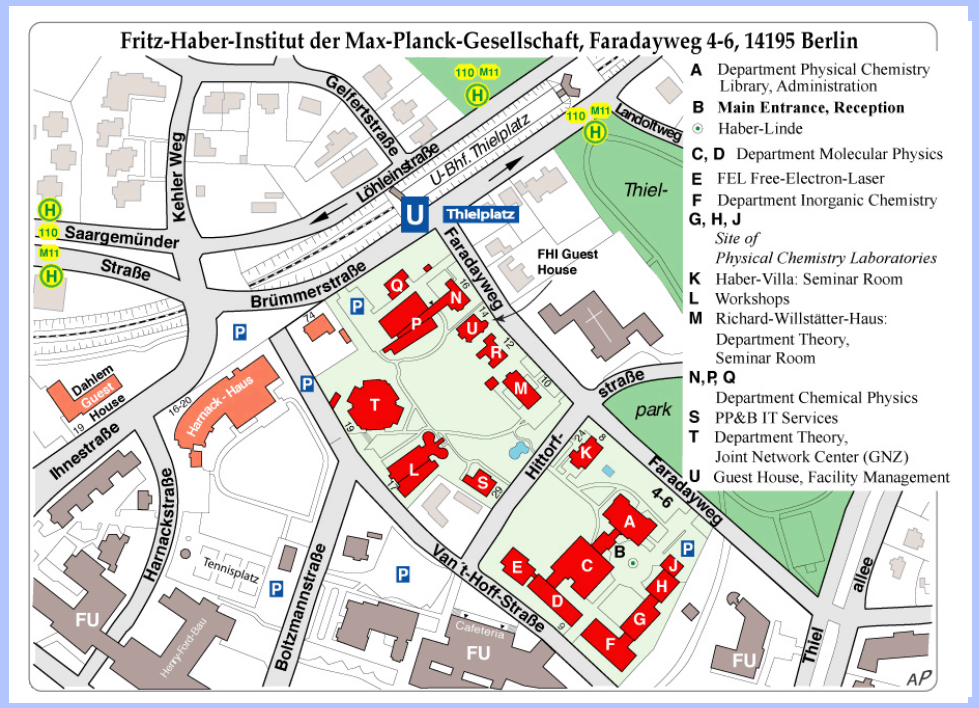
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs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

By Air from Schönefeld Airport:

Take the S-Bahn train S45 in the direction of Westend. Get off at Heidelberger Platz and change to the underground line U3 in the direction of Krumme Lanke. Get off at Thielplatz and take the exit Faradayweg. Turn left and cross the street at the traffic light. Turn right into Faradayweg and follow it for about 200 m; the entrance to the institute is opposite the park. The travel takes between 45 and 60 minutes. The ticket costs 2.30 EUR. A taxi from Schönefeld travels about 45 minutes outside the rush hour and costs about 30 EUR.

By Car:

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



Fritz-Haber-Institut der Max-Planck-Gesellschaft

Faradayweg 4 – 6

14195 Berlin

Germany

You can find more information about timetables, alternative routes, etc. at BVG or VBB

Preface

Director:
Prof. Dr. Robert Schlögl
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Fax: **49 30 8413 4401**
E-mail: **acsek@fhi-berlin.mpg.de**

The department of Inorganic Chemistry at 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.

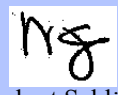
The study of MgO in pure and in deliberately doped forms continued at present gives valuable insights into the mode of operation of the OCM reaction. A thorough statistical analysis of the about 2600 literature reports on OCM (with M. Baerns) yielded some insight into the nature of a possible catalyst 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 arouse. 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.

The mission of the MPI CEC is to understand and develop the chemical processes that we require in order to convert chemical energy carriers. Catalysis is the underlying science and technology. The foundation concept of the Institute assumes that catalysis has a common science base independent of molecular or interfacial catalytic systems. Further, a combination of theory and experiment can deliver the knowledge for designing and optimizing chemical energy conversion reactions. This mission is pursued considering the basic processes of energy storage from renewable primary electricity and its integration into the energy system. The reactions of water splitting and of hydrogenation of N_2 and CO_2 were chosen as key reaction systems. As the AC department forms a bridge between the two institutes FHI and MPI CEC, the activities of the AC department were re-structured to effectively transfer solid-state chemical knowledge to MPI CEC and to benefit from the knowledge on molecular systems available at MPI CEC.

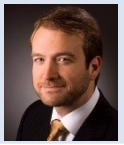
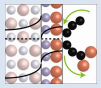
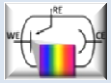
Co-operations are essential for the department. Theory and modeling as well as all the rigorously defined model systems and alternative synthetic concepts are incorporated into the projects through our partners inside and outside of FHI. Academically the department focused on a broad collaboration with 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.

Numerous smaller collaborations are conducted within our BESSY group supporting the broad usage of the ambient pressure XPS facility which was upgraded by an instrument for ambient pressure (500 mbar) XAS spectroscopy.
Latest big achievement is the joint HZB-MPG project called “EMIL”, a high-end photon energy beamline with several end stations. 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 “Carbokat” (with M. Muhler). Industrial collaborations : With BASF our various collaborations are focused through a joint laboratory installed at TUB within the framework of UniCat. With BAYER we collaborate within the “INNOCNT” platform. Further collaboration projects exist with VOLKSWAGEN. 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. Theory support we are receiving form K. Hermann who is strengthening our activities in evaluating X-ray absorption and EELS spectroscopy.



Robert Schlögl

Internal Structure

Reactivity	Electronic Structure	Nanostructures
GL: Dr. Annette Trunschke  	Dr. Axel Knop-Gericke  	Dr. Malte Behrens  
Tel: 49 30 8413 4457	49 30 8413 4422	49 30 8413 4408
E-mail: trunschke@fhi-berlin.mpg.de	knop@fhi-berlin.mpg.de	behrens@fhi-berlin.mpg.de
Scientific Field: Nanostructured MoV catalysts in activation of light alkanes	Metals in selective oxidation reactions	Nano-structured copper and nickel catalysts in CO_2 conversion reactions
Instrumentation: Synthesis, Vibrational and UV-vis spectroscopy, Reactor technology and Catalytic testing	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
Members: 15	18	14
Charge Transport in Catalysis	**Electron Microscopy**	**Electrochemistry**
GL: Dr. Maik Eichelbaum  	Dr. Marc Willinger  	Dr. Julian Tornow  
Tel: 49 30 8413 4566	49 30 8413 4643	49 30 8413 4640
E-mail: me@fhi-berlin.mpg.de	willinger@fhi-berlin.mpg.de	tornow@fhi-berlin.mpg.de
Scientific Field: Semiconductor physics of oxidation catalysts	Microstructural characterization, geometric and electronic structure, in-situ electron microscopy	Li-ion batteries and water splitting
Instrumentation: In situ microwave cavity perturbation technique; In situ microwave Hall effect setup; X-band cw-EPR Bruker ESP 300E; LCR meter Agilent 2 MHz E4980A; Keithley DC Hall effect setup	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
Members: 3	13	7

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

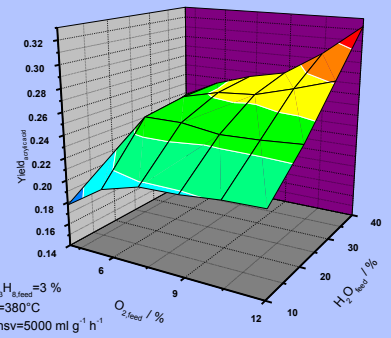
Dr. A. Trunschke

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

The sophisticated formulation and complexity of current heterogeneous catalysts requires the application of controlled synthesis conditions and well-defined chemical precursors 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.

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



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

Examples of the technical equipment:

- Automated laboratory reactor system (Mettler-Toledo Labmax®), analytic autoclave HPM-PT-040 (Premex), parallel microwave reactors Speed*wave* MWS-3 (Berghof)
- Lambda 650 (Perkin Elmer) / Cary 5000 (Agilent) UV-vis spectrometer with Harrick DR accessory for *in-situ* and low-temperature measurements
- Cary 680 (Agilent), 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)

ELECTRONIC STRUCTURE AND ADSORPTION

Dr. A. Knop-Gericke

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

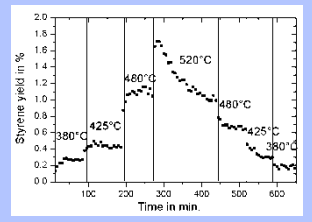
In situ XPS endstation at ISISS

ISISS: Soft X-ray station at BESSY:

The FHI and BESSY installed the ISISS facility (Innovative Station for In Situ Spectroscopy) which 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.) Amongst others these investigations aim e.g. at the identification of correlations between the electronic surface structure of a working catalyst and its catalytic performance or the detection of subsurface species forming under reaction conditions by depth profiling with varying photon energies.

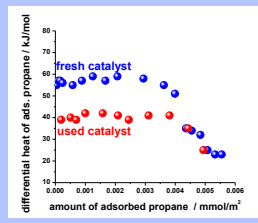
Combined TDS, XPS and reactivity studies of low surface area (model) catalysts

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

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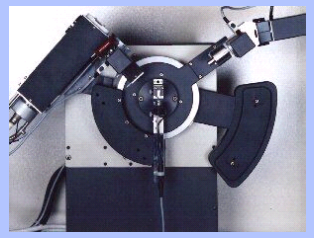
Scaleable and reproducible preparation under controlled conditions is a prerequisite for knowledge-based catalyst design. Precursor phases, intermediates during the preparation process and the final catalyst have to be submitted to comprehensive characterization using various analytical tools. The facilities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

- **Automated laboratory reactor system** (Mettler-Toledo Labmax, photo) for controlled precipitation 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)

ELECTRON MICROSCOPY

Dr. M. Willinger

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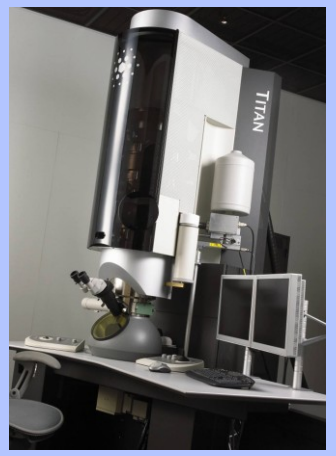
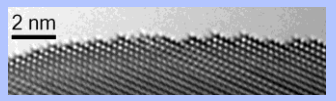
The Electron Microscopy group is equipped with a laboratory for sample preparation and the facilities for ex- and in-situ morphological, compositional and structural characterization of catalyst materials from the millimeter to the Sub-Ångstrøm scale.

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-Ångstrøm 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.



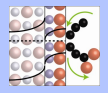
FEI Titan 80-300 aberration corrected TEM.



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

Instrumentation

CHARGE TRANSPORT IN CATALYSIS



Dr. M. Eichelbaum

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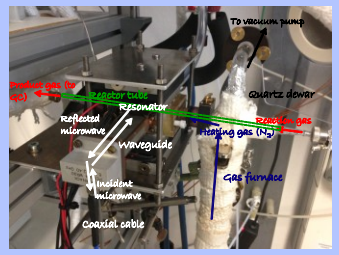
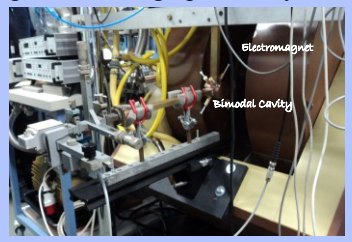
In order to study charge transport in polycrystalline catalysts a new in situ methodology has been developed based on the absorption of microwave radiation. The developed setups allow the absolute determination of the complex permittivity, electrical conductivity, mobility, charge carrier density of powder samples under catalytic operation conditions, overcoming typical problems of conventional conductivity methods such as ill-defined electrode-sample contact resistances.

In situ microwave cavity perturbation technique

MCPT relies on the adiabatic change of the characteristics (resonance frequency, quality factor) of a microwave cavity upon the introduction of a sample with defined permittivity. The developed setup using the TM110 and TM0n0 modes of cylindrical cavities operating between 1 and 20 GHz enable the characterization of powder catalysts in a flow-through fixed-bed quartz reactor with on line gas chromatographic analysis of reaction gases.





In situ microwave Hall effect technique

The method relies also on MCPT, uses a cylindrical bimodal TE112 cavity and is being developed to determine contact-free and in situ the Hall mobility, majority charge carrier type and charge carrier concentration in catalysts under operation conditions.

Complementary techniques

For performing frequency-dependent conductivity measurements an **LCR meter** (Agilent 2 MHz E4980A) and a Keithley van-der-Pauw **DC conductivity** and **Hall mobility** setup are used.
A Bruker ESP 300E X-band **cw-EPR spectrometer** (Figure) is available to characterize paramagnetic metal ions, defects, and radical reaction intermediates on catalysts and to analyze radical reaction intermediates in the gas phase by spin-trapping.

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.

Inert gas atmospheres

Lithium batteries are air sensitive, so we mount and disassemble the cells in argon purged and water free gloveboxes. For the post-cycling analysis we do the spectroscopy either inside a glovebox or use transport systems as we do also for the microscopy.

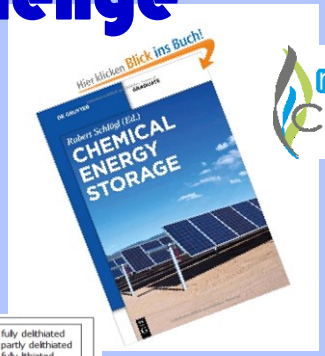
Electrochemical characterization

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 multipotientiostat/-galvanostat (ARBIN BT2143).

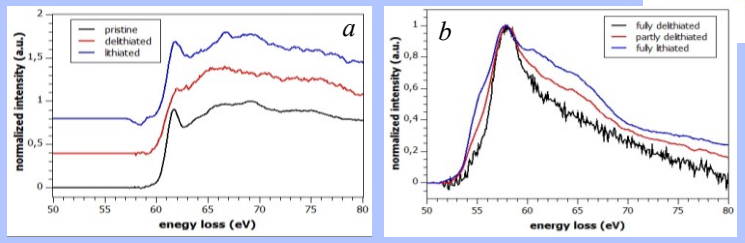
Thin film deposition

For materials to investigate 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. Furthermore we deposit thin metallic films with only a few nanometers thickness by a metal evaporator (Edwards FL 400) for in-situ experiments, either as electrical contacts or as the investigated electrode itself.

The Energy Challenge



We currently focus on electrode materials that are state-of-the-art in battery technology. Our aim is to understand where the charge is stored inside the cathode material and explicitly if the lithium retains also part of the charge.



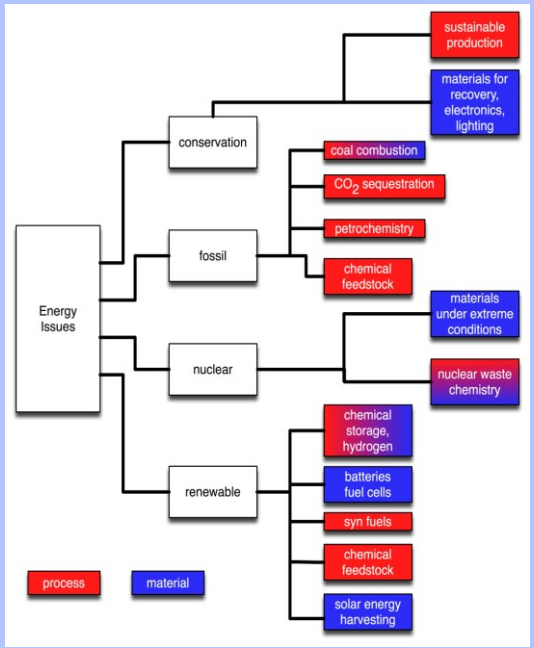
Lithium K-edge and metal M-edge EELS of a) $LiCoO_2$ and b) $LiFePO_4$ at different states of charge.

Systems Approach as a Key for a Sustainable Energy Supply:

- ✓ Fossil energy has a great historical advantage.
- ✓ Energy storage requires excessive activation as the reaction occurs uphill. Kinetics requires a stable product (there is no waste of excess hydrogen as often assumed!).
- ✓ The energy challenge is systemic. (Despite 100 Mtons CO_2 saving through renewable electricity more CO_2 emissions in 2012: rebound effects of the system; despite massive tax advantage little acceptance of compressed natural gas (CNG) as alternative fuel for passenger cars.
- ✓ The solar refinery concept power to chemicals as initiator for power to gas.
- ✓ New catalysts needed (e.g. Pt carbon for water electrolysis).
- ✓ Catalysis as chemo-, electro- and photocatalysis is the enabling basic science of energy storage.

The universal role of chemistry in the energy challenge both for efficiency optimization and for novel processes

From "The solar refinery" by R. Schlögl in Chemical Energy Storage, De Gruyter, Berlin 2013



Chemistry is a platform science in the energy challenge. All major areas of energy conversion and use requite materials or processes provided by chemistry.

Although chemistry is indeed a central science for addressing the energy challenge becomes evident that any meaningful treatment of science and technology for the energy system must be in contact with the non-scientific aspects. Science and technology further must transport its insights to those responsible for decision-making. This is clearly true for the aspects of implementing ready technologies. It is required in addition already at the earliest stages of fundamental scientific knowledge in order to account for the request of modern societies to be "knowledge societies" in which all members participate in detailed decisions on the functioning of the society. As energy supply in all its form is the cross-sectional enabling basis of all individual and collective activities of men it may be concluded that the evolution of the energy system is one of the central activities of organizing a society.

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: *"Nano-structured Copper and Nickel Catalysts in CO_2 Conversion Reactions"*

Electronic Structure and Adsorption: *"Metals in selective oxidation reactions"*

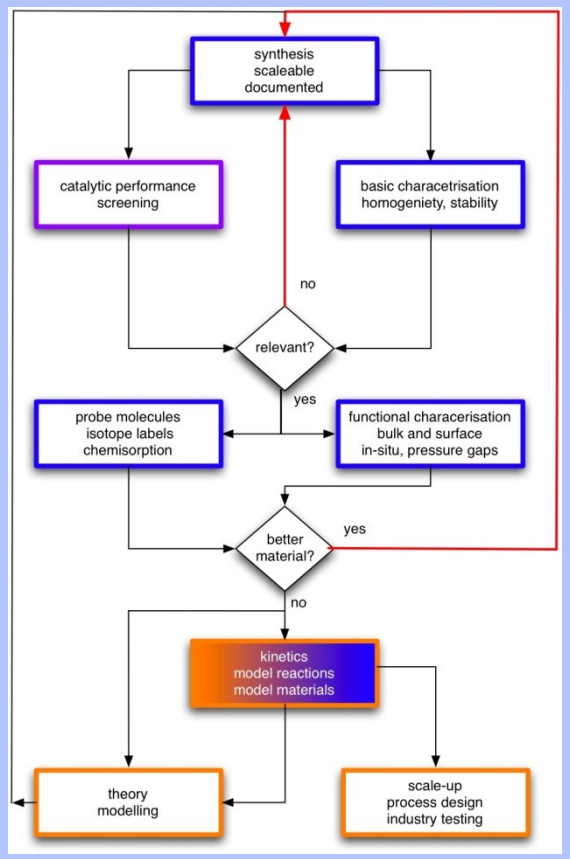
Electrochemistry: *"Li-ion batteries and water splitting"*

Charge transport in catalysis: *"Semiconductor physics of oxidation catalysts"*

Electron Microscopy: *"Microstructural characterization, geometric and electronic structure, in-situ electron microscopy"*

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).

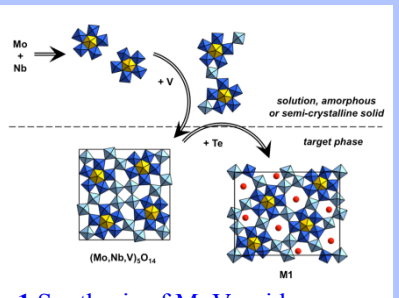
→ We are interested in generic effects: always reproduction of every single experiment.

→ We need quantitative results:
- multiple steady state kinetics
- pressure gaps, wide variations of process conditions
- quantification of structural data.

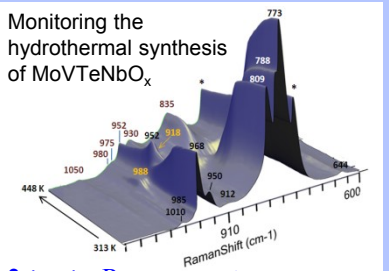
→ We want high-quality representation of results in graphics and images.

Scientific Progress

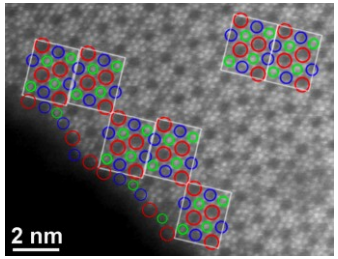
Nanostructured MoV catalysts in activation of light alkanes



1 Synthesis of MoV oxides



2 *in-situ* Raman spectra



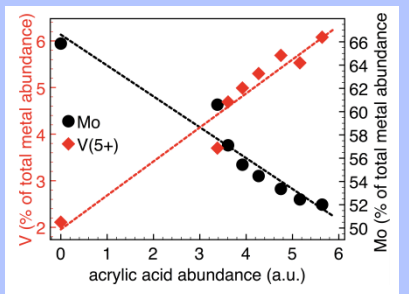
3 HRTEM image of M1 viewed along the <001> zone axis

Background and objective

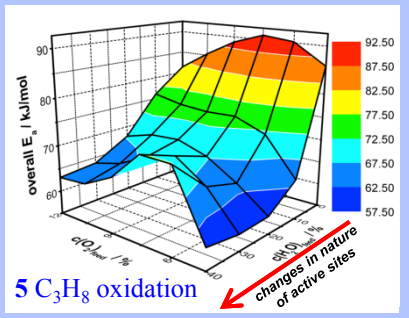
The project is aimed at understanding the factors that primarily determine the reactivity of MoV oxide-based bulk catalysts in oxidative dehydrogenation and selective oxidation of C2-C4 alkanes to valuable olefins, unsaturated aldehydes or acids. The research analyzes similarities and specifics of these reactions addressing the effects of (i) molecular structure of active ensembles on the catalyst surface and nature of defects, (ii) structural motives in the catalyst framework, (iii) chemical and structural complexity, (iv) oxidation state of the elements under reaction conditions, (v) the collective electronic properties of the solid, and (vi) the dynamics of the catalyst surface under varying operation conditions. Doped alkaline earth oxides are included as a model catalyst for the oxidative coupling of methane. Dispersed metal oxide species supported on mesoporous silica and metal oxide free functionalized nano-carbons are applied as model systems to investigate the oxidative dehydrogenation that generally represents the first reaction step in selective oxidation of alkanes. Metathesis and alkane dehydrogenation reactions are involved to understand reactivity at high O_2 conversions. Approaching the redox system of Mo and V from low oxidation states, synthesis and reactivity of carbides are studied.

Results

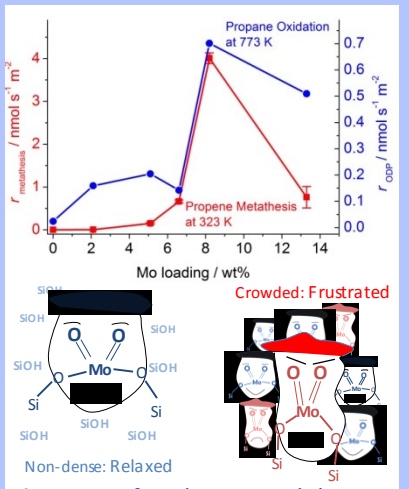
New approaches in hydrothermal synthesis of complex mixed metal oxides are pursued. Target structures are prepared by assembling secondary building units stepwise (**1**). The inorganic synthesis is guided by monitoring reaction intermediates using *in-situ* Raman spectroscopy (**2**). Correlations between structural characteristics, surface termination and catalytic properties in the selective oxidation of propane to acrylic acid have been studied over $MoVTeNbO_x$ model catalysts consisting of an orthorhombic phase called M1 (ICSD 55097, **3**). Acrylic acid formation correlates with surface depletion in Mo^{6+} and enrichment in V^{5+} sites in presence of steam in the feed (**4**). Kinetic analysis confirmed that the active surface changes dynamically with the reaction conditions (**5**). Model catalysts composed of highly dispersed molybdenum oxide supported on silica show a steep increase in metathesis of propene and oxidative dehydrogenation of propane at 8% of Mo loading. Based on DFT calculations, NEXAFS spectra at the O-K-edge at high Mo loadings are explained by distorted MoO_4 surface species. Limited availability of anchor silanol groups and lateral interactions at high loadings forces the MoO_4 groups to form more strained configurations with increased reactivity (**6**).



4 *In-situ* XPS: Surface composition of working M1



5 C_3H_8 oxidation



6 Impact of strain on reactivity

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Financial support:
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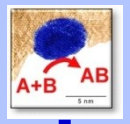
BMBF 03X0204C

Scientific Progress

Nano-structured Copper and Nickel Catalysts in CO_2 Conversion Reactions



1. CO_2 Reduction Reactions

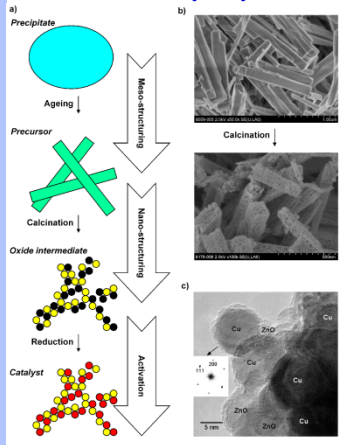
Methanol synthesis

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

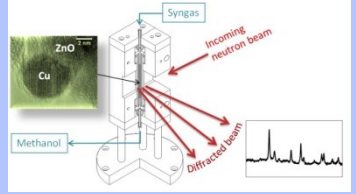
Dry Reforming of Methane

$CH_4 + CO_2 \rightarrow 2CO + 2H_2$

2. Cu/ZnO Catalyst Synthesis



3. In-situ Neutron Diffraction



Cu/ZnO/(Al_2O_3) for Hydrogenation of CO_2 to Methanol

Methanol is one an important base chemical in chemical industry and a potential clean fuel. Furthermore, it has the potential to act as a sink for the greenhouse gas CO_2 by chemical fixation. Nanostructured Cu/ZnO/Al_2O_3 is industrially applied in the methanol synthesis process, but details of the reaction mechanism and the understanding of the so-called Cu-ZnO synergy are still under investigation.

Goal of our work is to understand the multi-step catalyst synthesis (2) to establish a basis for further and more rational optimization. We aim at finding (micro)structure-performance relationships to better understand the nature of catalytically active ZnO-promoted "methanol copper". Careful synthesis is always followed by a comprehensive characterization of the nano-structured ensemble present in highly active catalysts using a variety of complementary (in-situ) techniques. For example, in-situ neutron diffraction was applied to study an industrial-like catalysts under true working conditions (3).

In cooperation with a theory group, this approach was recently applied to elaborate a model for the active site of methanol synthesis based on a defect-function-relationship (4).

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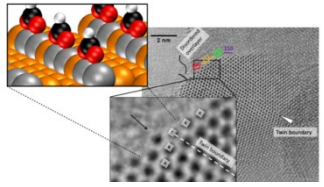
Technical University Berlin (T. Ressler)
Ruhr-University Bochum (M. Muhler)

The synergetic effect of ZnO on the Cu-based catalysts was studied by comparison of a Cu/ZnO (CZ) with a Cu/MgO (CM) catalyst prepared by co-precipitation (5). Only after subsequent addition of ZnO by impregnation (CMZ) was a high performance in CO_2 hydrogenation obtained, supporting the formation of unique Cu-Zn sites for this reaction. Interestingly, the performance in a CO_2-free CO/H_2 feed was much higher without ZnO indicating the presence of different sites for CO or CO_2 hydrogenation.

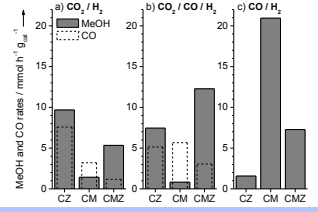
Novel Catalysts for CO_2-Reforming of Methane

The catalytic conversion of anthropogenic CO_2 to useful chemicals is the goal of the BMBF-funded CO_2RRECT project ("*CO_2-Reaction Using Regenerative Energies and Catalytic Technologies*"). We have developed a novel Ni-based catalyst for the dry reforming of methane that converts CO_2 and CH_4 into synthesis gas (CO/H_2). The material was prepared by a precursor route and consists of a Ni-nanoparticles embedded in a matrix of $MgAl_2O_4$ (6). This composite catalyst shows an excellent thermal stability against sintering, thus allowing applications of high reactions temperatures that were found to suppress undesired coking of the catalyst.

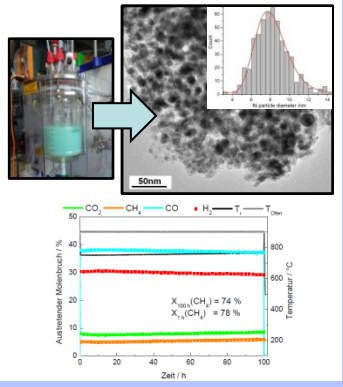
4. Active Site Model



5. The Role of Zinc Oxide



6. CO_2 Conversion with CH_4



External collaborations :
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MPI for Chemical Energy Conversion (M. Bukhtiyarova)
Helmholtz-Zentrum Berlin (D. Wallacher, M. Hävecker)

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.

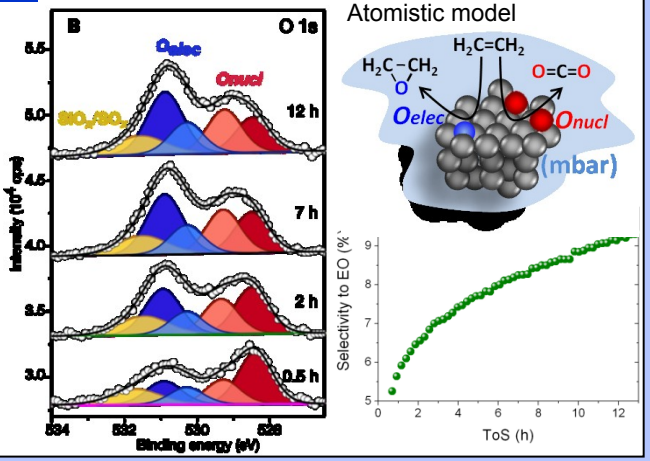
Ethylene epoxidation

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

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

A closer look at the active sites on Ag

Correlation of catalytic performance with surface chemistry



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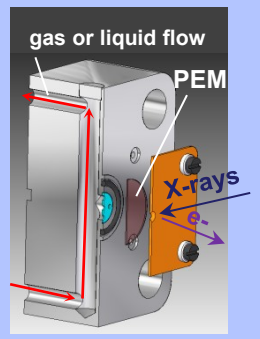
Scientific Progress

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 electro-catalyst. 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 beam-line (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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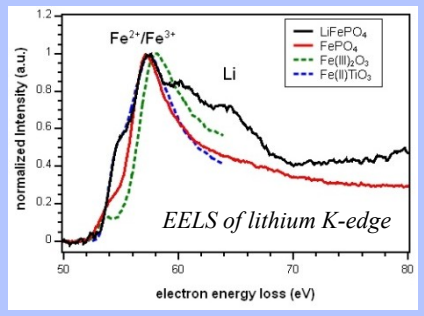
Scientific Progress

Electrochemistry

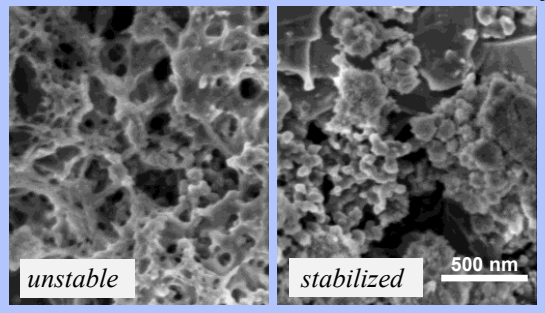
Electrochemical processes in lithium-ion batteries



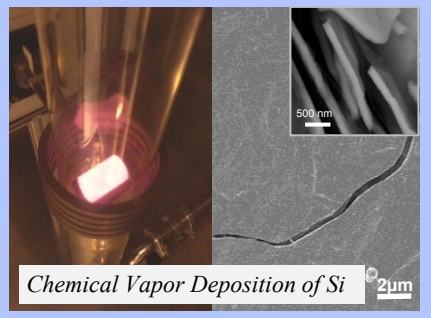
Among energy storage devices, lithium ion batteries exhibit a large gravimetric and volumetric energy density. Nonetheless substantial enhancements in energy storage capacities, charging times and long term stability are necessary to meet today's and future demands. New materials and concepts need to 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 $LiFePO_4$ as the cathode material and a silicon based battery anode. Electron energy loss spectroscopy for $LiFePO_4$ indicates that lithium in the olivine structure is not purely ionically bonded. This deduces a new understanding of the charge storage mechanism towards a more complex charge distribution model, since the lithium keeps part of its charge.

A breakthrough on the anode side would be silicon as material for battery electrodes, since it shows an about 10 times higher charge storage capacity compared to conventional carbon based anodes. Itse major drawback is an insufficient cycling stability. This electrode degradation is dependent on the interface chemistry, which is determined by the electrodes surface and the electrolyte composition. Anodes with low stability show a continuous growth of an interface layer with cycling, while additives to the electrolyte impede the growth rate of this so called solid electrolyte interphase

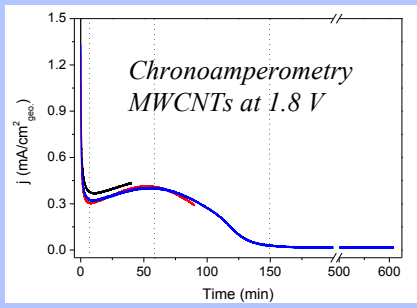


SEM of silicon based anodes after 100 cycles



(SEI), which results in stabilized batteries. Elemental analysis shows that silicon is partly dissolved into the SEI. Hence this is a degradation mechanism assuming that charge is predominantly stored in the bulk silicon phase, which was verified by thickness dependent charge capacity measurements on silicon thin films, prepared by chemical vapor deposition (CVD). Our main focus lies on the influence of the interface chemistry on the battery stability, so we also vary the silicon interface chemistry by modification with CVD. Besides a better understanding of the chemical processes upon electrode degradation this provides also an electrolyte independent route to stabilize silicon based anodes for lithium ion batteries.

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 oxygen evolution reaction (OER), which operate at a low overpotential and are stable even under alternating load. Besides the catalyst a stable electrically conducting support is needed to increase the surface area of the catalyst. A standard catalyst support with sufficient conductivity is carbon, but it is thermodynamically unstable under OER conditions. Our investigatins show that unlike in thermal oxidation processes under electrochemical OER conditions a stable oxide forms on multiwall carbon nanotubes ,which hinders the dissoluton of carbon and stabilizes them. This opens their suitability as a support material.

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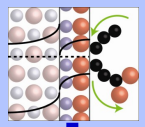
MPI for Colloids and Interfaces (Prof. Antonietti)

Financial support:
Volkswagen AG

Scientific Progress

Charge transport in catalysis



While the bonding and reaction of molecules on metal oxide surfaces is usually described by localized surface molecular models, macroscopic collective electronic properties of the catalyst – that can control the surface charge density, surface oxidation state, surface oxygen vacancy density, etc., and hence the formation of local active sites – have to be considered as well for a complete description of the catalytic working mode.

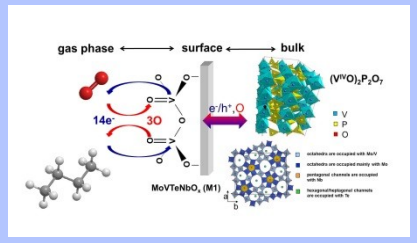


Fig. 1

Moreover, many oxidation reactions, e.g., the oxidation of alkanes to oxygenates, are accompanied with the transfer of a high number of electrons and oxygen atoms across phase boundaries. The aim of our research is thus 1) to determine the (collective) electronic bulk and surface properties, 2) to investigate the kinetics and thermodynamics of charge transport across bulk/surface interfaces of real and model catalysts under reaction conditions, and 3) to understand the consequences on the catalytic activity and the selectivity to the desired reaction products.

In order to investigate charge transport in working catalysts we are developing and applying novel in situ techniques such as a contactless electrical conductivity (Fig.2) and microwave Hall effect method (Fig. 3), both based on the microwave cavity perturbation technique, and try to rationalize the achieved insights into the charge transport in catalysts by studying the electronic and chemical surface and bulk structure with in situ X-ray photoelectron, X-ray absorption, and electron paramagnetic resonance spectroscopy.

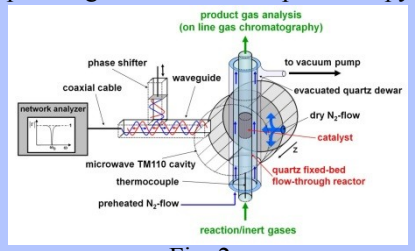


Fig. 2

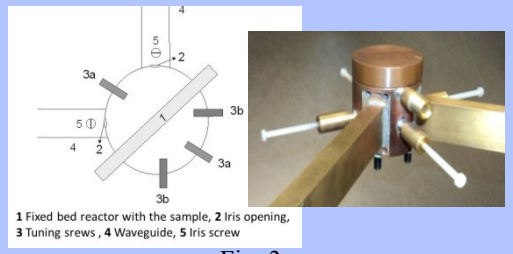


Fig. 3

Results: Microwave conductivity and X-ray photoelectron spectroscopy were applied to measure the response of the electrical conductivity (Fig. 4: vanadyl pyrophosphate (VPP), in n-butane (C4) oxidation), secondary electron cutoff, valence band (Fig. 5: VPP), and core level spectra, and the thus determined work function Φ, band bending qV_B, and electron affinity χ on different reaction conditions (e.g. under reducing (C4), oxidizing (O2), and selective C4 oxidation (C4/O2) conditions). We could prove that the selective phase-pure catalysts VPP and MoVTeNb oxide (orthorhombic M1 structure) react like semiconducting gas sensors on the different conditions. The electronic structure and modulated charge transport properties can be explained by a rigid band model of a semiconductor heterostructure comprising the bulk in contact with a 2-dimensional vanadium oxide surface layer and a Fermi level adjusted by the respective gas phase (Fig. 6: VPP). Whereas the gas phase dependent electron affinity is explained by the formation or modification of surface dipoles, the systematic valence band and core level binding energy shifts and hence band bending are caused by a Fermi level pinning to the surface state potential modulated by the gas phase.

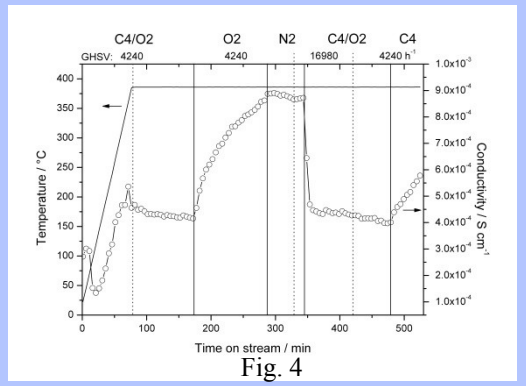


Fig. 4

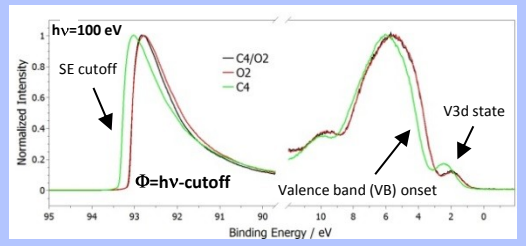


Fig. 5

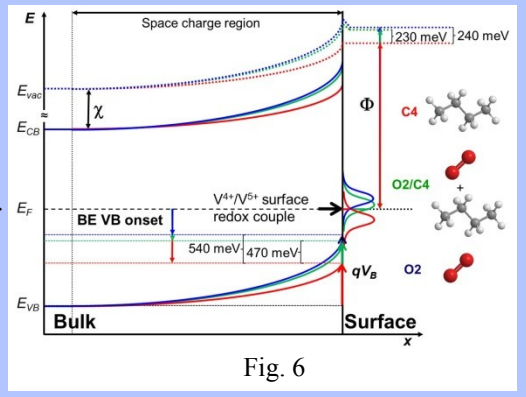


Fig. 6

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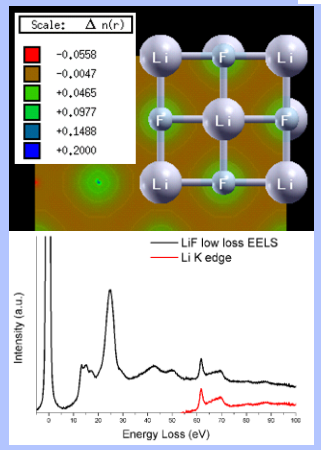
Scientific Progress

Structural and chemical information at the atomic scale

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 $LiFePO_4$ 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 imperfectness. Further research is aiming on improved cycling behavior of $LiFePO_4$.

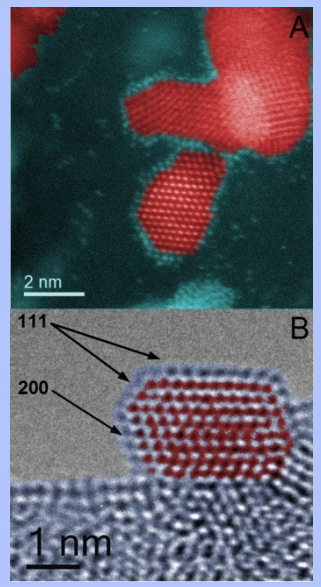


Electron density plot (top) and EELS spectrum of LiF

Surface termination and metal-support interactions

Using a combination of electron microscopy tools such as HRTEM, HAADF STEM and EELS we investigate the role of catalyst preparation, support structure and Pt particle size on the degradation of fuel cell catalysts. Observation of the dissolution and sintering behavior of Pt particles on the atomic scale combined with a detailed study of the geometric and electronic structure of the carbon support provides a deeper understanding of the involved degradation mechanisms.

For an atomistic understanding of the "Strong Metal Support Interaction" (SMSI), we study industrial catalysts as well as realistic model systems using aberration corrected TEM. Information about surface termination and interface structure is complemented by simultaneously acquired information about the electronic state via EELS.



A: HAADF STEM image of Pt on modified carbon. B: FeO SMSI overgrowth on a supported Pt particle.

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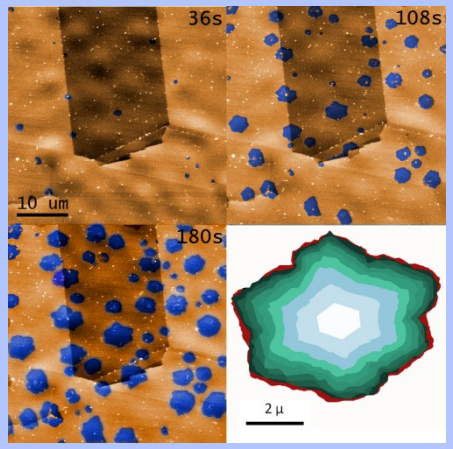
Scientific Progress

Electron microscopy of dynamic processes

In-situ studies by Environmental SEM

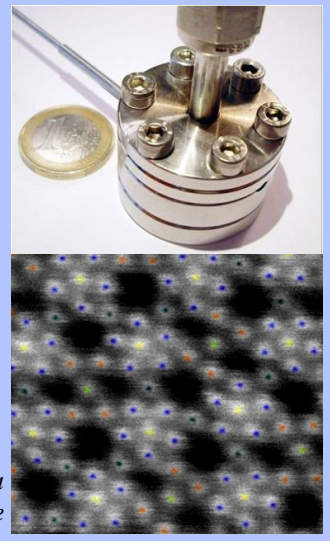
For in-situ studies of dynamic processes, we use a modified ESEM (Environmental Scanning Electron Microscope). The instrument is equipped with a laser heating stage, a gas feeding system with mass flow controllers and a mass spectrometer. The set-up allows direct observation of reaction induced morphological 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, nickel and platinum catalysts.



Snapshots recorded during in-situ low pressure metal catalyzed CVD growth of graphene on copper in the ESEM at 1000 C and $2 \cdot 10^{-2}$ Pa.

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.

Scientific Progress

Theory Support

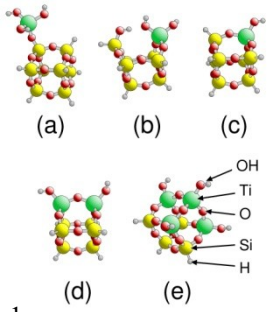


Fig. 1a

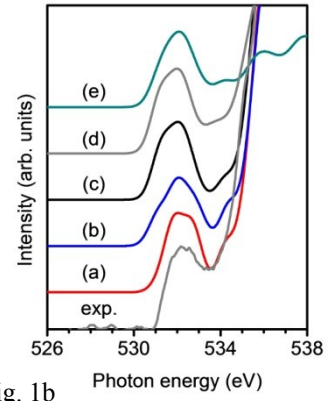


Fig. 1b

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_2, 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_4 units dominate the experimental spectrum Further, the theoretical results suggests 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.

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 simulation yield detailed information about possible reaction steps that can help the experimentalist to get deeper insight into properties of realistic catalysts.

As an example, we have studied the selective catalytic reduction (SCR) of NOx with NH_3 over vanadium based metal-oxide catalysts (VOx) where details of the reaction mechanism are still under discussion. Here adsorption and (de)hydrogenation of NH_3, 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 $V_2O_5(010)$ surface. NH_3 is found to interact only with the $V_2O_5(010)$ surface in the presence of OH groups (Brønsted acid sites) where it can form a rather strongly bound surface NH^{4+} 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_2NO intermediates.

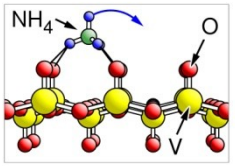


Fig. 2

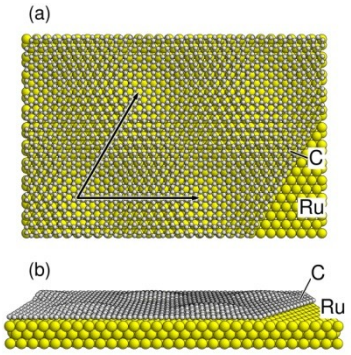


Fig. 3

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)Rα overlayers and explains the surprising behavior of moirons as well as their shapes, see Fig. 3.

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Distinguished scholar, Institute of Computational and Theoretical Studies, Department of Physics, Hong Kong Baptist University, 2011- 2014.

Photo of the AC department members

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

AC Department trip from 18. - 20. June 2013 to Dessau

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The library of the FHI, together with the scientists, has developed an elaborated and well established Open Access workflow. Thereby we have achieved 30% of Open Access publications. The publications are collected in the repository of the MPS, MPG PuRe. Our perspective for the next decade is to increase our Open Access publications.

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.

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

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Publications

The following publication list 2011 – 2013 is generated by PubMan. http://pubman.mpdl.mpg.de

2011

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Inventors: R. Schlögl, A. Trunschke

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

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Patents

1993 - 2013

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

Guest - lectures
2011 - 2013

Date	Speaking Guest	Titel
12.01.2011	**Prof. Vera Bolis** 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	**Prof Wolfgang Bensch** Inst.f.Anorg.Chemie, Uni Kiel	Following chemical reactions with in-situ scattering techniques
16.02.2011	**Prof. Martin Schmal** COPPE Rio de Janeiro, Brazil	$LaCoO_3$ and $LaCoMeO_3$ Perovskite for Partial Oxidation of Methanol and Selox reaction
23.02.2011	**Prof. Thorsten Ressler** Technische Universität Berlin	Structure function relationships of molybdenum oxide based model systems for selective oxidation catalysts
09.03.2011	**Prof. Ronald Imbihl** Institut für Physikalische Chemie und Elektrochemie Leibniz-Universität Hannover	Facts and fiction in the electrochemical promotion of catalytic reactions
14.03.2011	**Prof. Markus.Antonietti** MPI of Colloids and Interfaces, Dept. of Colloid Chemistry, Research Campus Golm	A Chimie Douce of metallic and semiconducting Carbon-nanostructures
23.03.2011	**Prof. Dr. Liu Hao Tjeng** Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden	Hard x-ray photoelectron spectroscopy: recent developments and new opportunities
11.04.2011	**Prof. Serena DeBeer** Cornell University, Chemistry and Chemical Biology	Valence to Core X-ray Emission as a Probe of Biological and Chemical Catalysis
15.04.2011	**Dr. Vladimir V. Roddatis** National Research Center "Kurchatov Institute"Moscow	High Resolution Scanning Transmission Electron Microscopy of Heterostructures
17.05.2011	**Prof. Reinhard Stößer** Humboldt University of Berlin, Institute of Chemistry, Dept. of Physical Chemistry	ESR application to selected solids and fluids using probes of different spin states

Date	Speaking Guest	Titel
27.05.2011	**Dr. Nicole Grobert** University of Oxford.Department of Materials	Tailoring Carbon-based nanomaterials
23.06.2011	**Prof. Christian Pettenkofer** Helmholtz Zentrum Berlin	Energy converting interfaces-surface science on semiconductor junctions
28.06.2011	**Prof. Gary L. Haller** Dept. of Chemistry Yale University	Aqueous Phase Reforming over Carbon Nanotube Supported Catalysts for Hydrogen Production
17.08.2011	**Prof. Dr. Christian Hess** Eduard-Zintl-Institut für Anorg. Chemie und Phys. Chemie Technische Universität Darmstadt	Probing catalysts, batteries and gas sensors at work
22.08.2011	**Dr. Karl J. J. Mayrhofer** Max-Planck-Institut für Eisenforschung, Düsseldorf	Catalysis in electrochemical reactors - fundamental investigations for real applications
07.10.2011	**Professor Wolfram Jaegermann** Technische Universität Darmstadt	Innovative photovoltaic energy converters: A challenge for materials science and thin film technology
12.10.2011	**PD Dr. Werner Lehnert** 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	**Dr. Karl Doblhofer** Fritz-Haber-Institut der MPG	Struktur einer zukunftsfähigen Energieversorgung
29.02.2012	**Dr. Dirk Niemeyer, Dr. Jörg Wölk** SASOL Germany GmbH Werk Brunsbüttel	Development of tailor made Catalyst Supports from an industrial perspective
11.04.2012	**Prof. Dr. Michael Smith** Department of Chemical Engineering Villanova University	Catalysis on Real Surfaces - Studies on the effect of surface roughness

Guest - lectures

2011 – 2013

Date	Speaking Guest	Titel
30.05.2012	**Dr. Dominik Samuelis** Max Planck Institute for Solid State Research, Stuttgart, Germany	Ionic / electronic wiring of lithium ion battery electrodes
13.06.2012	**Prof. Dr. Israel Wachs** Lehigh University Department of Chem. Engineering Bethlehem, PA, USA	Pervasiveness of Surface Metal Oxide Phases in Mixed Metal Oxide Catalysts
19.06.2012	**Prof. Dr. Dieter Vogt** Eindhoven Uni. of Technology Schuit Institute of Catalysis Laboratory of Homogeneous Catalysis	Catalytic Cascade Reactions Involving Hydroformylation
25.06.2012	**Prof. Dr. Israel Wachs** 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 WOx/SiO_2 Catalysts
27.06.2012	**Prof. Dr. Israel Wachs** Lehigh University Department of Chem. Engineering Bethlehem, PA, USA	New Insights into the Water-Gas Shift Reaction over Bulk Cr_2O_3*Fe_2O_3 Mixed Oxide Catalysts: A Combined Operando Raman-IR-XAS-MS Investigation
11.07.2012	**Prof. Dr. Lars C. Grabow** Assistant Professor of Chemical and Biomolecular Engineering University of Houston	Computational Catalysis Approaches for the Synthesis of Chemicals and Liquid Fuels
25.07.2012	**Prof. Dr. Jaeyoung Lee** Ertl Center for Electrochemistry & Catalysis Gwangju Institute of Science and Technology (GIST), South Korea	Oxygen catalysts in electrochemical energy technologies
25.07.2012	**Prof. Dr. Jeffrey D. Rimer** 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	**Prof. Dr. Anders Nilsson** SLAC National Accelerator Laboratory, Stanford University	In-situ X-ray Studies of Photo-and Electrocatalysis

Date	Speaking Guest	Titel
29.08.2012	**Prof. Dr. Michael R. Buchmeiser** Lehrstuhl für Makromolekulare Stoffe und Faserchemie Institut für Polymerchemie, Universität Stuttgart	Oxidic and Non-Oxidic Ceramic Fibers: Synthesis, Structure and Applications
23.10.2012	**Prof. Dr. Elena R. Savinova** 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	**Maya Kiskinova Ph.D. Sc.D.** Elettra Laboratory, Trieste, Italy	Microscopic insights on chemical state and morphology of key components in operating model fuel cells
06.11.2012	**Dr. Cristina Africh** CNR-IOM Laboratorio TASC, Trieste,Italy	Graphene growth on Ni(111): STM movies under in-operando conditions

Date	Speaking Guest	Titel
12.02.2013	**Dr. Claudia Weidenthaler** MPI für Kohlenforschung, Mülheim an der Ruhr, Germany	In situ powder diffraction studies of functional nanomaterials
06.03.2013	**Dr. Valeriya G. Makhankova** National Taras Shevchenko University of Kyiv, Chemistry Department, Ukraine	Direct synthesis: alternative approach to obtain heterometallic complexes as water-splitting catalysts and precursors of binary oxides
30.05.2013	**Prof. Dr. Thorsten Ressler** TU Berlin, Germany	Mo and V containing model catalysts supported on nanostructured oxides for selective oxidation of propene
17.06.2013	**Dr. Felix Studt** SLAC, Berkley, USA (Group of Prof. Jens K. Nørskov, SUNCAT/Photon Science (SLAC))	Activity and Selectivity in syngas conversion to higher alcohols - A DFT study
17.09.2013	**Prof. Dr. Helmut Baltruschat** Institut für Physikalische und Theoretische Chemie der Uni. Bonn, Abt. Elektrochemie	Monoatomic steps and monoatomic chains on surfaces: their role in electrocatalysis and tribology
24.10.2013	**Prof. Cécile Hebert** EPFL Lausanne, Switzerland	Spectroscopy in electron microscopy: 3D EDX with the focused ion beam, large dataset acquired by EFTEM and cathodoluminescence in the STEM

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.			MPG	2004 continuing	Dr. A. Trunschke	Prof. Dr. S. Klokishner (, Acad. Sci. Moldova)	

MAX-PLANCK-GESELLSCHAFT

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	2012 - 2015	Dr. M. Willinger	Dr. A. Gajović (Zagreb, Kroatien)	Dr. A. Gajović

DAAD

External Funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Oxidnitride 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
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)	
Nanostructured Ta-oxide nitride and Chalcopyrite-based Thin Film Composites and Co-Catalysts for Visible Light-driven Overall Water Splitting	SPP 1613	BE 4767/2-1	DFG	2012-2015	Dr. M. Behrens	Prof. M. Lerch, Dr. A. Fischer, Dr. Th. Schedel-Niedrig	
In-situ Neutron Diffraction of Solid Catalysts	BE 4767/1-1		DFG	2010	Dr. M. Behrens	Dr. K.D. Liss (BRAGG Institute, AUS)	
Neue kostengünstige und nachhaltige Materialien für die PEM-Elektrolyse zur Herstellung von H_2 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	http://www.unicat.tu-berlin.de	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. 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
Neue Katalysatoren für die saure Wasserelektrolyse		PSFHI 261	BASF	7.1.2013- 2016	Prof. R. Schlögl Dr. M Willinger	Prof. R. Schlögl	
Mo-based catalysts in olefin metathesis		PSFHI 255	Mitsubishi Chemicals	2008-2012	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. 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_2 als Kohlenstoff-Baustein unter Verwendung überwiegend regenerativer Energie	CO_2RRECT	PSFHI 109	BMBF	01.04.2011 - 31.03.2014	Prof. R. Schlögl Dr. M. Behrens		
Contruction of a photon energy beamline and several endstations @ BESSY	EMIL		BMBF HZB MPG	2010-2012	Prof. R. Schlögl 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

Cluster of Excellence CoE

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

unicat
Unifying Concepts in Catalysis

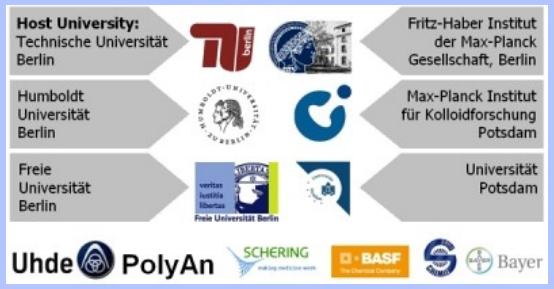
What is UniCat ?

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

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



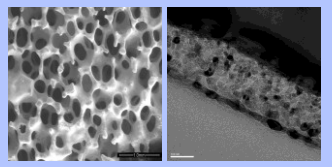
http://www.unicat.tu-berlin.de

Coordinator of the FHI der MPG, Dept. of AC until 06/ 13:
Prof. Raimund Horn
horn@tuhh.de

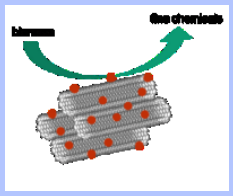
Prof. R. Horn (Pincipial Investigator and junior scientist in Research Fields A1, C3, D1, and D2 in Prof. Schlögl's group) has accepted an appointment at the Hamburg University of Technology [Technische Universität Hamburg-Harburg (TUHH)]. R. Horn succeeds Prof. Frerich Keil at the Institute of Chemical Reaction Engineering of TUHH on 1st July 2013. Being involved in BasCat Raimund Horn will still be connected to UniCat.

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, Dr. S. Mavlyankariev, P. Schwach, Dr. H. Schwarz, Dr. A.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
(Dr. S. 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

Grafol

Graphene Chemical Vapour Deposition: Roll to Roll Technology

What is Grafol ?

Because of its unique electrical, mechanical, surface and thermal properties a single layer of sp^2 bonded carbon, also known as Graphene, is considered as a well suited component in next generation electronic, optoelectronics and microsystems. However, large scale mass production with high quality and large lateral extensions has been proven difficult to achieve. The Grafol project aims to develop the first roll-based chemical vapour deposition (CVD) machine for the mass production of few-layer graphene (FLG) for transparent electrodes for LED and display applications, and adapts the process conditions of a wafer-scale carbon nanotube growth system to provide a low-cost batch process for graphene growth on silicon.

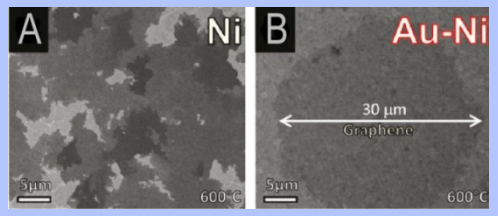
Cooperation Partner:

Fritz-Haber-Institute, University of Cambridge, AIXTRON, Philips, IMO, Thales Research and Technology, Intel Performance Learning Solutions, CEA, Cambridge CMOS sensors, EPFL, CNRS, Technical University of Denmark, Graphenea

Catalyst-support and catalyst-carbon interactions during the chemical vapor deposition (CVD) of graphene are systematically analyzed by combining various structure sensitive methods, such as environmental TEM, Raman Spectroscopy and XRD, with time-resolved *in-situ* XPS.

In-situ XPS Characterization of Graphene growth on various substrates:

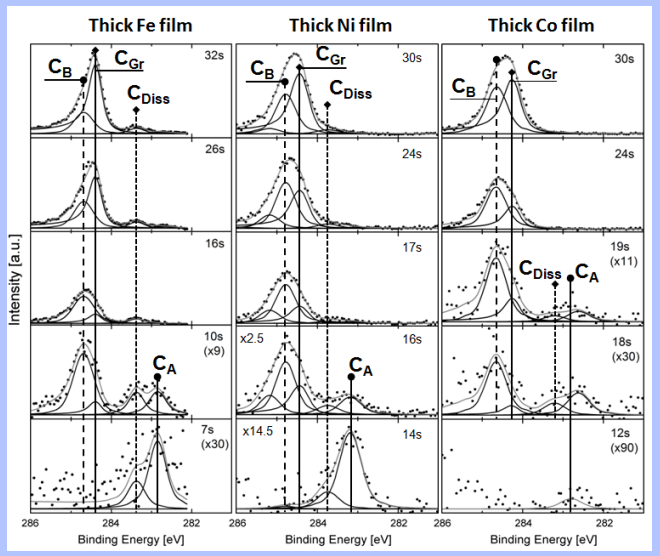
A key to the large scale growth of Graphene and FLG is the carbon solubility in the catalyst. While graphene can be grown solely via a surface carbide at considerably low temperatures and pressures (< 400 C, 10^{-7} mbar), the resulting graphene film quality is rather poor with respect to island size, growth rate and defect density.



SEM micrographs of as-grown graphene (C_2H_2 CVD in $2x10^{-6}$ mbar for 2min at 600 C, cooled at ~25 C/min) on Ni (A) and Au(3 nm)Ni(530nm) (B) representative of an intermediate stage of growth.

Contact:
Dr. Axel Knop-Gericke or Dr. Raoul Blume
knop@fhi-berlin.mpg.de, raoul@fhi-berlin.mpg.de

A more suitable growth mode yielding in less defective graphene involves higher temperatures (~550 C) and moderate pressures in the 10^{-6} to 10^{-5} mbar range. Utilizing transition metal films of moderate thickness (0.1-1µm), carbon atoms dissociated on the metal surface can easily diffuse into the bulk of the film. Due to the limited thickness, a saturation is quickly reached and the surplus carbon atoms start to form graphene and FLG. Several growth mechanisms are involved which are manifested by distinct peaks in C1s XP spectra recorded during the growth. After an incubation time, depending on substrate thickness and carbon solubility, a surface carbide (C_A) is formed while simultaneously dissolved carbon (C_{diss}) appears near the surface. Graphene growth is then initiated in form of epitaxial graphene (C_B) forming out of the surface carbide and decoupled, rotated graphene (C_{Gr}) forming at a high rate at defective surface sites. Hence, a crucial factor to limit the surface carbon yield to form graphene is the exposure time. Formation of FLG or graphite is manifested by further increase of the C_{Gr} intensity.
Alloying the catalyst with Au not only improves the quality of the grown graphene but also increases the lateral extension of the obtained graphene islands.



Left to right: C1s spectra recorded during the onset of graphene growth during C_2H_2 CVD of 100 nm Fe (550 C, 10^{-6} mbar), 530 nm Ni (600 C, $2x10^{-6}$ mbar) and 300 nm Co (550 C, 10^{-6} mbar) films deposited on SiO_2. The time scale illustrates the incubation time.

http://www.grafol.eu

PIRE: PARTNERSHIPS *for* INTERNATIONAL RESEARCH & EDUCATION

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

University of New Mexico, USA

Iowa State University, USA

Universtiy 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

Utrecht University, Netherlands

Twente University, Netherlands

The University of Turku, Finland

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.

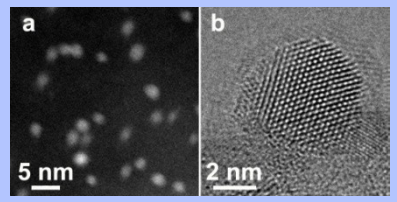
The UNM PIRE Program is funded by NSF grant OISE 0730277.

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

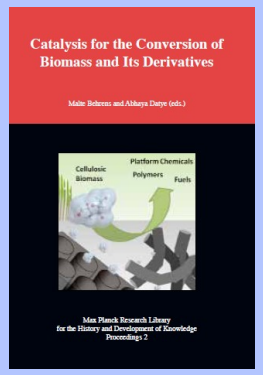
In the framework of the PIRE program, the Department of Inorganic Chemistry at FHI acts as a German host for student from the US sites. It offers its infrastructure and expertise to resolve scientific questions in a collaborative manner ideally within short-term projects of several months.

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



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

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

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

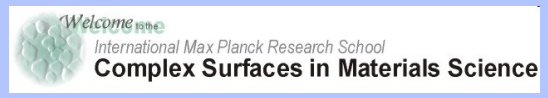
Teaching Activities

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.ht
"Modern Methods in Heterogeneous Catalysis Research" is a class aimed at giving advanced students, who are interested or involved in catalysis research, insight into the methods of catalyst preparation, catalyst testing, and catalyst characterization. The class consists of a series of individual and largely independent lectures given by different instructors.



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

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

Hong Kong Baptist University, Institute of Computational and Theoretical Studies, Department of Physics, Hong Kong
Instructors: K. Hermann
"Structural Properties of Surfaces"

Practical Courses

jugend forscht

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

Gerrit Anders (18) *August 2013*

Nach den zwei Wochen am Fritz-Haber-Institut im August 2013 bin ich mir sicher: Ich möchte später selbst forschen. Besonders faszinierend war für mich das "In-situ-Rasterelektronenmikroskop". Damit ist es möglich, Reaktionen auf einem Katalysator zu beobachten, während sie ablaufen. Zu sehen war das Graphen-Wachstum auf Metalloberflächen. Graphen ist der Stoff mit dem ich mich auch in meinen Jugend-forscht-Experimenten beschäftigt habe. Doch auch viele andere Apparaturen und Arbeitsmethoden, mit denen man Katalysatoren charakterisieren kann, konnte ich kennenlernen wie: XRD, IR-Spektroskopie, Mikrokalorimetrie oder auch die Transmissionselektronenmikroskopie. Aber nicht nur mit der Analyse von Katalysatoren, sondern auch mit deren Synthese konnte ich mich beschäftigen. So lernte ich unter anderem die Synthese mittels Sprühtrockner und die Hydrothermalsynthese in einem Autoklaven, einem speziellen Druckgefäß. kennen. Ganz herzlichen Dank an die Wissenschaftler am Fritz-Haber-Institut, die sich viel Zeit genommen haben, mich in Ihre Arbeitsfelder einzuführen.

Spray drying in technical scale for rapid and continuous solidification and drying.

LetteVerein

Occupation practical course

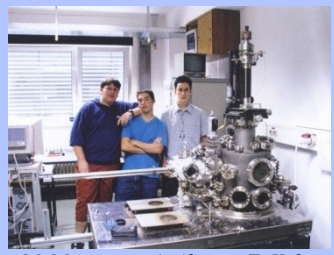
Today the Lette Foundation incorporates five more or less independent educational institutions. Courses are currently offered for the following diplomas in the following departments: Technical Assistant in Metallography and Physical Material Analysis Chemistry and Biology Electronics and Data Processing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

Nadine Schechner *(3.-18.1.2005)*

Das 4-wöchige Berufspraktikum am FHI verging viel zu schnell. Es waren eindrucksvolle 4 Wochen. Ich lernte viele neue Labor-Geräte und Labor-Apparaturen kennen sowie neue Messtechniken, konnte aber auch gelerntes anwenden. Alles war sehr spannend für mich.

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

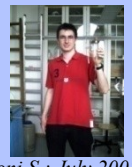
Pupil practical course

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. VOx/SBA-15) bei tiefen (flüssiger Stickstoff) und höheren Temperaturen. Die FTIR – Spektroskopie war meine dritte und letzte Station. Neben Probenvorbereitungen in KBr – Pressling und selbsttragender Presslingsform, untersuchte ich zunächst Karbonatgruppen auf LiMgO und anschließend Brönstedt/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

Early insight into the world of science

Schoolgirls visited the FHI (2005 …2013).

Have a go at a real chemical laboratory and

- **Prepare a chemical compound that really pops**
- **Test your jewelry on nickel**
- **Distinguish different colored foils**

24 preschoolers visited the FHI (2013).
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

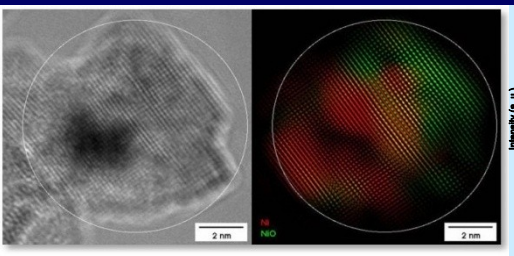
Children examining each other with a magnifying lens

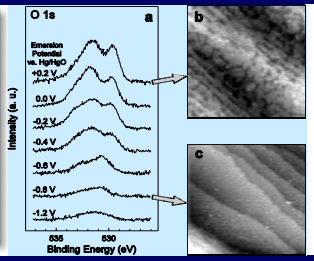
Visiting the library

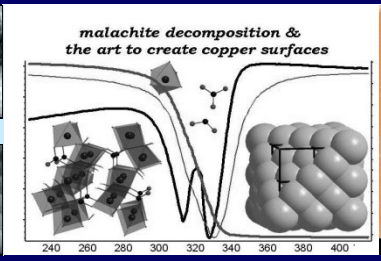
The children used both stereo and optical microscopes to examine flies, moldy bread, leaves, and more

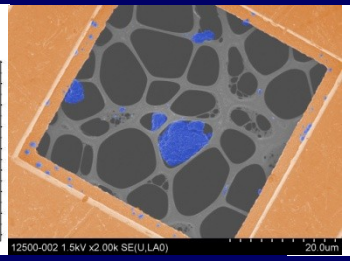
http://www.fhi-berlin.mpg.de/acnew/department/pages/youngpeople.html

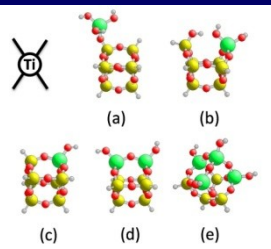
Notes

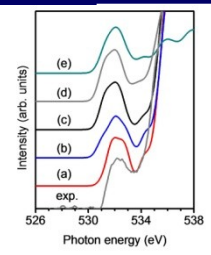


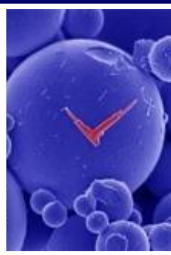




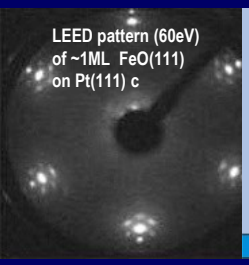


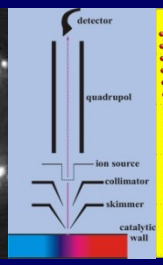


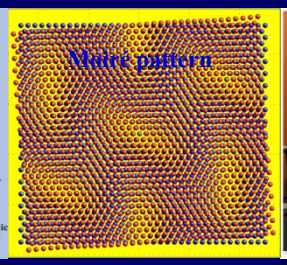


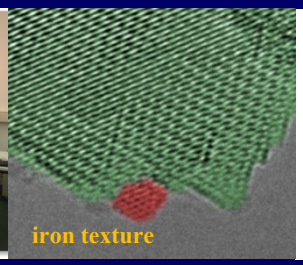


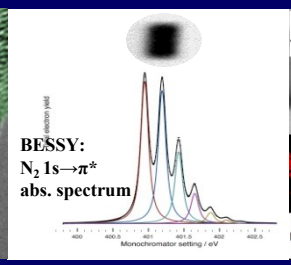
http://www.fhi-berlin.mpg.de

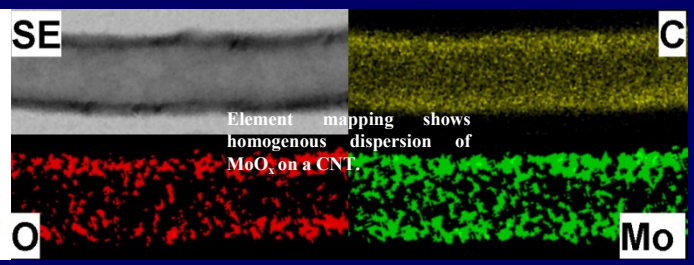












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