DEPARTMENT OF

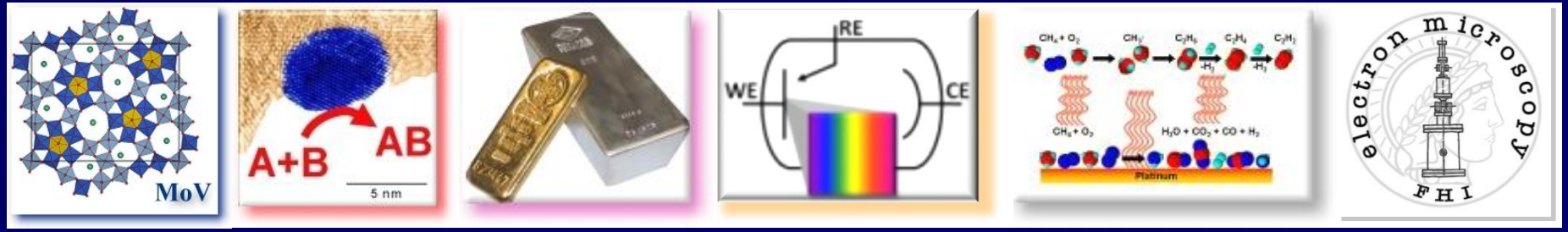
MAX-PLANCK-GESELLSCHAFT

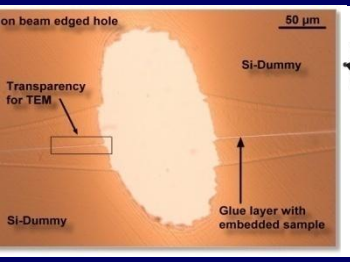
INORGANIC CHEMISTRY

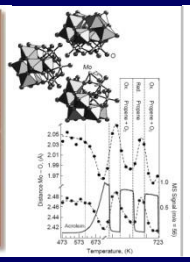
AC FHI

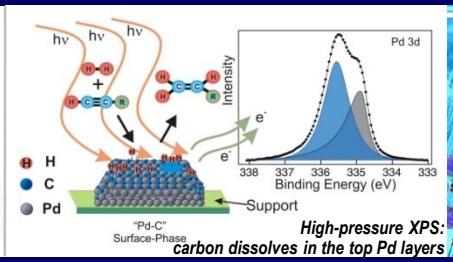
FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT

October 2011 / 7th Edition

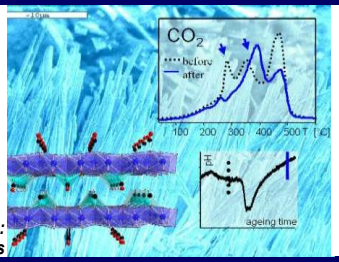


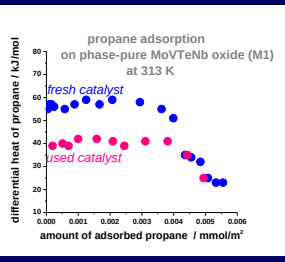


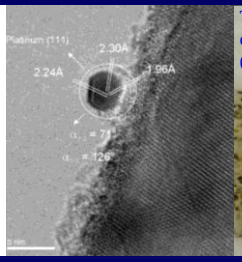




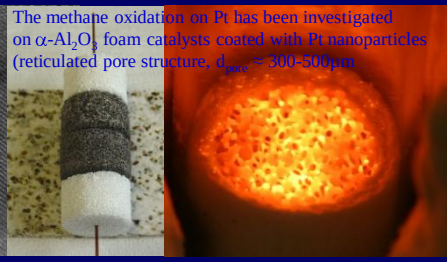
High-pressure XPS: carbon dissolves in the top Pd layers







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)



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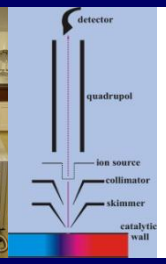
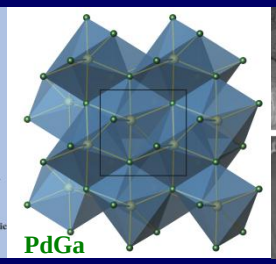
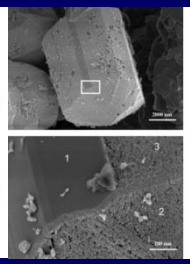
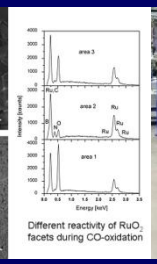
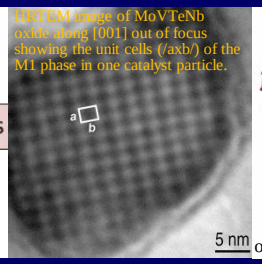


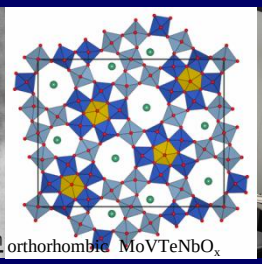




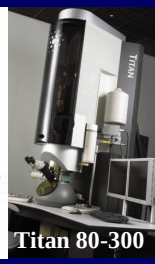




HRTEM image of MoVTeNb oxide along [001] out of focus showing the unit cells (/axb/) of the M1 phase in one catalyst particle.



orthorhombic $MoVTeNbO_x$



Titan 80-300

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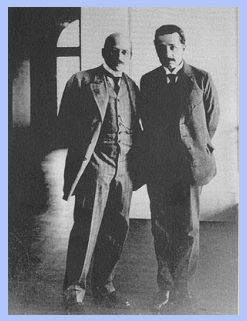
History of the Fritz-Haber-Institut

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

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

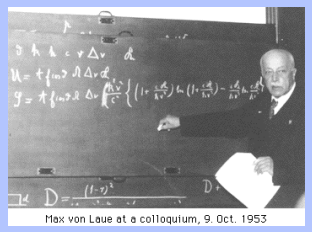
What is now called the Fritz-Haber-Institut of the Max-Planck-Gesellschaft was founded in 1911 as the Kaiser-Wilhelm-Institut for Physical Chemistry and Electrochemistry, together with the Kaiser-Wilhelm-Institut for Chemistry. These were in fact the first two institutes of the Kaiser-Wilhelm Society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



Fritz Haber (left) and Albert Einstein (right) at the "Fritz-Haber-Institut" (1915).

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

In 1951, at the age of 71, Max von Laue became chief director of the institute. This started a new period of consolidation in which Max von Laue applied all his influence and his great scientific reputation to the task of rebuilding the institute.



Max von Laue at a colloquium, 9 October, 1953

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

How to reach the Institute

MAX-PLANCK-GESELLSCHAFT

By Train from Bahnhof Zoologischer Garten:

Take U-Bahn U9 direction Rathaus Steglitz. Change at Spichernstrasse. Take U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 30 min. Costs are about Euro 2,00. Taxi takes about 20 minutes outside rush hours. Costs are about 15 Euro.

By Air from Flughafen Tegel:

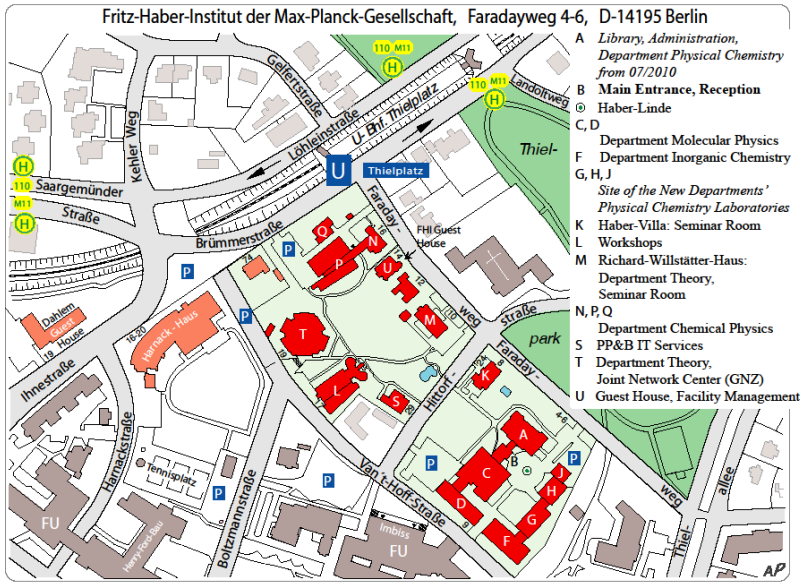
Take bus 109 to Jakob-Kaiser-Platz (about 3km away). From there take subway U7, direction Rudow. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 50 min. Costs are about Euro 2,00. A Taxi is somewhat faster, about 25 minutes outside rush hours. Costs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

By Air from Flughafen Tempelhof:

Take subway U6 direction Alt-Tegel, change at Mehringdamm, take U7 direction Rathaus Spandau. Change at Fehrbelliner Platz to U3 direction Krumme Lanke. Go off at Thielplatz. Travel takes about 30 min. Costs are about Euro 2,00. Taxi takes about 20 minutes outside rush hours. Costs are about 15 Euro.

By Car:

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



Fritz-Haber-Institut der Max-Planck-Gesellschaft

Faradayweg 4 – 6

14195 Berlin

Germany

Preface

Director:
Prof. Dr. Robert Schlögl
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E-mail: **acsek@fhi-berlin.mpg.de**

The department AC in the Fritz-Haber-Institute aims to gain a generalized understanding of heterogeneous catalysis as a multi-scale phenomenon. To achieve this goal the department develops and applies in situ methodology and combines the obtained information with kinetic data. The rationale behind this approach is the realization that catalysts are dynamic materials whose active centres are formed or transformed under reaction conditions.

A substantial evolution occurred with the dedication of our research towards energy-related topics. In particular, the activation of small molecules such as water, CO_2 and CH_4 are long-standing issues in catalysis bearing now a much larger relevance in the context of storing regenerative energy in chemical bonds. This insight and the results from the collaborative Max-Planck research network enerchem together with the successful integration of electrochemistry into the department gave rise to the recent developments.

All projects in the departments are directed towards the relation between a chemical reaction of interest and its coupling to the material dynamics of the catalyst used to achieve the transformation. We continued finding multiple evidences that this coupling is strong in the sense that a given catalyst performs differently beyond pure surface coverage effects under different reaction environments. This has the consequence that in-situ analysis is not a pleasant addition to catalyst characterisation but is essential in finding the working catalyst structure. It also has the consequence that a catalyst can perform qualitatively different under modified reaction conditions trough enhancing various parts of the complex reaction network standing behind most desired target reactions. Kinetic analysis of systems thus requires studying the performance in a field of relevant parameters rather than at a fixed set of conditions. This is being executed at present with the M1 system in selective oxidation of propane and with copper in C1 hydrogenation. With metal catalysts this behaviour was studied for the quite dynamical systems of silver and ruthenium. To our surprise also the quite stable intermetallic compound Pd2Ga seems to exhibit this behaviour acting as “palladium-like” at low temperatures and as “alloy-like” at high temperature counter-intuitive to expectations about segregation and to the results of scaling law analysis.

These examples confirm our general approach that the separation of a catalytic problem in independent studies of its kinetics and its material science gives at best information about the boundary case of minimal reactivity but will fail in describing the structure-function relation under high-performance conditions. The traditional view that structural complexity is an addition to performance of a catalytic system but can be neglected in first approximation when analyzing the function is questionable from our collected experience.

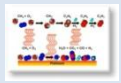
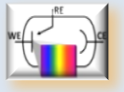
An illustrative example for this insight is the evolution of the CoE project on OCM catalysis. Only due to the intense collaboration between the model studies led in the CP department and performance studies led by the AC department in collaboration with the TUB it was possible to prove convincingly that the “well-known” Li-MgO system is only a transient system with continuous degradation to a residual small activity of defects in pure MgO and not the over 800 times studied prototype catalyst of methane activation.

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

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

Co-operations are essential for the department. Theory and modelling as well as all the rigorously defined model systems and alternative synthetic concepts are incorporated into the projects through our partners inside and outside of FHI. Academically the department focussed on a broad collaboration with the Technical University Berlin (TUB) through the collaborative research network SFB 546 and through the CoE UniCat (anchoring partner: R. Schomäcker). International major collaborations: the synthesis mechanism of nanocarbon is studied with the University of Cambridge (J. Robertson) partly supported by EU projects. The biomass conversion activity partly initiated by the CoE UniCat is now conducted within the PIRE collaboration (A. Datye) centred at Iowa State University (B. Shanks) and Univ. of Albuquerque. Numerous smaller collaborations are conducted within our BEESY group supporting the broad usage of the ambient pressure XPS facility which was upgraded by an instrument for ambient pressure (500 mbar) XAS spectroscopy as announced in the last report. In collaboration with Uppsala university (J. Nordgren) and with the ALS we explore the potential of RIX as in-situ method using as example the silver-oxygen system in selective oxidation. Other collaborative projects are the “Pd project” encompassing groups in Austria (B. Klötzer, M. Rupprechter) and the US (D. Zemlianov), the “intermetallics” project conducted with the MPI CPFS (Dresden) (J. Grin, M. Armbrüster), the contribution to “Carboscale” (with M. Muhler and W. Wirth) and various other projects within the framework of the national competence network on nanocarbon “INNOCNT”. Industrial collaborations : We expect to start in the CATLAB cooperation with Clariant (former SüdChemie) . With BASF our various collaborations will be focussed through a joint laboratory installed at TUB within the framework of UniCat. With BAYER we collaborate within the “INNOCNT” platform and together with the TU Berlin in a multi-national project on the chemo- and electro-catalytic oxidation of HCl to chlorine (“Deacon”). The FHI-internal collaboration is continuing on multiple projects. With the CP department we collaborate on the issue of ultra-thin oxide over-layers and are deeply connected through the OCM issue. A visual element of the collaboration with the TH department is the continuation of the work of K. Hermann after his formal retirement in the AC department where he will strengthen our activities in evaluating X-ray absorption and EELS spectroscopy. With the MP department we will engage in searching for adequate uses of the new FEL facility for advanced applications of low-energy radiation in catalysis science.

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	Copper and palladium catalysts in C1 chemistry
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 desortion, TP reaction, calorimetry, BET	Synthesis, Elemental analysis, X-Ray and Neutron diffraction, TG, DSC, EXAFS
Members: 18	18	19
High Temperature Catalysis	**Electron Microscopy**	**Electrochemistry**
GL: Dr. Raimund Horn  	Dr. Marc Willinger  	Dr. Julian Tornow  
Tel: 49 30 8413 4420	49 30 8413 4643	49 30 8413 4640
E-mail: horn_r@fhi-berlin.mpg.de	willinger@fhi-berlin.mpg.de	tornow@fhi-berlin.mpg.de
Scientific Field: High temperature catalysis research	Microstructural characterization, geometric and electronic structure	Li-ion batteries and water splitting
Instrumentation: High temperature high pressure reactor for spatial profile measurements, Laser Spectroscopy (Raman, LIF), Molecular Beam Mass Spectrometry (MBMS)	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	Potentiostats/Galvanostats, Gloveboxes, Metal evaporation
Members: 7	9	11

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

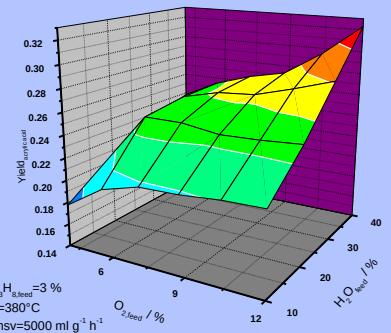
Dr. A. Trunschke

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 chemicals for their reproducible preparation. The work of the group is targeted on a deeper understanding of **catalyst synthesis** ranging from the assembly of molecular building blocks in solution to phase transformations during thermal pretreatment procedures. New synthetic concepts are developed using **automated laboratory reactor systems for precipitation and hydrothermal synthesis** equipped with probes for measuring pH, conductivity, turbidity, viscosity, pressure, temperature, RAMAN and UV-vis spectra. The thermal treatments are performed in rotating furnaces under controlled atmosphere.

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

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:

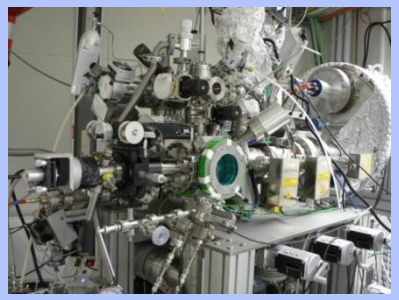
- Automated laboratory reactor system (Mettler-Toledo Labmax®), analytic autoclave HPM-PT-040 (Premex), parallel microwave reactors Speed*wave* MWS-3 (Berghof)
- Lambda 650 UV-vis spectrometer (Perkin Elmer) with Harrick DR accessory
- IFS 66 FTIR (Bruker) and Spectrum 100 FTIR (Perkin Elmer) for in-situ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

ELECTRONIC STRUCTURE AND ADSORPTION

Dr. A. Knop-Gericke

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

ISISS: Soft X-ray station at BESSY :

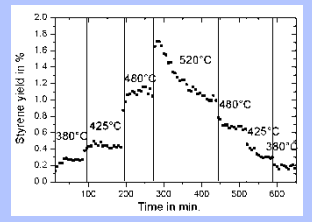


In situ XPS endstation at ISISS

BESSY and the FHI installed the facility ISISS (Innovative Station for In Situ Spectroscopy). ISISS consists of 3 main parts: a) the in situ XPS endstation, b) a state of the art soft X-ray beamline, and c) a permanent infrastructure on site for experiments with a chemical background. This facility allows measurements of XP and XA spectra in the soft energy range under reaction conditions (mbar pressure range, T <700 C.) One aim of these investigation is the identification of correlation between the electronic surface structure of a working catalyst and its catalytic performance. Subsurface species were observed under reaction conditions by the help of photon energy variation (depth profile).

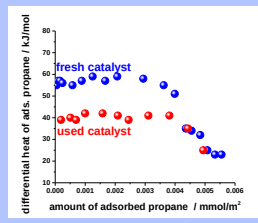
Combined TDS, XPS and reactivity studies of low surface area (model) catalysts

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



Measurement of isotherms & differential heats of adsorption by microcalorimetry

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



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

Instrumentation

NANOSTRUCTURES

Dr. M. Behrens

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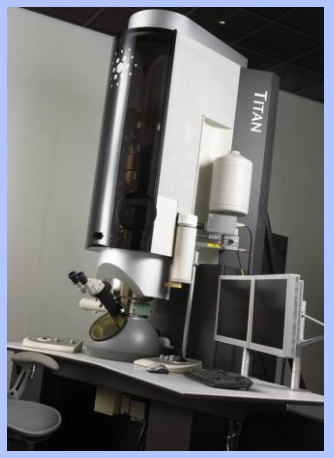
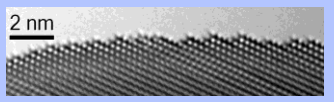
The Electron Microscopy group is equipped with a laboratory for sample preparation and the facilities for ex- and in-situ morphological, compositional and structural characterization of catalyst materials from the millimeter to the Sub-Ångstrøm scale.

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.



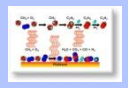
FEI Titan 80-300 aberration corrected TEM.



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

Instrumentation

HIGH TEMPERATURE CATALYSIS



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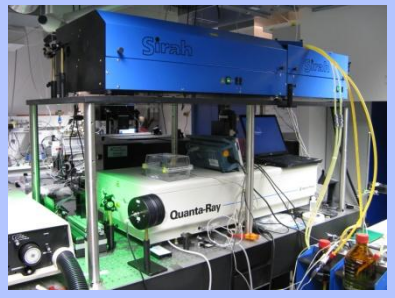
Dr. R. Horn

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

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

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

• **Various pulsed and CW lasers** are operated in the high temperature catalysis lab as excitation source for in-situ Fluorescence and Raman Spectroscopy (Spectra Physics Stabilite 2018 Ar+/Kr+, Spectra Physics Series 2000 Ar+, Coherent Verdi-V10 Nd:YVO4, Spectra Physics Wave Train, Quanta Ray Pro 230 30Hz Nd:YAG, Sirah Cobra Stretch Dye Laser).



ELECTROCHEMISTRY

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The analysis of electrochemical reactions by only electrical measurements gives a rather speculative picture upon the occurring chemistry. Consequently we have the infrastructure to prepare and perform electrochemical experiments, but additionally apply microscopic and spectroscopic techniques provided by the electronic structure and the electron microscopy group. Furthermore we develop experiments to combine these methods towards in-situ investigations of electrochemical reactions.

Gloveboxes

Battery cells are mounted before and disassembled after a cycling experiment in an argon purged and water free glovebox. A second argon purged glovebox is designed for direct electrochemical water splitting experiments. Both gloveboxes allow for an inert transportation of the electrochemically tested materials to further analytics.

Potentiostats/Galvanostats

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

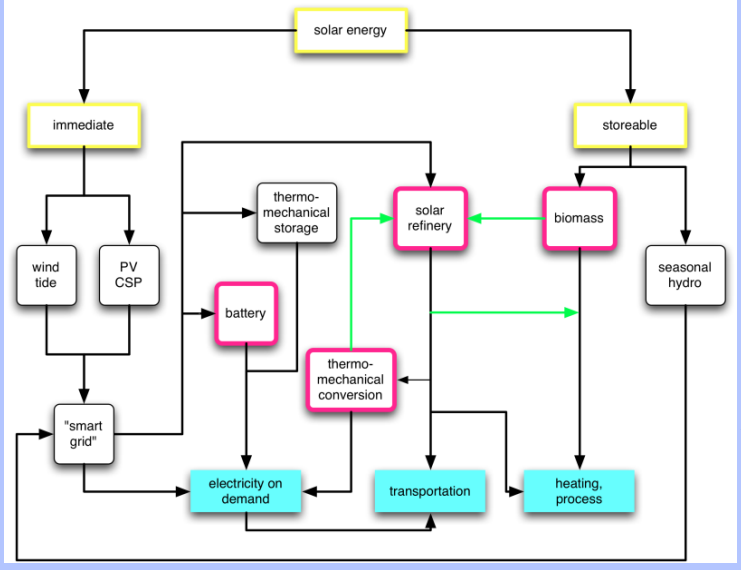
Metal evaporator

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

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. Defining priority areas for basic catalysis science as outlined in Figure 2 led to the development of the concept of a solar refinery recently published. A research strategy resulted towards the fundamentals for such a refinery discriminating the MPG approach from multiple shorter-term oriented efforts going straight for the solution of phenomenological partial solutions.



Simplified flow chart for the grid-scale use of regenerative solar energy. Red boxes indicate areas where catalysis science is critical. Developments of biological systems beyond the sustainable use of biomass are omitted.

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

Scientific Progress

The Department AC is uniquely positioned at the crossroads of synthetic inorganic chemistry and metrology augmented by method development capabilities. Using these elements it seems possible to arrive at the development of truly rational synthesis procedures of nanostructured (defined in several dimensions of size) catalytic materials that can be used as intermediate systems to build the experimental bridge between complex technical and the present model systems. It will be necessary to develop in addition to the bare materials also suitable handling forms for in-situ experimentation such as thin films or nanocrystals. Such catalyst forms require the adaptation of testing environments to allow the novel systems to be used for static model experiments with validated functional performance.

The target of the Department that will be pursued in six of the research areas :

Reactivity : *"Nanostructured MoV catalysts in activation of light alkanes"*

Nanostructures: *"Copper and palladium catalysts in C1 chemistry"*

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

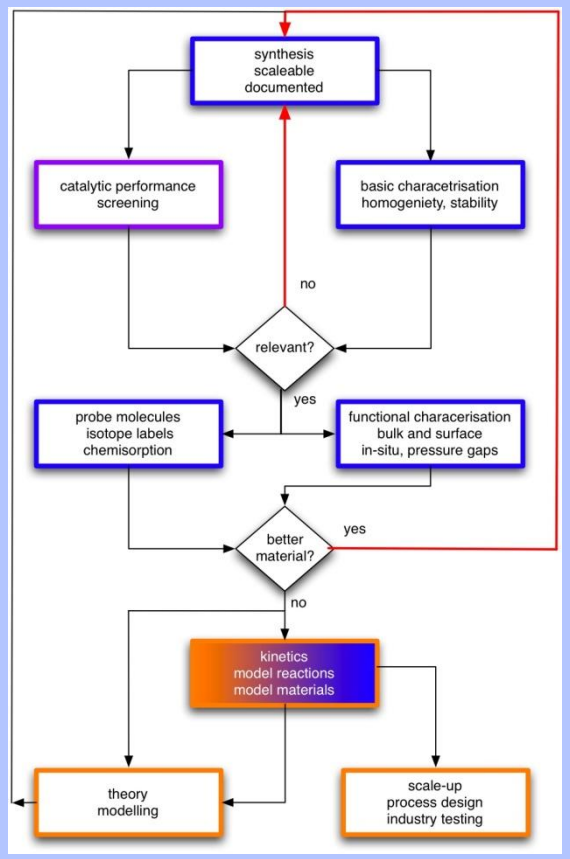
Electrochemistry: *"Li-ion batteries and water splitting"*

High Temperature Catalysis: *"High temperature catalysis research"*

Electron Microscopy: *"Microstructural characterization, geometric and electronic structure"*

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

Research concept



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

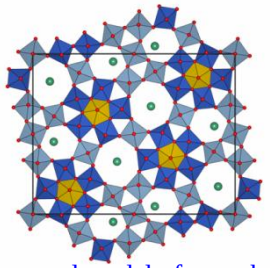
→ We are interested in generic effects: always reproduction of every single experiment.

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

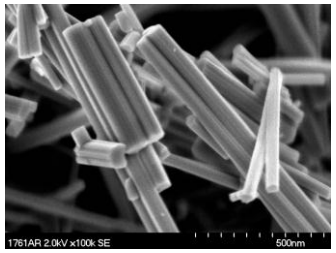
→ We want high-quality representation of results in graphics and images.

Scientific Progress

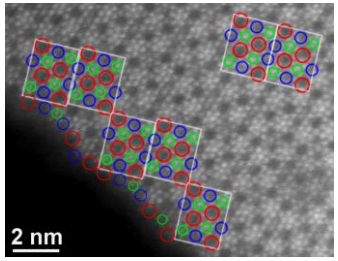
Nanostructured MoV catalysts in activation of light alkanes



1 Structural model of an orthorhombic $MoVTeNbO_x$ phase



2 SEM image of phase-pure M1



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

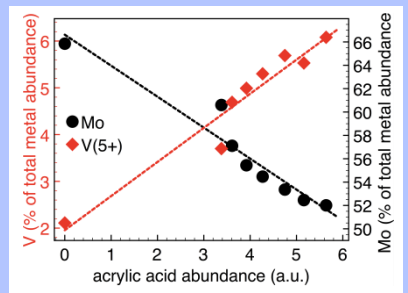
Background and objective

The project is aimed at understanding the factors that primarily determine the reactivity of MoV oxide based catalysts in oxidative dehydrogenation and selective oxidation of C2-C4 alkanes to valuable olefins, unsaturated aldehydes or acids. The research analyzes similarities and specifics of these reactions addressing the effects of (i) molecular structure of active ensembles on the catalyst surface, (ii) structural motives in the catalyst framework, (iii) chemical and structural complexity, (iv) oxidation state of the elements under reaction conditions, (v) the collective electronic properties of the solid, and (vi) the dynamics of the catalyst surface under varying operation conditions.

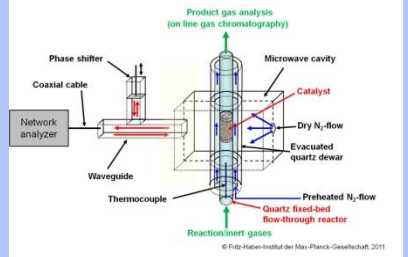
Our research subjects include V phosphates and Mo oxide based bronze structures, which are efficient catalysts for selective oxidation of alkanes. Dispersed metal oxide species supported on mesoporous silica and metal oxide free functionalized nano-carbons are applied as model systems to investigate 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

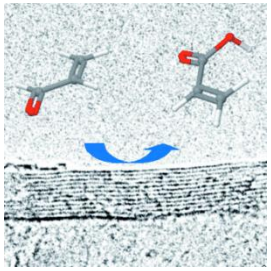
Correlations between structural characteristics, surface termination and catalytic properties in selective oxidation of propane to acrylic acid have been studied over phase-pure $MoVTeNbO_x$ model catalysts consisting of an orthorhombic bronze-like phase denominated as M1 (ICSD 55097, **1-3**). The surface of a highly crystalline M1 has been analyzed by infrared spectroscopy, microcalorimetry, and *in situ* photoelectron spectroscopy. Acrylic acid formation correlates with surface depletion in Mo^{6+} and enrichment in V^{5+} sites in presence of steam in the feed (**4**). The rate of selective oxidation can be limited by electronic and/or ionic transport properties. We have developed a contactless method based on the microwave cavity perturbation technique (MWCPT) to probe the electrical conductivity of heterogeneous catalysts under reaction conditions (**5**). First results show remarkable sensitivity of this method towards gas-phase induced changes on the catalyst (VPO, M1) surface. Applying carbon nanomaterials in oxidation catalysis, we have shown that the graphitic carbon has the potential to selectively mediate the insertion of an oxygen atom into an organic molecule, i.e., acrolein revealing substantial similarities between metal oxide- and carbon-catalyzed reactions (**6**).



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



5 Setup for conductivity measurements with MWCPT



6 Black matter in catalysis: Graphitic carbon catalyzes the insertion of O atoms into acrolein.

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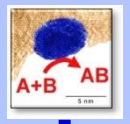
BMBF 033R028B, 03X0204C, SFB 546, Unicat

Scientific Progress

Copper and palladium catalysts in C1 chemistry



1 Methanol chemistry

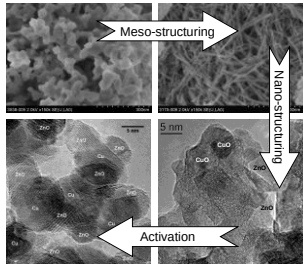
Methanol steam reforming

$CH_3OH + H_2O \rightarrow CO_2 + 3H_2$

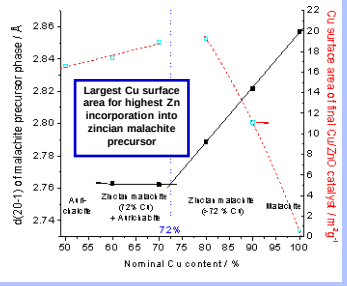
Methanol synthesis

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

2 Preparation of Cu/ZnO



3 Precursor effects



Cu/ZnO/(Al_2O_3) in methanol chemistry

Methanol is one of the most important basic chemicals in chemical industry. Furthermore, it has the potential to act as a sink for the greenhouse gas CO_2 by chemical fixation. In the future, it might also serve as a chemical hydrogen carrier for mobile applications of fuel cells via the methanol synthesis and steam reforming reaction network (1). Nanostructured Cu/ZnO/Al_2O_3 is active in both reactions, but increasing demand and variations in feed gas composition require further optimization.

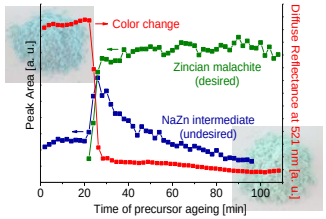
Goal of our work is to understand the industrially applied multi-step catalyst synthesis to establish a basis for further and more rational optimization. We also develop new methods of preparation using novel precursor systems. We aim at finding (micro)structure-performance relations to better understand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

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

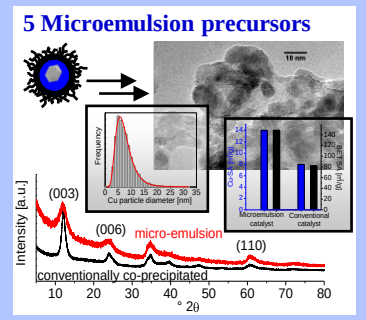
Intermetallic Pd/X catalysts (X=Ga, Zn, …)

Pd/X model systems have been successfully investigated in our department for several years. In order to transfer the fundamental results obtained on model samples to high performance catalysts, the focus of the work in the Nanostructure group is on exploring co-precipitation methods as routes to Pd-based intermetallic catalysts by application of similar preparative concepts as for Cu/ZnO. As first results, a nanoparticulate Pd_2Ga catalyst supported on MgO/Ga_2O_3 has been developed (6). The average size of the intermetallic particles is below 20 nm, which is impossible to achieve by conventional melt synthesis.

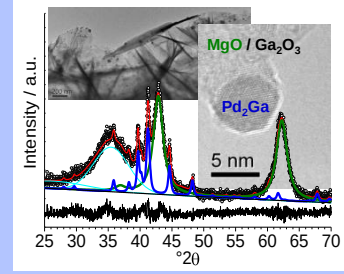
4 Chemistry of ageing



5 Microemulsion precursors



6 Pd_2Ga intermetallic catalyst



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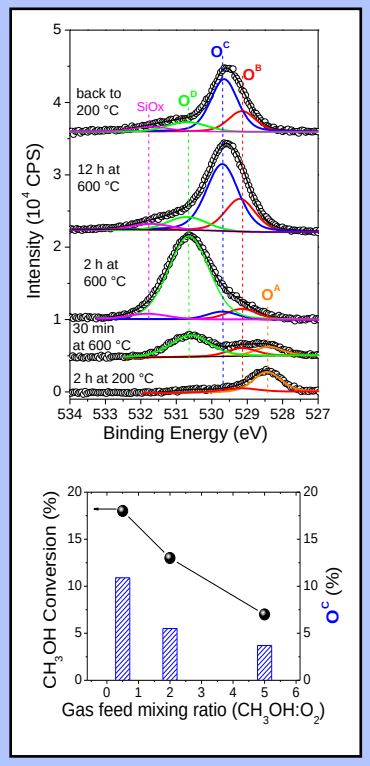
University of Innsbruck (B. Klötzer, S. Penner)
Technical University Vienna (G. Rupprechter)
Federal University of Rio de Janeiro, COPPE (M. Schmal)

Scientific Progress

Silver in partial oxidation reactions

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



In order to shed some light on these questions, we have investigated Ag catalysts in equilibrium with gas phase under reaction conditions with pressures in the mbar range by *in situ* XPS.
The upper panel in the figure shows the oxygen 1s spectra of a Ag foil at different temperatures relevant for ethylene (200 C) and methanol oxidation (600 C) reactions. Briefly, four different oxygen species were identified with distinct binding energies, thermal stability and associated formation of ionic Ag.
The different thermal behavior and spectroscopic characteristics of these species arises from their dissimilar bonding with the Ag, which leads to different roles in oxidation reactions
For instance, under methanol oxidation reaction at 600 C, the species named $\mathbf{O^A}$ is not present, $\mathbf{O^b}$ nearly vanishes, and $\mathbf{O^D}$ does not change. On the other hand, the species $\mathbf{O^C}$, which appears only at high temperatures under pure O_2, present a good correlation with the methanol conversion, as can be seen in the lower panel, which suggests its role as a relevant site for this reaction.

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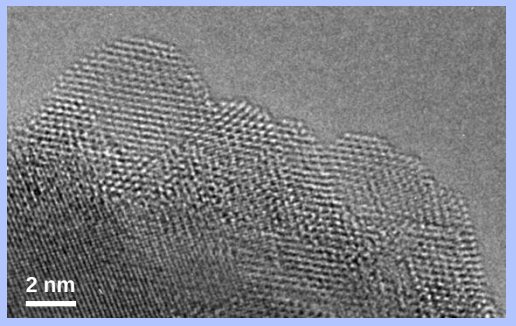
Scientific Progress

Oxygenated Ruthenium in oxidation reactions

The CO oxidation over oxygenated ruthenium was thought to be a model reaction for the investigation of a reaction mechanism in detail. In contrast our previous results on polycrystalline RuO_2 indicated a strong change of the catalyst under reaction conditions in the surface/bulk structure or in the composition up to complete reduction to ruthenium as confirmed by in situ XRD. Our new experiments on single crystalline Ru(0001) confirm this findings. An initially prepared RuO_2/Ru(0001) film with sharp LEED spots completely loose this LEED pattern after reaction in the micro-flow reactor. Starting from clean Ru(0001) or RuO_2/Ru(0001) similar surface states are reached after prolonged reactions under different conditions as revealed by conversion measurements and ex-situ TDS, LEED and AES.

Chlorine is one of the essential basic chemicals of the chemical industry, because a large portion of processes require at certain steps chlorine. On the large scale, it is produced using electrolysis of NaCl (or HCl) solutions and very recently by the heterogeneous gas phase oxidation of HCl (Deacon Process). Interestingly both processes rely on RuO_2-based materials! Currently, we are involved in characterizing electrode materials and find that the surface-near region of the samples undergoes strong modification (phase changes, segregation) during electrolysis. In the Deacon catalysts RuO_2 is in the form of 2-4 nm sized particles, often in epitaxial relation to the support with rutile structure. As shown by the high resolution TEM image below, the nanoparticles expose nicely facetted surfaces, many of them belonging to the {110} and {101} families. These catalysts if prepared with a binder material allows industrially relevant stable long-term operation. Despite these catalysts being state of the art, by using in situ Prompt Gamma Activation Analysis experiments we could show that during Deacon reaction Cl adsorbs strongly on these surfaces with coverages high enough that only a low portion of the surface is in fact active during reaction.



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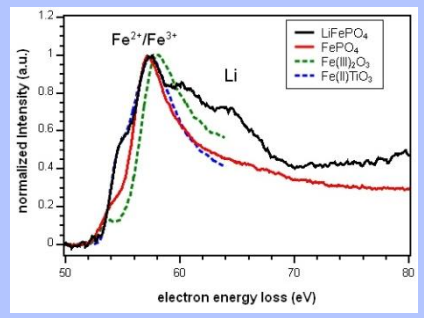
External collaboration:
Institute of Isotopes
(Budapest)

Scientific Progress

Electrochemistry

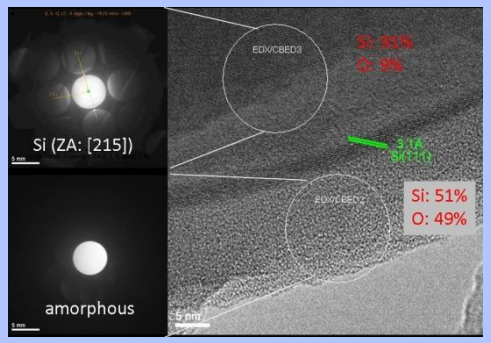
Charge storage mechanism in lithium ion batteries



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 which requires a fundamental understanding of the electrochemical processes in current batteries. These are not revealed at an atomistic level by solely electrical battery characterization, but an additional spectroscopic investigation is supposed to illuminate the understanding on that level.

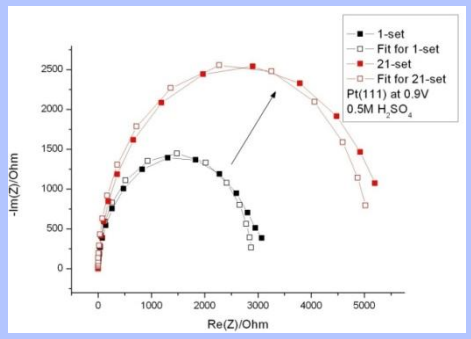
This project focuses on a battery system with LiFePO4 as the cathode material and a silicon/carbon composite as anode material. Electron energy loss spectroscopy is one of the rare methods giving a direct information about the electronic structure of lithium. Such a loss spectrum for LiFePO4 indicates that lithium in the olivine structure is not purely ionically bonded. This would deduce a new understanding of the charge storage mechanism and it is currently under verification by a comparison with theoretical modeling performed in the electron microscopy group.

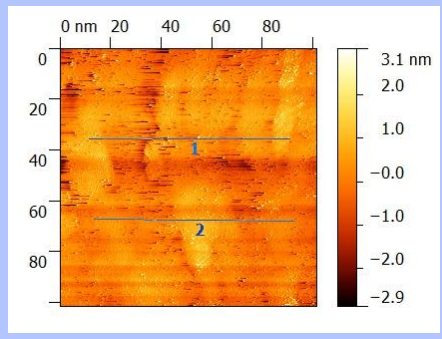
A composite system of silicon nanoparticles enclosed in a carbon matrix has shown high performance, but a collaborated study in the framework of Enerchem depicts a strong dependency on the formation of an amorphous oxide layer on the silicon nanoparticles. While this oxide might help to improve the cycle stability, transmission electron microscopy studies reveal that it has a thickness of up to 20nm. This impedes the charge transfer, which significantly decreases the anode capacity.



Electrocatalitic water splitting

Electrochemical water splitting comes with many challenges which have remained inspite of decades of research work and recurring interest in the reaction. The challenges come from the anodic part of the reaction which involves oxygen evolution at potentials 1.2V or higher. The complexity of transferring 4 electrons and 4 protons for evolution of every molecule of oxygen renders the reaction kinetically difficult. The best catalysts IrO2, RuO2 operate between 0.2 – 0.4V of overpotential when operated at 10mA/cm2 of current output. The overpotentials for catalysts like MnO2 and Pt are even higher around 0.4 - 0.5V. Another enormous challenge is the long term stability of catalysts. The anodic electrochemical conditions are extremely oxidizing and this makes catalysts corrosion a serious issue. Our approach is to understand the reaction on model systems like single crystals of Pt, Ru, Ir, IrO2, RuO2 in order to understand the oxygen evolution reaction (OER) and corrosion on these surfaces using all available electrochemical techniques. On Pt single crystalline electrodes, the activity for OER depends on the surface orientation. Of the three Pt low index surfaces Pt(111) showing the highest and Pt(110) showing the lowest activities. Electrochemical impedance spectroscopy under in situ OER conditions show a changing impedance spectra overtime. This shows that processes occur on the surface in the potential regime of OER, but their nature remains unclear. We are currently developing photoelectron spectroscopy and scanning probe microscopy under in situ conditions to get insights into the surface chemistry of OER.





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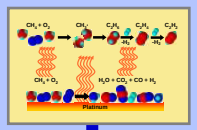
MPI for Colloids and Interfaces (Prof. Antonietti, Dr. Titirici)

Financial support:
Volkswagen AG

Scientific Progress

High temperature catalysis research



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

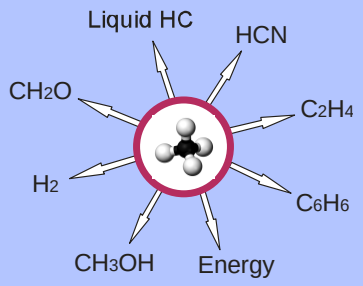


Fig. 1

Fig. 2

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

Results: The methane oxidation on Pt has been investigated both, on α-Al_2O_3 foam catalysts coated with Pt nanoparticles (reticulated pore structure, $d_{pore} \approx$ 300-500µm, Fig. 3) and polycrystalline Pt tubes with 4.4mm inner diamater (Fig. 4).

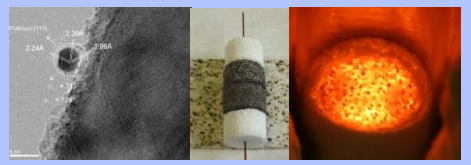


Fig. 3

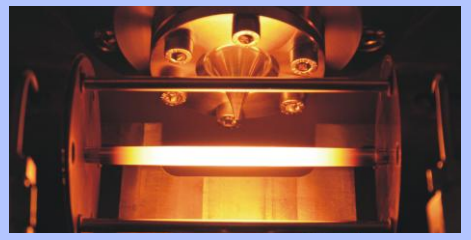


Fig. 4

Reactor measurements on the foam catalysts with a geometric surface to volume ratio of about 160cm^{-1} show H_2, CO, H_2O and CO_2 as reaction products. Spatially resolved species and temperature profiles (Fig. 5) reveal that these products are formed at the Pt surface by partial and total oxidation of methane followed by steam reforming. CO_2 reforming is not observed.

Methane oxidation in a Pt tube with only ~7cm^{-1} surface to volume ratio leads at temperatures below 1100°C also to H_2, CO, H_2O and CO_2. However, above 1100°C surface temperature, a sudden formation of C2 products (C_2H_6, C_2H_4, C_2H_2) is observed (Fig. 6). Quantitative measurements of gas phase CH_3· radicals reveal the onset of gas phase chemistry at this point. C2 products are obviously formed by reaction of CH_3· radicals with CH_4 molecules in the gas phase and subsequent dehydrogenation. H_2, CO, H_2O and CO_2 are formed by surface oxidations supplying heat to drive the gas phase chemistry.

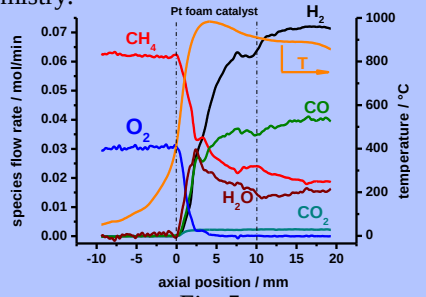


Fig. 5

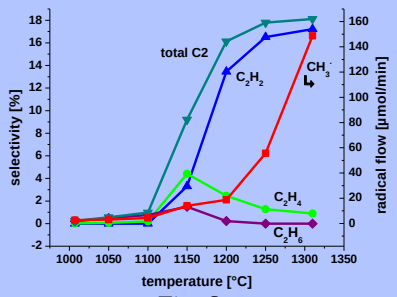


Fig. 6

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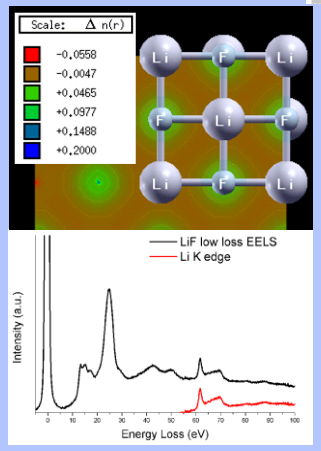
Scientific Progress

Simulation and experiment in electron microscopy

Li Ion Battery materials

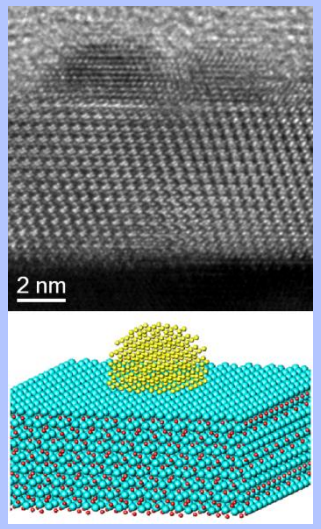
In a joined project with the Electrochemistry group, we are studying the way in which Li is stored in battery materials by analytical electron microscopy. High resolution TEM analysis and morphological studies are combined with spectroscopic information recorded in electron energy loss spectrometry (EELS). To assist the interpretation of the experimental data and in order to understand the features in the acquired spectra, density functional theory based calculations of the electronic structure and simulations of energy loss spectra are performed for a set of reference systems. This provides fundamental insights on the Li bonding state, transport and storage.



Electron density plot (top) and EELS spectrum of LiF

Geometric structure of model systems

In cooperation with the CP department we are investigating model catalysts consisting of metal nanoparticles that are supported on well defined oxide surfaces. In order to reveal details of the particles shape, termination and interfaces samples are prepared for cross-section imaging in the preparation lab of the group and investigated by high resolution electron microscopy. Interpretation of the experimental data is supported by image simulation. Comparison between simulation and experiment enables the reconstruction of the three-dimensional shape of the platinum and palladium nanoparticles from the two-dimensional lattice fringe images.



HRTEM image of $Pd/Fe_3O_4/Pt$ (top) and a model for image simulation (bottom)

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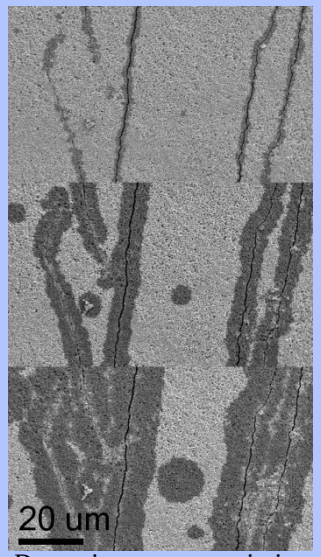
Observation of dynamics in electron microscopy

Ethylene decomposition on Ni catalysts

Using an environmental SEM that is equipped with a heating stage and a feeding system with mass flow controllers for reaction gases we study the decompositions of Ethylene on polycrystalline Ni films. This in-situ studies complement in-situ, time- and depth-resolved X-ray photoelectron spectroscopy and X-ray diffraction experiments. We investigate effects of hydrogen addition and Ni catalyst pretreatment on the dynamics of carbon precipitation and graphene nucleation. Dynamic contrast variations are observed under the addition of hydrogen. Their nature and the underlying contrast mechanisms are presently under study.



Dynamic contrast variation observed during in-situ Ethylene decomposition

Grain growth in Ag

In order to complement in-situ XPS studies that are performed by the Electronic Structure group, we study the effect of oxygen on silver at elevated temperature at similar conditions in the environmental SEM. This allows to monitor the development of structural modifications which can otherwise not be observed in-situ. In contrast to the static description of oxygen species obtained by the classical surface science approach, a very dynamic picture of the silver-oxygen interaction is revealed. An enhancement of grain boundary mobility and grain growth in silver is observed upon oxygen exposure, giving rise to changes in the surface morphology. This observations can be related to the XPS data and provide valuable insight for the description of the kinetics of oxygen species formation at different temperatures.

FHI Library

FHI Library

The library collects special literature covering the research fields of the institute. The library has about 15.500 monographs and several eBook collections (i.e. RSC eBook Collection 1968-2009). In addition, the library offers about 30.000 currently subscribed electronic journals, most of them based on central MPG agreements. The range of electronic services of the FHI Library includes various databases, access terms and conditions for e-journals as well as catalogues. Therefore, the qualified library personnel will remain indispensable also in the new age of electronic „libraries without walls“. The acceptance of electronic media is very high within the FHI due to constant efforts and the regular training of the users.
The traditional services as interlibrary loan service, acquisition of books and other information material, literature searches and reader service are also available. Furthermore, the library participates in the development and maintenance of the Max Planck Virtual Library (VLib).

Move of the library

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

External Collaborations

The library cooperates with various institutions, for example with:

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

Max Planck Virtual Library (VLib)

Max Planck Virtual Library VLib

This system is a portal to various information resources available to members and guests of the Max Planck Society. To support that system the library is giving feedback to VLib by intensely testing the user interface and integrating library catalogs that run with the library system Allegro.

Open Access

Open Access @ Max Planck Society

The library is constantly monitoring the publication market, especially in respect of to new trends, e.g. Open Access. The FHI is practicing open access to scientific results as stated in the „Berlin Declaration on Open Access to the Knowledge in the Sciences and Humanities“ in two ways: Publication in Open Access Journals and institutional self-archiving on the eDoc Server. Currently about 1650 open access documents from FHI scientists are available on the eDoc Server.
The library attended with some activities on the International Open Access Week in October 2009 and October 2010 (http://www.openaccessweek.org/).
The head librarian is member of the workgroup for open access in the MPS.

PubMan

eSciDoc.PubMan

PubMan is the electronic repository of the Max Planck Society and provides the possibility to represent the research output of the Institutes. In 2011 the data migration from eDoc to PubMan proceeded successfully.

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

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Guest - lectures
2009 - 2011

Date	Speaking Guest	Titel
21.01.2009	**Prof. Douglas J. Buttrey** Center for Catalytic Science and Technology, Department of Chemical Engineering, University of Delaware/USA	Using Aberration-Corrected STEM Imaging to Explore Chemical and Structural Variations in the MoVNbTeO and Related Systems
13.05.2009	**Prof. Claude F. Goldsmith** Massachusetts Institute of Technology, Department of Chemical Engineering,	Predicting Combustion Properties of Hydrocarbon Fuel Mixtures
03.07.2009	**Dr. E. Emilio Bunel** Director Chemical Sciences and Engineering Division , National Laboratory Argonne/USA	Applications of Homogenous Catalysis to the Pharmaceutical Industry
14.07.2009	**Prof. Alberto Morgante** Laboratorio Nazionale TASC-CNR-INFM, and	Resonant photoemission spectroscopy in organic thin films
21.08.2009	**Prof. Dan V. Goia** Clarkson University/Center for Advanced Materials Processing, , /	Highly dispersed uniform metallic particles: Preparation and Applications
21.08.2009	**Prof. Brent H. Shanks** for Biorenewable Chemicals, Iowa State University/USA	Biorenewable Chemicals: Creating a Generalized Production Paradigm
10.12.2009	**Prof. Jens K. Nørskov** the Lundbeck Foundation's Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, Lyngby/Denmark	**Winner of the Gerhard Ertl Lecture Award 2009**

Date	Speaking Guest	Titel
17.02.2010	**Dr. Benoit Louis** LMSPC (Strasbourg, France)	Rational design of zeolite catalysts: toward a green organic chemistry
05.05.2010	**Prof. François Beguin** Centre de Recherche sur la Matière Divisée Centre National de la Recherche Scientifique and Orléans University Orléans, France	Carbon based electrochemical capacitors
02.06.2010	**Prof. Dr. Christian Limberg** Humboldt-Universität zu Berlin, Institut für Chemie	From surface-inspired oxovanadium models to active catalysts for the oxidation of alcohols with O_2
14.06.2010	**Dr. Cornelia Jäger** Laborastrophysik- und Clusterphysikgruppe des Max-Planck-Institutes für Astronomie, am Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena	Formation and spectral properties of carbonaceous cosmic dust analogs
13.08.2010	**Prof. John Robertson** University of Cambridge, UK	Catalytic growth mechanism of Carbon Nanotubes
30.09.2010	**Dr. Tobias Rüffer** TU Chemnitz, Institut fuer Chemie	Verbrennen/Oxidieren dünner Filme von mehrkernigen Übergangsmetall-komplexen
17.11.2010	**Dr. Jong Hoon Joo** Max-Planck-Institut für Festförperforschung	In-situ XPS of adsorbed oxygen and protonated species on mixed conducting perovskites cathode under close to SOFC operation condition
01.12.2010	**Dr. Ekatarina Skorb** MPI für Kolloid- und Grenzflächenforschung in Golm	Ultrasound Induced Formation of Mesoporous Multi Metal Catalysts
08.12.2010	**Dr. Oleksiy Khavryuchenko** Kiew National Taras Shevchenko University, Ukraine	Active carbon and spin catalysis: a quantum chemical insight
17.12.2010	**Prof. Dr. De Chen** Department of Chemical EngineeringNorwegian University of Science and Technology	Carbon nanotube based nanoelectrode array for energy storage

Guest - lectures

2009– 2011

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

External Funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
ENERCHEM Nanochemical Concepts for a Sustainable Energy Supply Projects of Max Planck Institutes	ENERCHEM	M.IF.A.FHI 08025	MPG	2005 continuing	Prof. R. Schlögl Dr. D. S. Su	Prof. F. Schüth (MPI für Kohleforschung), Prof. J. Maier (MPI für Festkörper-forschung), Prof. K. Müllen (MPI für Polymerforschung)	Verbundprojekt
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	
Nonstructural catalysts for environment protection and green chemistry			MPG	2002 continuing	Dr. D. S. Su	. M. Najbar	Dr. D. S. Su
Cooperation "TEM and Raman spectroscopy of nanostructured transition metal oxides"		K 500Z	MPG	2004 continuing	Dr. D. S. Su	Dr. K. Furic (Zagreb, Kroatien)	Dr. D. S. Su
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)	

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
Interaction of Surface and Gas Reactions in High Temperature (max ca.1300 C) High Pressure (max. ca. 5 M Pa) Catalytic Alkane Oxidations	Emmy-Noether-Nachwuchs-gruppe	EM.FHI 707	DFG	2008 - 2013	Dr. R. Horn		
Novel Pd-based catalysts for non-oxidative methane activation	DFG	444 BRA-113/56/0-1	DFG	2009-2011	Dr. M. Behrens	Prof. Dr. M. Schmal (Centro de Technologia, COPPE, Rio de Janeiro, Brazil)	

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	starting 2007	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)

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Mischoxide		PSFHI 253	Südchemie	2007 - 2011	Prof. Dr. R. Schlögl Dr. A. Trunschke	Südchemie AG	Prof. Dr. S. B. Abd Hamid
Electrochemistry		PSFHI 990	VW	01.07.2011-30.06.2013	Prof. R. Schlögl Dr. J. Tornow		Prof. R. Schlögl
Mo based catalyst in selective oxidation of hydrocarbons		PSFHI 255	Mitsubishi Chemicals	2008-2012	Prof. R. Schlögl Dr. A. Trunschke		Prof. R. Schlögl

External Funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Development of a long-term stable methanol synthesis catalyst	Cu IX	PSFHI 256	Bayerisches Staatsministerium für. Wirtschaft, Infrastruktur, Verkehr u. Technologie	Starting 2010	Prof. Dr. R. Schlögl Dr. M. Behrens	Südchemie, Prof. M. Muhler (Ruhr-Uni. Bochum), Prof. Hinrichsen (TU München)	Südchemie
Joint project with Bayer AG Teilprojekt AP1: "Aufklärung, Reaktionsmechanismus und Optimierung des bestehenden Katalysatore"	CarboScale	PSFHI 105	BMBF Fkz: 03X0040H	2007 - 2012	Prof. Dr. R. Schlögl Dr. R. Arrigo	TU Berlin Ruhr-Uni. Bochum Univ. Erlangen Univ. Clausthal Future Carbon GmbH Bayer Ehrfeld Mikrotechnik - BTS GmbH Leibnitz-Inst, Dresden TU Ilmenau Frauenhofer-Gesellschaft München H. C. Starck GmbH	Bayer AG
Effizienzsteigerung bei der Chlorherstellung		PSFHI 257	BMBF	2009-2012	Prof. R. Schlögl Dr. D. Teschner	Bayer MaterialScience TU Berlin Universität Giessen Universität des Saarlandes Ruhr-Universität Bochum Universität Erlangen NANO-X GmbH	Bayer AG
Ressourceneffiziente AlkanSelektiveOxidation an neuen kristallinen Festkörperphasen. TP2: High-end In-situ-Analytik unter realistischen Bedingungen- Ermittlung verbesserungswürdiger Strukturmotive	ReAlSelOx	FHI 107	BMBF Fkz : 033R028B	01.07.2009 – 30.06.2012	Prof. R. Schlögl Dr. A. Trunschke	Prof. Dr. Glaum (Uni. Bonn), Prof. Dr. Kniep (MPI CPfS), BASF, hte	BASF
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	Dr. M. Behrens		
Contruction of a photon energy beamline and several endstations @ BESSY	EMIL		BMBF HZB MPG	2010-2012	Dr. A. Knop-Gericke	HZB	

External Funds

Project Name	Akronym	Referenz No.	Funds Provider	Funding Period	Project Leader at FHI	Cooperation Partner	Coordinator
Integrated Design of Nanostructured Catalytic Materials for a Sustainable Development ERIC provides services to improve effectiveness of research	IDECAT / ERIC European Research Institute on Catalysis (ERIC)	PSFHI 805	European Union	2005 – 2010 ERIC -Nov. 2008 continuing	Prof. Dr. R. Schlögl	Prof. H.J. Freund Prof. M. Scheffler Prof. M. Reetz Prof. F. Schüth and other (17 European partners) http://.idecat.org	Prof. Dr. G. Centi
Technology for Wafer-Scale Carbon Nanotube Applications	Technotubes	PSFHI 872	European Union NMP-2008 4.0.3. CP-IP 228579-1	2009-2012	Dr. Axel Knop-Gericke	, AIXTRON, AG, Philips GmbH, IMEC, Thales Research and Technology, Thales Electron Devices, CMOS sensors, Technical Uni. , Technical Uni. , ETH Zürich, CNR-Trieste	Prof. Dr. J. Robertson
Graphene chemical vapour deposition: roll to roll technology	Grafol		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

European Union - Network of Excellence / NoE

At the Lisbon summit in March 2000, EU governments called for a better use of European research efforts through the creation of an internal market for science and technology - a 'European Research Area' (ERA). FP6 is the financial instrument to help make ERA a reality.

http://cordis.europa.eu

http://idecat.org

NoE IDECAT: "Integrated Design of Catalytic Nanomaterials for a Sustainable Production" NMP3-CT-2005-011730

What is a Network of Excellence

- An instrument to mobilize transnational research collaborations between partners sharing a commitment to long-term integration
- A series of common initiatives on integration, research, spreading of excellence and transfer to companies with the final goal to create a self-sustaining **Durable Integration Structure (DIS)**

- The DIS of IDECAT is the **European Research Institute on Catalysis** (ERIC) which started operations in Nov. 2008
- ERIC , with headquarter in Belgium, operates in close partnership with industry to create a long-term scientific, institutional, industrial and societal awareness on catalysis
- ERIC provides services to improve effectiveness of research

ERIC a.i.s.b.l. European Research Institute of Catalysis

Scientific vision of IDECAT

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

IDECAT: numbers

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

IDECAT successfully terminated in 2010 – final goal achieved

ERIC European Research Institute of Catalysis

- Final objective of IDECAT was the creation of an European Research Institute of Catalysis (ERIC) which offers to companies and public sponsors the possibility to realize top level project in the field of catalysis and catalytic functional materials using the unique and integrated research facilities and competence of ERIC.
- After the termination of IDECAT the ongoing activities are coordinated by ERIC. Successive projects are under preparation.

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

Technotubes

Technology for Wafer-scale Carbon Nanotube Application

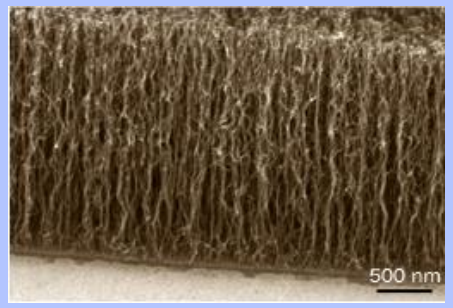
What is Technotubes ?

Carbon nanotubes (CNTs) are characterized by unique electrical, mechanical, surface and thermal properties. However, their high potential for a variety of industrial applications has been limited by mass production of carbon nanotubes on surfaces. The **Technotubes project** aims at the design, engineering, process control, quality assurance, qualification and process development of applications such as cathodes for time resolved X-ray tomography as well as for high power microwave amplifiers, interconnects for VLSI and integrated sensors on CMOS, among others.

Cooperation Partner:

Fritz-Haber-Institute, University of Cambridge, AIXTRON, Philips, IMEC, Thales Research and Technology, Thales Electron Devices, Cambridge CMOS sensors, Technical University of Berlin, Technical University of Denmark, Swiss Ferderal Institute of Technology Zürich, CNR-Trieste

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

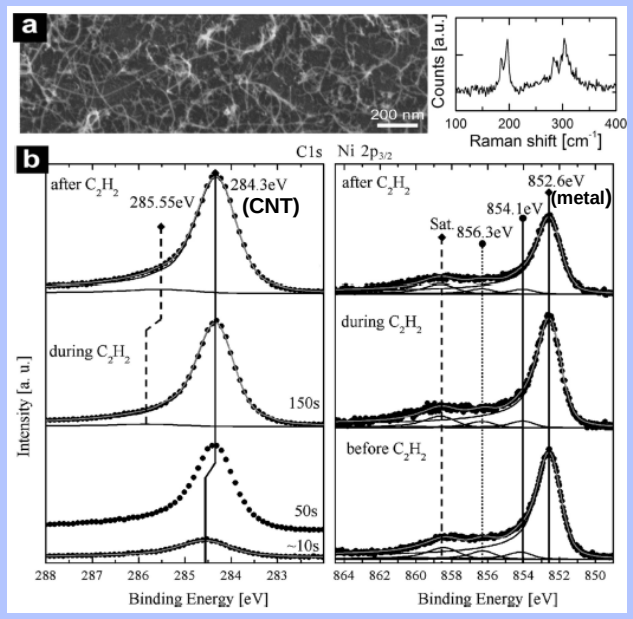


SEM image of CNTs catalysed by Al_2O_3-supported Fe films. The catalyst film was annealed prior to growth in NH_3. CVD at 2.5 x 10^{-3} mbar of C_2H_2 for 5 min. at 500 – 580 C from an ex situ deposited Fe film (0.5nm).

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

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

On SiO_2 substrates prior to the exposure to the reactive gas, C_2H_2, Fe is only reduced and dispersed by simultaneous heating to the reaction temperature and NH_3 exposure, whereas thermal treatment only is sufficient for Ni. During C_2H_2 exposure both, metallic Fe and Ni catalyst particles are active towards SCNT growth with a comparable yield. The catalyst metal surfaces supply sites to dissociate the hydrocarbon precursor and then guides the formation of a carbon lattice and the liftoff of a carbon cap as evidenced by the C1s peak at 284.3eV.
In the case of Fe under the same experimental conditions changing the substrate to Al_2O_3 significantly increases the CNT yield due to an increased Fe/substrate interaction yielding in large CNT forests (bottom). This interaction more efficiently pins the Fe particles and can also be used to tune the particles size and hence the CNT diameters.



(a) Postgrowth SEM and Raman radial breathing mode and (b) in situ XPS C1s and $Ni2p_{3/2}$ core level lines of 0.25 nm Ni film on SiO_2 after being heated to 500 C, pretreatment in 10^{-3}mbar O_2 and 0.6 mbar NH_3, and before/ during/ after C_2H_4 exposure at $2x10^{-3}$mbar in two intervals, for 3 and 10 min, respectively. The time of C_2H_4 exposure is indicated. The C1s intensity are normalised to highest C1s intensity.

http://www.technotubes.org

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.

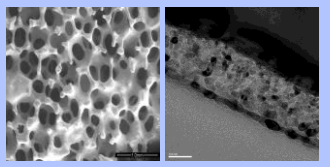
UniCat is currently being developed by the

Coordinator of the FHI der MPG, Dept. of AC:
Dr. Raimund Horn
horn_r@fhi-berlin.mpg.de

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

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

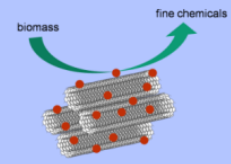
1. Oxidative coupling of methane to ethylene
(Dr. R. Horn, Sardor Mavlyankariev, Dr. Hugo Petitjean, Pierre Schwach, Heiner Schwarz, Dr. Annette Trunschke)



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

2. Conversion of biomass on the MWCNT-supported metallic nanoparticles
(Sylvia Reiche)

Goal: Design and application of MWCNT-supported metallic catalysts for conversion of biomass into building blocks for the production of biodegradable polymers.



What is BIG-NSE? 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

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

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.

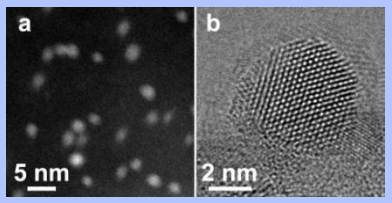
Moreover, the department contributes to the program by sending staff to research stays abroad, which are integrated into PhD or post-doctoral studies.

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.

Utrecht University, Netherlands

Twente University, Netherlands

The University of Turku, Finland



Pd nanoparticles on carbon

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

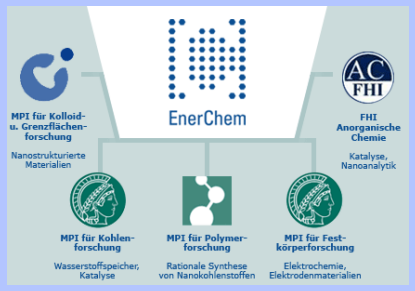
http://www.unm.edu/~pire/

EnerChem

Projects of Max Planck Institutes
Nanochemical Concepts for a Sustainable Energy Supply

What is EnerChem ?

EnerChem is a research association, initiated by five Max Planck institutes. The aim is to combine the chemical expertise and capacities of these institutes to generate solutions to the emerging problems of energy supply, storage and saving The worlds energy consumption is at present based to nearly 90% on fossil sources, like coal, oil and natural gas. Low efficiency of energy utilization has accelerated the depletion of fossil fuels and global warming. With the establishment of "nanochemical concepts for a sustainable energy supply – EnerChem", a scientific basis for a renewable mobile energy storage and more effective methods of energy production was founded.

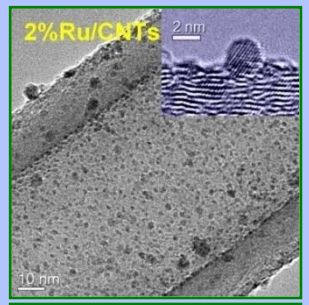


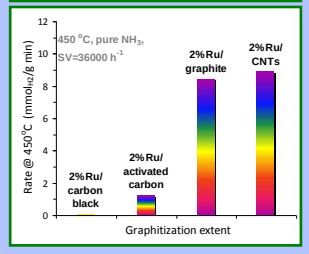
The projects of the AC department in EnerChem are:

1. Ammonia as energy carrier

Ammonia decomposition ($2NH_3 \rightarrow N_2+3H_2$) is free of CO_x and environmentally benign. Conversion of nearly 100% can be achieved at 400°C on the supported metals. Carbon nanotube is the best support due to its high electric conductivity and thermal/chemical stabilities. The graphitic structure as the electron reservoir greatly enhances the reaction rate via optimizing electron exchange on the local domain of active sites.

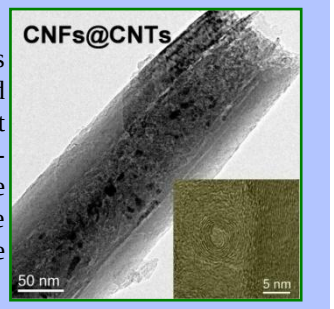
Structure of carbon was found to determine the activity of supported metals, *i.e.* the higher the graphitization, the higher the activity. As revealed by *in-situ* XPS at a near-ambient pressure, the decomposition activity shows a positive dependency on the efficiency of electron transfer inside the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





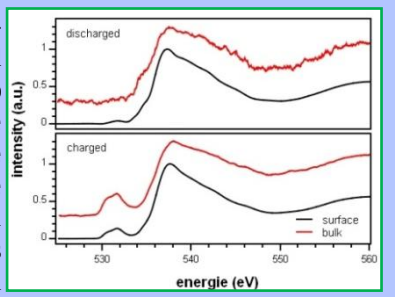
2. Novel nanocarbons for electrochemical energy storage

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



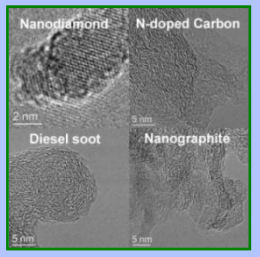
3. Charge storage in Li-ion batteries

The current atomistic picture of charge storage in Li-ion batteries is predominantly based on electrical and crystallographic measurements. But these methods do not directly resolve how charges in the electrode are stored. On the contrary, information about the electronic structure and by this about the charge distribution in the electrode material can be gathered by x-ray absorption spectroscopy. This method is either surface sensitive by collecting the total electron yield or bulk sensitive in the fluorescence yield spectra. Currently we apply this method to analyse the O K-edge and the Fe L-edge spectra of solvothermally prepared nanostructured LiFePO4.



4. Structural characterization of novel nanocarbons

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



Contact:
Dr. Dangsheng Su, dangsheng@fhi-berlin.mpg.de
Dr. Julian Tornow, tornow@fhi-berlin.mpg.de

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

Financial support:
MPG

K

Teaching Activities

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

The AC Department covers teaching aspects within the IMPRS (International Max Planck Research School; http://www.imprs-cs.mpg.de) of the FHI on the chemistry of heterogeneous catalysts and on the aspects of preparation of inorganic solids.

Modern Methods in Heterogeneous Catalysis Research

Robert Schlögl, Annette Trunschke et al.

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

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

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

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

unicat Unifying Concepts in Catalysis

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).

Tsinghua University Beijing, China
Instructor: D. S. Su
"Electron Microscopy and Its Application in Heterogeneous Catalysis: A basic lecture to understanding electron microscopy"

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. of AC
Instructor: D. S. Su
"Basics Course on Electron Microscopy and Its Applications"

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

Technische Universität Berlin (WS 2010/2011)
Instructor: R. Horn
Vorlesung Technische Chemie I

Humboldt Universität Berlin (WS2011/2012)
Instructors: R. Horn
Vorlesung Physikalische Chemie 20250

Long Night of Science

LANGE NACHT DER WISSENSCHAFTEN 2011

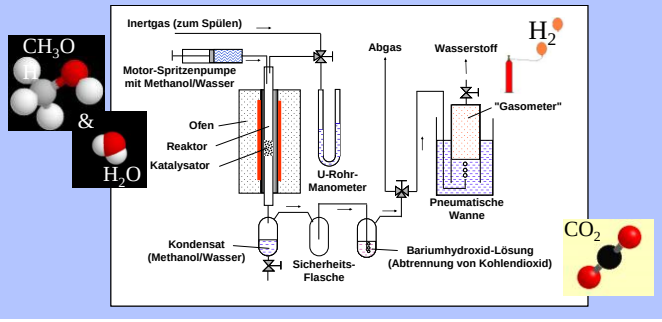
Hydrogen Technology

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

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

Where does hydrogen come from?

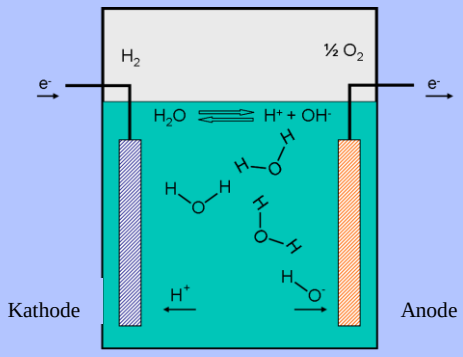
z.B. aus Methanol CH_3OH



Future Research and Perspective

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

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



$2\,H^+ + 2\,e^- \longrightarrow H_2$ $\qquad$ $2\,OH^- \longrightarrow H_2O + \frac{1}{2}\,O_2 + 2\,e^-$

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

DMFC – Direct Methanol Fuel Cell

The DMFC converts methanol and oxygen electrochemically into electrical power, heat, carbon dioxide and water. At the anode (negative electrode), the methanol is first split into hydrogen and carbon dioxide before the same catalyst splits the hydrogen into protons and electrons. These reactions require a special platinum/ruthenium catalyst. The protons then diffuse across the polymer membrane to the cathode (positive electrode), while the electrons pass as current through the external circuit. At the cathode, the electrons then recombine with the protons that have passed across the membrane and with oxygen to form water. The cathode reaction is catalyzed by e.g. platinum particle. The voltage generated by a single DMFC cell is 0.3-0.9 V.

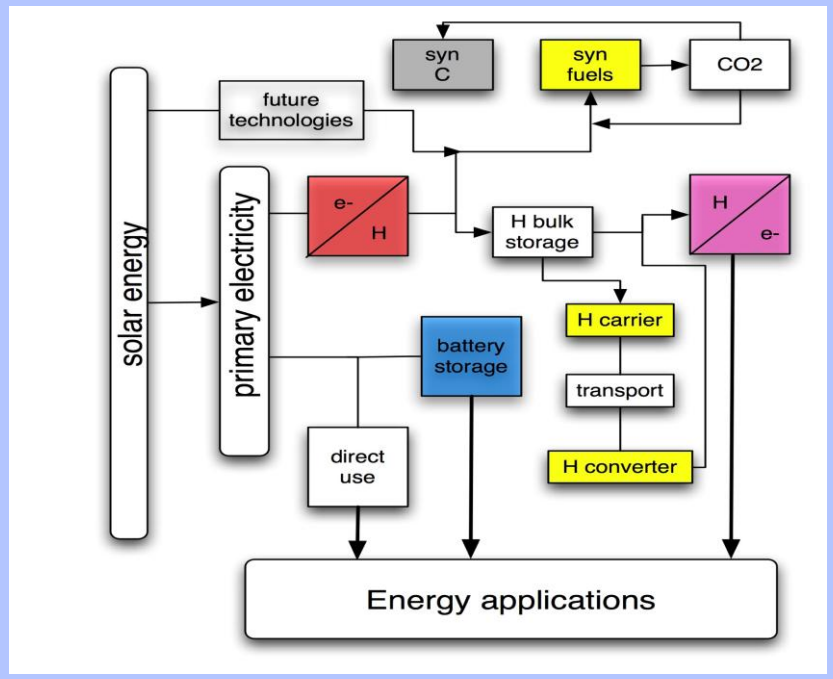
Reformer/ Katalysator: $CH_3OH + H_2O \longrightarrow CO_2 + 3H_2$

Anodenreaktion: $H_2 \longrightarrow 2H^+ + 2e^-$

Kathodenreaktion: $\frac{1}{2}\,O_2$ (Luft) $+ 2H^+ + 2e^- \longrightarrow H_2O$

M

A Global Energy Scenario



Exposition on the Long Night of Sciences

On occasion of the Long Night of Sciences, the IC department gave a general overview of the physical and chemical basis for the use of hydrogen as a source of energy. Various experiments and exhibits were illustrating to the visitors the development and techniques of hydrogen economy. By means of a sterling motor basic principles of energy transformation were shown. A fuel cell demonstrated the state-of-the-art.

Feedback on the Long Night of Science

Fritz-Haber-Institut der Max-Planck-Gesellschaft
Prof. Dr. Robert Schlögl
Geschäftsführender Direktor
Faradayweg 4-6
14195 Berlin

Beuth Hochschule für Technik Berlin
Der Präsident / Vorsitzender des Vereins „Lange Nacht der Wissenschaften"
Prof. Dr.-Ing. Reinhard Thümer

25.06.2010

Lange Nacht der Wissenschaften

Sehr geehrter Herr Prof. Schlögl,

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

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

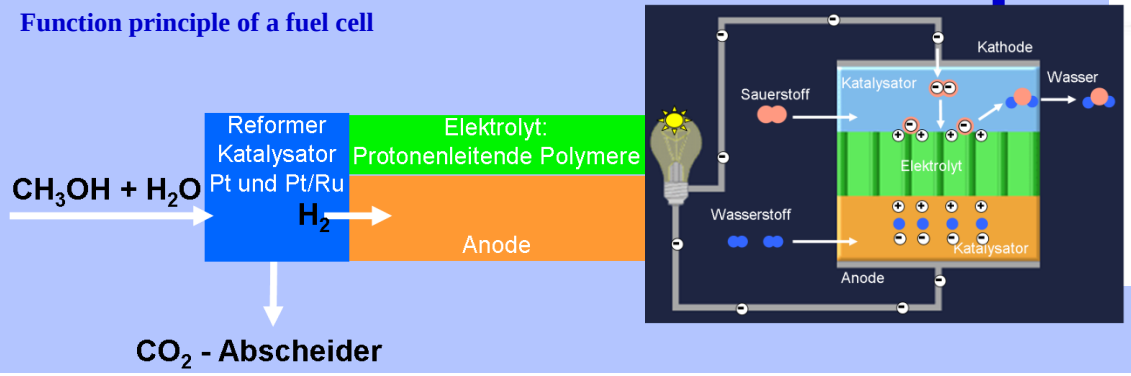
Ein besonderes Jahr war 2010 für die Lange Nacht der Wissenschaften auch dadurch, dass aus dem bisherigen Kuratorium heraus ein gemeinnütziger eingetragener Verein (LNDW e.V.) gegründet wurde, der nun als Veranstalter für die Gesamtorganisation verantwortlich zeichnet. Es würde uns außerordentlich freuen,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

Mit freundlichen Grüßen

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

www.beuth-hochschule.de

Function principle of a fuel cell



Application

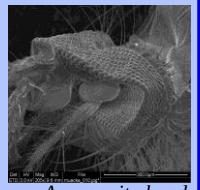
Practical Courses

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.

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

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



A mosquito head

LetteVerein

Occupation practical course

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

Nadine Schechner *(3.-18.1.2005)*

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

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

On April 14, 2011, schoolgirls visited the FHI.

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**

On February 25, 2011, 24 preschoolers visited the FHI.
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

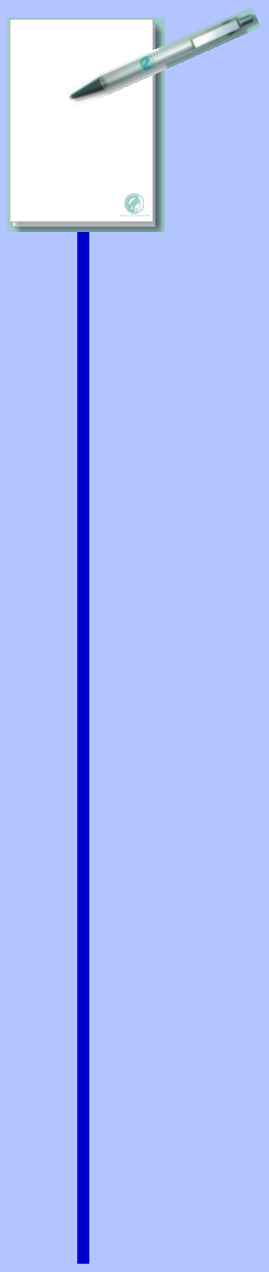
Children examining each other with a magnifying lens

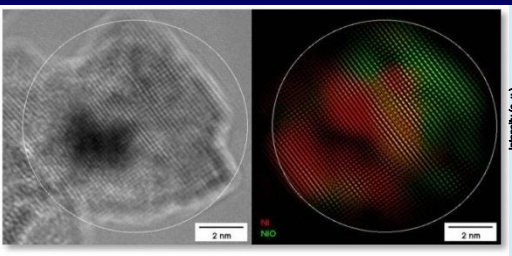
Visiting the library

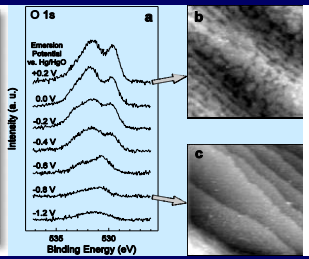
The children used both stereo and optical microscopes to examine flies, moldy bread, leaves, and more

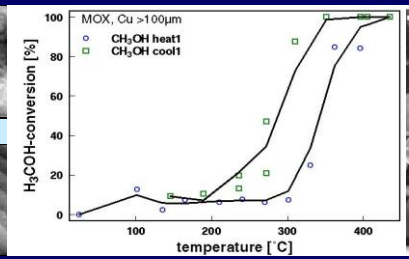
http://www.fhi-berlin.mpg.de/acnew/department/pages/youngpeople.html

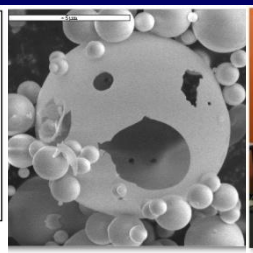
Notes

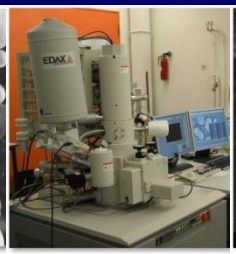


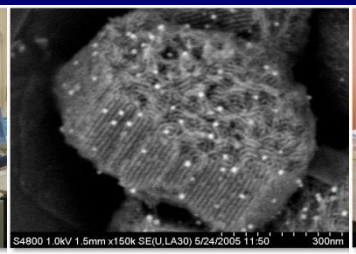




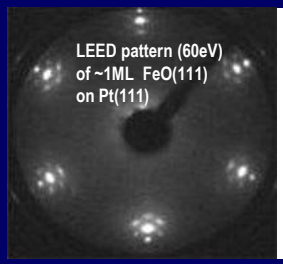


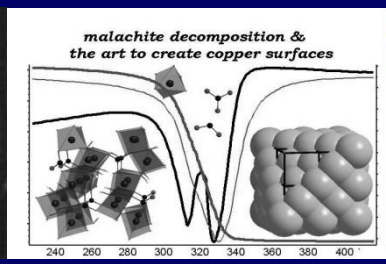


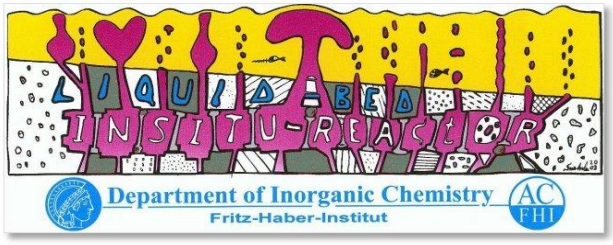


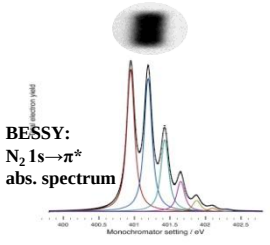


http://www.fhi-berlin.mpg.de

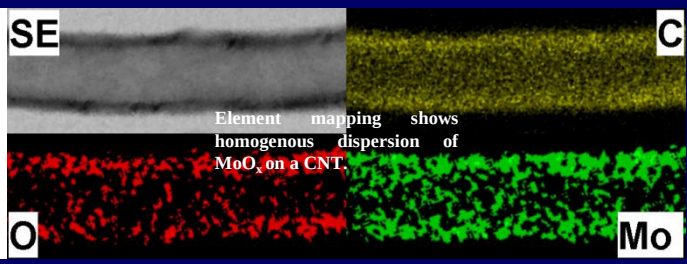




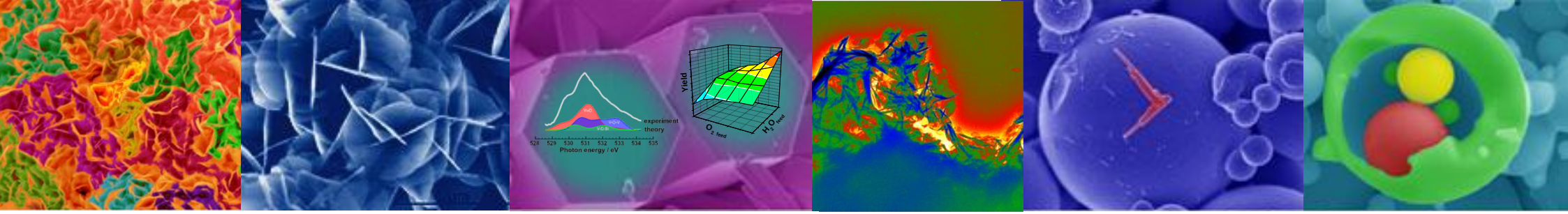




BESSY:
N_2 1s→π* abs. spectrum



Element mapping shows homogenous dispersion of MoO_x on a CNT.



Scientific Art Gallery

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