Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin

14th Meeting of the Fachbeirat

Berlin, 11th - 13th November 2007

Reports

Fritz-Haber-Institut der
Max-Planck-Gesellschaft
Berlin

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Reports

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Report of the Executive Director

Within the reporting period 2005 – 2007, work at the institute has led to many important scientific findings and the scientific output has remained at a constantly high level. The main activities of the institute continue to concern investigations into the basic processes of heterogeneous catalysis and other surface-, interface-, and cluster-related phenomena as well as the manipulation, control, and study of gas-phase molecules. In all these areas the institute has developed and built up a unique set of experiments, together with the tools that are required to accurately treat such systems theoretically. The institute has strengthened its involvement in national and international collaborations as well as its efforts in fostering academic talent, and it has actively conveyed its activities to the general public. These activities have taken place in the face of considerable challenges. These challenges are not only related to the still ongoing renovation of several buildings and the refurbishment of (part of) the ageing infrastructure on the FHI campus, but also to the unexpected delay in the appointment of a new director at the FHI.

During the last meeting of the Fachbeirat, in November 2005, we informed you that the board of directors of the FHI was planning to nominate Professor Richard Berndt, University of Kiel, for appointment as director on the vacant position formerly held by Professor Gerhard Ertl. The appointment procedure within the MPG went very smoothly, and a formal offer by the president of the MPG was made in the summer of 2006. In spite of considerable efforts from the side of the FHI, and after extensive negotiations, Professor Berndt declined the offer in early 2007 for – predominantly – private reasons. In the meantime, a new candidate with a very attractive field of research that fits very well with the interests of the institute has been identified. At the moment of this writing, the formal documents to start up the appointment procedure for this future colleague director are being prepared; this will be reported upon in more detail during the meeting of the Fachbeirat.

In March 2006, Professor Joachim Sauer (Humboldt University, Berlin) was appointed as External Scientific Member of the FHI, strengthening the close ties he and his group have had with the FHI over the years. Since the summer of 2006, Professor Hardy Gross (Free University, Berlin) has been a Max Planck Fellow at the FHI. These Max Planck Fellow positions are a new initiative of the MPG to support – for a period of five years – outstanding senior university lecturers, and to provide them with some financial support by the MPG.

By many benchmarks, the institute has maintained its leading status among German and international research institutions. According to the most recent evaluation of the Alexander-von-Humboldt Foundation, for example, the Fritz Haber Institute ranks first among German non-university institutions in terms of hosting scholars and prize winners funded by the Foundation. This is in absolute numbers, i.e. not even normalized to the size of the institute, and is a clear sign of the high esteem that the institute enjoys in the international community. Over the years, a post-doctoral or group-leader position at the FHI has also proven to be an excellent stepping stone towards an independent academic career. In the first call for Starting Grants of the European Research Council (ERC) earlier this year, four young scientists of the FHI have been invited to submit a full proposal in the final round (559 of more than 9000 applicants, covering all fields of science throughout Europe, have been admitted to the second round). Two of them plan to perform their ERC project at the FHI, while the other two will go abroad, or, more accurately, “back home”. Over the last ten years, the publication output has remained remarkably constant, and about 230-250 papers are published by members of the FHI per year. These papers are well received, as testified by the number of citations as well as by the number of invited lectures that the members of the FHI are asked to present.

The scientific achievements of the FHI are described in detail in the reports of each of the five departments. Here, I only want to mention the successful completion of two major FHI projects during the last years. The first of these is a beamline at the BESSY synchrotron radiation source, specifically geared towards experiments involving the use of reactive chemicals, that has been commissioned and is fully operational now, including the high pressure photoemission end-station. The second of these is the SMART photoelectron microscope, which has set a world record in spatial resolution within the LEEM mode. The commissioning of the PEEM mode is in its final stage.

The institute continues to be involved in several collaborative research centers [Sonderforschungsbereiche (SFB)] that strengthen the interaction with the Berlin universities as well as with other research institutes in Berlin:

SFB 450	Analyse und Steuerung ultraschneller photoinduzierter Reaktionen (Analysis and control of ultra fast photo-induced reactions)
SFB 546	Struktur, Dynamik und Reaktivität von Übergangsmetalloxid-Aggregaten (Structure, Dynamics and Reactivity of Aggregates of Transition Metal Oxides)

SFB 555	Komplexe nichtlineare Prozesse: Analyse-Simulation-Steuerung-Optimierung (Complex Nonlinear Processes: Analysis–Simulation-Control-Optimization)
SFB 658	Elementarprozesse in molekularen Schaltern auf Oberflächen (Elementary Processes in Molecular Switches at Surfaces)

The FHI is also actively involved in a proposal for establishing a so-called Cluster of Excellence entitled “Unifying Concepts in Catalysis” together with the Berlin universities in the framework of a competition launched by the Federal Government.

The achievements by scientists of the FHI have been recognized by various awards, distinctions, and memberships in professional bodies and committees.

- Professor Ertl has become honorary member of the Deutsche Bunsengesellschaft für Physikalische Chemie, and he has received the Gold Medal of the Slovak Chemical Society. He has given the Guptill Lecture at Dalhousie University, the Baker Lecture at Cornell University, and he has received the Faraday Lectureship of the Royal Society of Chemistry. He will receive the Otto Hahn Prize, awarded by the city of Frankfurt together with the German Chemical and Physical Societies, later this year.
- Professor Freund has been elected Fellow of the Institute of Physics (UK) and he has received an honorary professorship at the School of Physics and Astronomy at the University of Birmingham. He has become member of the Board of Trustees of the Fund of the German Chemical Industry, he has presented the Centenary Lecture for the Royal Society of Chemistry (UK) and he has received the Gabor A. Somorjai ACS award for Creative Research in Catalysis.
- Professor Schlögl has been elected Fellow of the Royal Society of Chemistry (UK). He has been Chairman of the Chemical-Physical-Technical Section (CPTS) of the Max Planck Society, and is Chairman of the panel on “Material and chemical sciences” of the ERC.
- Professor Scheffler has received a Dr. h.c. from Lund University, Sweden.
- Professor Meijer has been elected to the NWO-SPINOZA selection committee.
- Dr. Bretislav Friedrich has been appointed Honorary Professor in the Department of Physics of the Technical University of Berlin
- Professor Mikhailov has accepted the offer to take the International Solvay Chair in Chemistry in Belgium in 2009.

- Dr. Bruno Pettinger received the “Prix Jacques Tacussel” of the International Society of Electrochemistry.
- Four research group leaders have completed their habilitation: Dr. Günther Rupprechter, Technical University, Berlin, 2005; Dr. Catherine Stampfl, Technical University, Berlin, 2006; Dr. Knut Asmis, Free University, Berlin, 2006; Dr. Thomas Risse, Humboldt University, Berlin, 2007.
- Dr. Friederike Jentoft has been elected Associate Editor of “Advances in Catalysis”.
- Several young scientists have been honoured by the Otto Hahn Medal of the Max Planck Society: Dr. Jörg Behler and Dr. Svetlana Schauermann in 2006, and Dr. Jutta Rogal in 2007.
- Dr. Christian Hess and Dr. Timo Jacob have been granted an Emmy Noether Independent Junior Research Group by the DFG (at the FHI and at Ulm University, respectively) and Dr. Rick Bethlem has been granted a VIDI fellowship by NWO (Free University of Amsterdam).
- Dr. Swetlana Schauermann and Martin Sterrer have recieved a DFG-Fellowship, and Dr. Raimund Horn has received a Feodor Lynen Fellowship of the AvH foundation.
- Dr. Melanie Schnell has been elected as member of the “Junge Akademie an der Berlin-Brandenburgischen Akademie der Wissenschaften und der Deutschen Akademie der Naturforscher Leopoldina”.
- Dr. Thomas Schmidt has been awarded the BESSY Innovation Award on Synchrotron Radiation 2006.

Since the last meeting of the Fachbeirat, the following scientists have been appointed to academic positions:

- Professor H.-H. Rotermund, George Munro Professor of Physics, Dalhousie University, Halifax, Canada.
- Dr. Angelos Michaelides, Reader in Physics, University College London, UK.
- Dr. Günther Rupprechter, Professor of Physical Chemistry, Technical University, Vienna, Austria.

In terms of funding, the institute finds itself in a stable situation. Administrative handling of the day-to-day running of the institute has been made easier by the removal of certain regulations, in particular those applying to the budget within the institute. The diagram in

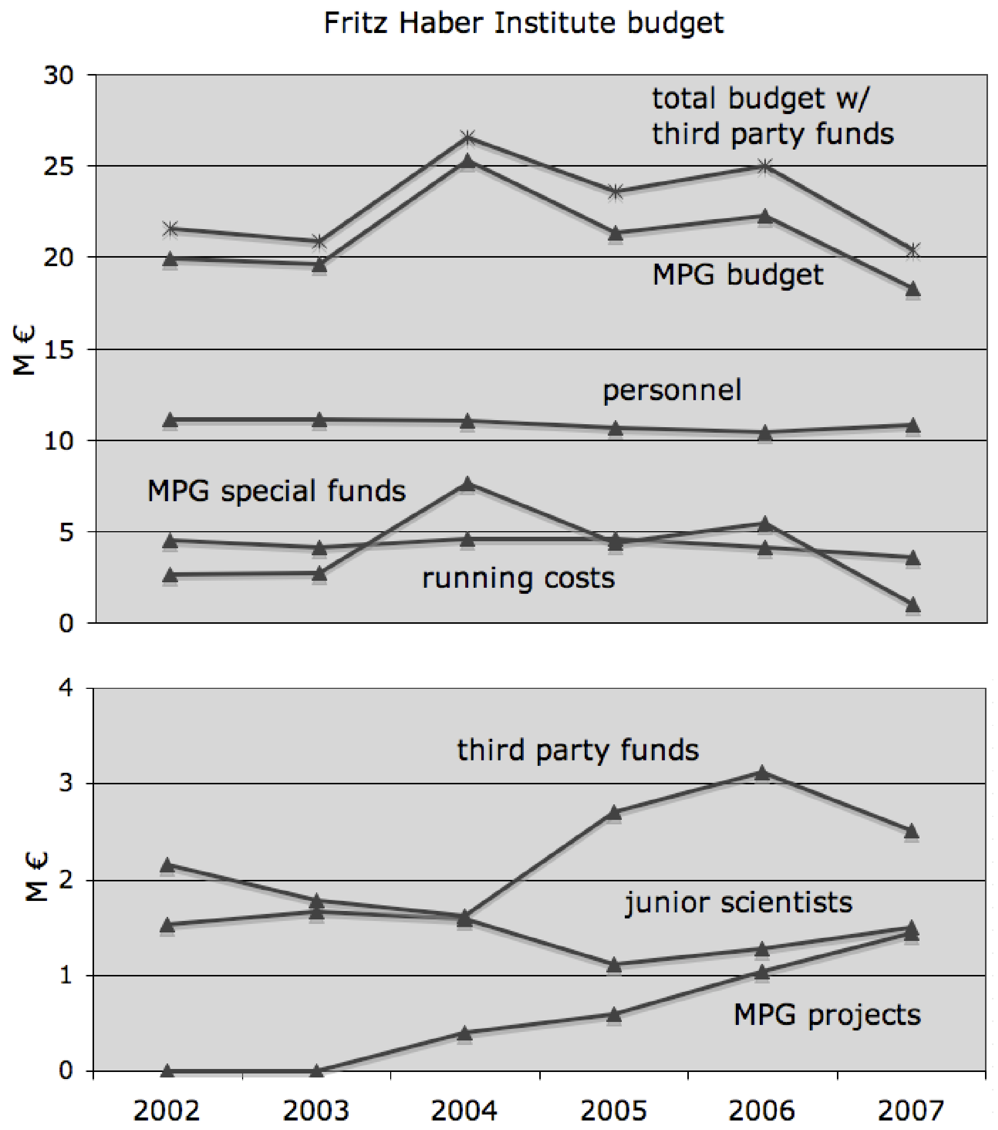


Figure 1: Budget of the institute broken down into specific sources of funding. MPG special funds relate to startup funds and grants for large equipment (e.g. TEMs). MPG projects are funds that are distributed by the Central Administration through proposal and peer review

Figure 1 shows, in M€/year, the development of funds over the last six years in terms of personnel costs, running costs, investment costs, funding for students and postdoctoral fellowships and outside contributions. The peaks in the years 2004 and 2006 were caused by large grants for major equipment, but other than that the overall budget has remained quite stable. A few years ago, a new financing scheme of providing a fixed core budget to the institutes, with extra funds being made available through a proposal system, has been implemented by the Central Administration of the MPG. This has worked well for the FHI, and via the proposal system the institute has attracted grants for the International Max Planck Research School (IMPRS), inter-institute collaborations, and international collaborations. The IMPRS "Complex Surfaces in Materials Science" has been very positively evaluated in the end of 2006. This evaluation, together with the explicit support from the Fachbeirat during the last meeting, has resulted in the decision to renew the school, thereby securing the funds for the 2009-2014 period. Third party funding continues at a level of around 2-3 M€/year. The institute currently has 202 full-time equivalent positions of which 53 (including the five director positions) are for scientists; of the latter, four are within scientific service groups. Including post-docs, Ph.D. and diploma students, apprentices and guests, about 350 persons are working in the institute on average. Most of the Ph.D. students earn their degree in one of the Berlin universities; occasionally, a thesis defense takes place elsewhere.

The institute has undergone a massive refurbishment of many of its buildings, some of which are almost 100 years old. In 2001 a master plan for the modernization of the institute's buildings and its infrastructure was arranged, with funds made available by the Central Administration. This process started with the renovation of buildings C and D for the new department of Molecular Physics in 2003, and of building F for the department of Inorganic Chemistry; there is a map of the FHI campus on the last page of this booklet, indicating the description of the various buildings. The service group for electronics (E-lab) and the mechanical workshop will all be housed in building L; the reconstruction of this building is now almost finalized. The master plan will be completed by the upcoming renovation of Fritz Haber's original institute building (A) for the department of the new director.

Throughout on the FHI campus, state-of-the-art cooling and laboratory air conditioning systems, energy-saving central heating, new electrical and network wiring, up-to-date fire alarm systems and related installations have been implemented. These systems serve the needs of experiments in terms of temperature stability, vibration isolation and other parameters. Such installations are indispensable for the new generation of experiments, but bring with them a heavy workload on the technical staff of the institute; this also is true for the entirely new control system (computer aided facility management, CAFM) which is currently being implemented. Not all of these building projects have gone as smoothly as one might have hoped for, which has caused several disruptions and delays of the ongoing research, in particular on the old part (southern part) of the FHI campus. We see an urgent need for a position of an FHI employed engineer, who will be in charge of the upgrade and maintenance of the complex technical infrastructure on the FHI campus, and we have applied for additional funds from the Central Administration for such a position.

A new collective wage agreement, which also applies to the Max Planck Society, was introduced for the employees of the public sector in Germany in 2005/6. This has removed many of the complexities of the old “Bundesangestellten-Tarifvertrag” (BAT), and replaced the former wage increases by seniority, with a scale that is influenced by the employees’ performance. We are still in a transition stage, so all consequences of the introduction of this agreement cannot be judged at present. For the scientific staff, employment on fixed term contracts was previously not permitted beyond a certain age limit. With the introduction of a new law, this barrier has now been lifted, subject to certain regulations, allowing employer and employee greater freedom in contract agreements.

To represent the activities of the various service groups at the FHI, all of whom are equally crucial for the harmonious operation of the institute, I will finish this report by briefly describing the activities of the Administration and the E-lab.

The Administration

The 15 staff-members in this group handle the usual accounting, procurement and inventory services, as well as all aspects of contract issues for all members of the institute. In all respects, the administration supports the scientists and offers direct contact and advice in administrative matters. It aims at reconciling individual requests and the specific requirements of the scientific groups, with the often complicated rules and regulations of the German civil service. The services offered by the administration go well beyond these tasks, however. Visa and passport issues are dealt with for our foreign staff and visitors, relieving them of tedious visits to the immigration department; also, help with accommodation and health insurance is offered. All aspects of business travel are organized, including ordering of tickets and hotel reservations and cost reimbursements. The administration is well experienced in dealing with the administrative complexities of project proposals, in particular for European Union projects, and provides assistance for the scientists in this respect.

Several persons in the administration are involved in pilot projects and work groups in the Central Administration of the Max Planck Society in Munich, where new methods aimed at streamlining administrative processes are planned and tested. These functions involve being key user for the Human Resources Management system, the central SAP accounting and reporting system, and for an online travel reservation system. The FHI was also pilot institute for the new e-procurement system for web-based ordering of goods and services. Our administrative manager, Mr. Rainer Fink, was recently elected speaker for the administrators in the Chemical-Physical-Technical Section of the Max Planck Society, a position in which he negotiates with the Central Administration at a high level. Beyond these tasks and services, the Administration strives to support young persons in their job training; several apprentices are being “trained on the job” in the administration at any one time.

Service group for electronics (E-lab).

In the E-lab, headed by Mr. Georg Heyne, there are 15 staff-members and, at present, two apprentices. The principal task of the E-lab is the development and construction of complex measurement and control equipment that is required for the ongoing and planned experiments at the FHI, equipment that is not commercially available. A close interaction of the E-lab with the scientists and research engineers in the scientific departments is crucial for its success; certain experiments can only be performed when the E-lab can produce the required electronic components, and *vice versa*. During the last two years, the development of the specialized high-voltage electronics for the various types of decelerators and traps that have been set up in the department of Molecular Physics have constituted a major part of the total work-load. The production of a multiple output voltage generator with amplitudes up to 300 Volt and operating from DC to 3 MHz has enabled the first demonstration of the deceleration of molecules on a chip. Equipment produced in the E-lab has also been instrumental in getting the EPR spectrometer in the department of Chemical Physics, as well as the SMART photoelectron microscope up and running. For the young scientists at the FHI, the E-lab organizes periodic practical training classes and seminars on electronic measuring methods, which are well attended and very well received. Although the members of the E-lab have suffered from the building reconstruction that was required to accommodate the mechanical workshop, they are also looking forward to the more efficient interaction that is anticipated when both service groups are housed in the same building.

Finally, on behalf of all directors and the rest of the institute, I wish to thank the Fachbeirat for their important help and the guidance they have given over the years, and I wish them an exciting and fruitful meeting.

Berlin-Dahlem, September 7, 2007

Gerard Meijer
(Chairman of the Board of Directors).

Fritz-Haber-Institut

Organization and Scientific Personnel

Legend
A: Departments
B: Scientific Personnel
* Group Leader
C: General Facilities

Board of Directors

AC	**Prof. Schlögl**
CP	**Prof. Freund**
MP	**Prof. Meijer**
PC	**Prof. Meijer (acting director)**
TH	**Prof. Scheffler**

A	**Inorganic Chemistry** **Prof. Schlögl**	**Chemical Physics** **Prof. Freund**	**Molecular Physics** **Prof. Meijer** **(Executive Director)**	**Physical Chemistry** **Prof. Meijer** **(Acting Director)**	**Theory** **Prof. Scheffler**	**Administration** **Prof. Horn** **(Admin. Director)**
B	Dr. Behrens Dr. Girgsdies Dr. Hävecker Dr. Hansen Dr. Hess Dr. Jentoft* Dr. Knop-Gericke* Dr. Kubias Dr. Su* Dr. Teschner Dr. Timpe Dr. Trunschke*	Dr. Heyde* Dr. Kuhlenbeck* Dr. Nilius* Dr. Risse* Dr. Rupprechter* Dr. Schauermann* Dr. Shaikhutdinov* Dr. Sterrer* Dr. Watanabe* N.N.	Dr. Asmis* Prof. Becker* Dr. Conrad* Dr. Fielicke* Dr. Friedrich* Dr. von Helden* Prof. Horn* Dr. Küpper* Dr. S. van der Meerakker* Dr. A.Osterwalder Dr. M.Schnell* Dr. Schöllkopf*	Dr. Eiswirth* Prof. Mikhailov* Dr. Pettinger* N.N. N.N. N.N. N.N. N.N.	Dr. Blum Dr. Carlsson* Dr. Gómez Abal Dr. Hanke Prof. Hermann* Dr. Hortamani Dr. Ireta* Dr. Michaelides* Prof. Kratzer* Dr. Rinke M.Fuchs **Independent Junior Research Group** **Dr. Reuter**	Personnel Budgets Purchasing Dept. Technical Services House Management Buildings
C	**Library** **Service Group Electron Microscopy**	**Crystal Processing** **PP&B Personal Computers,Realtime and Image Processing**	**Mechanical Workshops**	**Electronics Workshop**	**GNZ Joint Network Center**	

International Max Planck Research School
Complex Surfaces in Materials Science

Spokesperson:

Hans-Joachim Freund

Coordinator:

Thomas Risse

Members:

Klaus Christmann, FU
Hans-Joachim Freund, FHI
Paul Fumagalli, FU
Klaus Hermann, FHI (since 07/06)
Karsten Horn, FHI
Gerard Meijer, FHI
Horst Niehus, HU (until 07/06)
Klaus Rademann, HU
Karl-Heinz Rieder, FU (until 12/07)
Karsten Reuter, FHI (since 01/07)
Harm-H. Rotermund, FHI (since 03/06)
Joachim Sauer, HU
Matthias Scheffler, FHI
Robert Schlögl, FHI
Reinhard Schomäcker, TU (since 01/07)
Helmut Schwarz, TU (since 01/07)
Helmut Winter, HU
Martin Wolf, FU

FU: Freie Universität Berlin; HU: Humboldt-Universität zu Berlin; TU: Technische Universität Berlin; FHI: Fritz-Haber-Institut

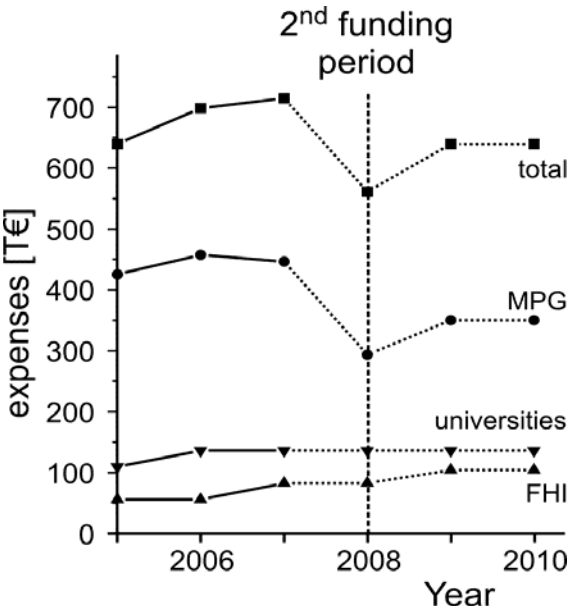
PhD-Student Members:

Micol Alemani, *Italy (until 12/06)*
Sebastian Arndt, *Germany (since 06/07)*
Rosa Arrigo, *Italy (since 11/05)*
Martin Baron, *Germany (since 03/06)*
Hadj M. Benia, *Algeria*
Juraj Bdzoch, *Slovakia (since 07/06)*
David Blauth, *Germany (since 01/07)*
Marta Borasio, *Italy (until 06/06)*
Jan Hugo Dil, *Netherlands (until 07/06)*
Katrin Domke, *Germany (until 12/06)*
Carsten Enderlein, *Germany (since 01/07)*
Jason Farmer, *USA (06/07 – 10/07)*
Christoph Freysoldt, *Germany (until 05/07)*
Mathis Gruber, *Austria (since 08/07)*
Philipp Grüne, *Germany (since 01/06)*
Sébastien Guimond, *Canada (until 06/07)*
Mahboubeh Hortamani, *Iran (until 06/06)*
Sarp Kaya, *Turkey (until 07/07)*
Ki Hyun Kim, *Korea*
Patrick Kirchmann, *Germany*
Karolina Kwapien, *Poland (since 09/07)*
Tanya Kumanova Todorova, *Romania*
Bo Li, *PR China*
Xinzheng Li, *PR China*
Jichun Lian, *PR China (since 08/06)*
Rhys Lloyd, *UK*
Junling Lu, *PR China (until 07/06)*
Helder Marchetto, *Italy (until 07/06)*
Erik McNellis, *Sweden (since 01/06)*
Michael Rieger, Germany *(since 03/07)*
Yuriy Romanyshyn, *Ukraine*
Pablo Sanchez Bodega, *Spain (since 06/06)*
Adnan Sarfraz, *Pakistan*
Viktor Scherf, *Kazakhstan (since 02/07)*
Philipp Schmidt-Weber, *Germany*
Andreas Schüller, *Germany*
Julia Stähler, *Germany (until 07/07)*
Konrad von Volkmann, *Germany*
Yongsheng Zhang, *PR China*

General Remarks:

The International Max Planck Research School (IMPRS) “Complex Surfaces in Material Sciences” (http://www.imprs-cs.mpg.de) aims at combining the expertise of several research groups, creating a unique opportunity in terms of cutting-edge research and a thorough training in the methods, concepts, and theoretical basis of the physics and chemistry of surfaces. Since the last visit of the Fachbeirat the number of participating groups has increased from 13 to 16. While the school was initially composed of groups from the Freie Universität Berlin, the Humboldt-Universität zu Berlin, and the Fritz Haber Institute, two groups of the Technische Universität Berlin (Schomäcker, Schwarz) were incorporated into the IMPRS after the successful evaluation of the school in late 2006. This renewal of the school provides funding for the time period from 2009-2014. A quote from the evaluation report may highlight the positive appreciation of the school: “The Research School has been very successful at implementing high quality graduate education in materials science as well as substantially increasing interaction and cooperation between the partner institutes. The reviewers were impressed by the enthusiasm of the graduate students and by their scientific success.”

At the moment the school has 28 students, 22 being financed by funds from the IMPRS. This is well within the range 25-30 participants proposed at the beginning. One of the goals for all International Max-Planck Research Schools is to attract especially foreign students to participate in these schools. In accordance with this guideline, currently 62 % of all participants IMPRS are foreign students which cover a broad range of 14 nationalities.



Budget of the IMPRS 2005 - 2010

The Figure presented on the left shows the total budget of the IMPRS as well as the individual contributions of the different participating organizations for the years 2005-2007. In addition, the expected evolution for the forthcoming years is drawn. The maximum of the budget in 2006 is due to the fact that the number of fellowships (nominal duration of 3 years) offered by the school, reaches its maximum after 4 of the 6 years. The reduction of the budget in 2008 is caused by the funding scheme which provides lower fund at the end of a funding period. Due to the fact that the school was positively evaluated, it is anticipated that additional funds will be made available to allow for a smooth continuation of the activities.

The plan of research of the IMPRS encompasses a wide range of complex surfaces and interfaces. Surface science has evolved, over the last two decades, from a predominance of studies on highly idealized, single-phase, single-crystalline materials, to address complex multi-phase systems such as nanoparticles, multiply layered systems, and combinations between different material classes such as metal-oxide structures. An excellent example of research in this field relates to chemical processes on surfaces. On oxide surfaces, elementary processes in heterogeneous catalysis are studied, while an understanding of reactions on semiconductors is important for a wide range of applications. Surfaces of other materials which so far have not been widely studied in surface science because of their complexity, such as nitrides and carbides, are also important from a technological point of view and will be investigated. Finally, magnetic films and multilayers are exciting topics in view of their emerging use in magnetic data storage.

The importance of turning towards a fundamental understanding of the properties of highly complex surfaces is highlighted, among other things, by an ever-increasing appreciation of the experimental methods and results of basic research in surface analysis by industrial scientists and engineers. Many of these techniques, such as atomic force microscopy, X-ray photoemission, and optical methods are nowadays routinely used in the industrial environment. This overlap of interest in surface processes is reflected in the high demand for well-trained scientific personnel with an excellent command of the concepts and techniques of modern surface science.

To accomplish the goals of the school, namely doing cutting-edge research and a thorough training in the methods, concepts, and theoretical basis of the physics and chemistry of surfaces, a variety of activities have been established. While the first issue is well covered by the individual PhD projects, the latter are addressed by a variety of teaching efforts. First, block courses on basic as well as advanced topics taking place every semester (for typical content see attached schedules). Since the school aims at recruiting chemists and physicists alike, the basic courses pay particular attention to the typical language barriers which exist between these fields. The lectures pay particular attention to this aspect, thus providing a common experimental and theoretical knowledge base for more advanced topics. The block courses are amended by lectures on special topics extending and deepening the knowledge provided in the compact block courses. (A list of lecture courses is attached below.) A central role plays the seminar program as well as a visiting researcher's program. The students are involved in the selection of the speakers at the seminar. Postdoctoral students are important in guiding the students and they are also involved in the teaching and advising efforts. It is particularly important to make sure that there is a lively exchange of ideas, and an open atmosphere of discussion across the various groups involved. To establish a suitable forum for this to happen, regular small workshops are organized where students report on the current development of their projects and discuss the achievements as well as exchange ideas for the future progress of their project with the other participants of the research school. Since most of the students will later be working in industry, excursions to industry (e.g. BASF) offer the possibility to get acquainted with the industry perspective of surface problems and the possibility to make contacts which may help in their future career.

Nowadays, so called soft skills play an increasing role for industry when recruiting scientists. Among others this includes communication skills, proper time management, or the ability to manage a project efficiently. The school offers a variety of courses to improve these skills. These include e.g. courses on scientific presentation or scientific writing. In order to combine the scientific and the soft skill aspects the students have organized a workshop at Schloß Ringberg for which all organizational details have been arranged by the students themselves including invitation of international speakers. The school only provided the funds. The response from the invited speakers was exceedingly enthusiastic, e.g.: "I would like to take that opportunity to point out that I was impressed by the workshop of the IMPRS at Schloß Ringberg. It was on a very high scientific level with a vivid discussion in a relaxed atmosphere. One can only compliment the students on this successful workshop". The students have greatly profited from the workshop and made an effort to publicize the idea. We include a report that was recently printed in "MaxPlanckIntern" (see below).

FRITZ-HABER-INSTITUT

Doktoranden üben den Ernstfall

Die Doktoranden der International Max Planck Research School for Complex Surfaces (IMPRS-CS) in Materials Science in Berlin absolvierten ein Softskill-Training der besonderen Art: Wie sonst nur etablierte Wissenschaftler haben sie eigenständig eine Konferenz nach ihren Wünschen organisiert.

Mit den International Max Planck Research Schools hat die MPG Doktorandenschulen geschaffen, in denen herausragende Doktoranden aus der ganzen Welt nicht nur fachlich, sondern vor allem auch in Softskills besonders gefördert werden. Über die gängigen Präsentations-, Schreib- und Redekurse hinaus hat die IMPRS-CS, die das Fritz-Haber-Institut mit FU Berlin und HU Berlin unterhält, ihren Doktoranden ein ganz spezielles Training finanziert: Die 25 Studenten organisierten eigenständig eine Konferenz, um so einen Einblick in die zusätzlichen Aufgaben etablierter Wissenschaftler zu gewinnen.

Die Vorbereitungszeit nahm ein gutes Jahr in Anspruch: Dass es ein konferenzähnlicher Workshop mit bekannten Forscherpersönlichkeiten als eingeladenen Gastrednern auf Schloss Ringberg werden sollte, war schnell entschieden. Auch auf das Thema „Bridging the gap" einigte man sich problemlos, denn die Kommunikationsprobleme zwischen Physikern und Chemikern sowie zwischen Experimentalisten und Theoretikern sind altbekannt und zeigen sich in der gemischten Doktorandengruppe der IMPRS-CS besonders deutlich. Eine weitere Brücke sollte zwischen den renommierten Professoren und den jungen Nachwuchswissenschaftlern geschlagen werden, denn Netzwerke erleichtern das Forscherleben ungemein, und nichts ist so wertvoll wie die professorale Plauderei aus dem Nähkästchen.

Weniger leicht war die Aufgabe zu bewältigen, wie man höchst demokratisch 25 unterschiedliche Meinungen zur Gestaltung des Workshops in ein Gesamtkonzept fasst. Obwohl in unzähligen Treffen des Organisationskomitees an jedem Wort des Einladungsschreibens bis zur Perfektion gefeilt und die Kaffeepausenzeiten präzise ausdiskutiert wurden, war man nach Versand der Einladungen doch eher skeptisch, ob die angesehenen Wissenschaftler aus der ganzen Welt sich auf ein solches „Doktorandenspiel" einlassen würden. Doch die positive Überraschung ließ nicht lange auf sich warten: Ein Großteil der geladenen Gäste sagte begeistert zu.

Dank der im Doktorandenalltag trainierten Fähigkeit, scheinbar unlösbare Aufgaben zu bewältigen, konnten alle (!) Wünsche der Gäste in Bezug auf den Rede-, An- und Abreisetermin berücksichtigt und trotzdem noch thematisch zusammenhängende Vortragsgruppierungen beibehalten werden. Und rechtzeitig vier Wochen vor Workshopbeginn ging sogar das Book of Abstracts in Druck.

Die Woche auf Schloss Ringberg war ein voller Erfolg: Seniors wie Juniors präsentierten überzeugend den neuesten Stand der Oberflächenforschung von Aerosolen bis zu Zirkoniumfilmen. Obwohl ausgiebige Diskussionszeiten angesetzt worden waren, zog sich der von Professoren und Studenten gleichermaßen getragene wissenschaftliche Diskurs, wie bei guten Tagungen üblich, immer bis in die Kaffeepausen und wurde während der Postersitzungen ergänzt und erweitert. Die Wettergötter waren milde gestimmt, – laut Mitarbeitern von Schloss Ringberg ist das immer vom Betragen der Gäste abhängig – sodass der sonnige Ausblick ins Tegernseer Tal und auf die glitzernden, schneebedeckten Berge die gute Workshopstimmung noch abrundete. Einzig der nach der Begrüßung von Bürgermeister Bierschneider geplante Konferenzausflug musste wegen der frühlingshaften Temperaturen von der Eisstockbahn ins Olaf-Gulbransson-Museum verlegt werden.

Foto: Fritz-Haber-Institut

Auch der Nachwuchs pflegt die Fachdiskussion in der Kaffeepause.

Die Professionalität der Schlossmitarbeiter, ebenso gute wie reichhaltige Mahlzeiten und nicht zuletzt die urige Ritterburgatmosphäre haben zum perfekten Gelingen des Workshops beigetragen. Fazit: Die Organisation hat viel Zeit – und natürlich auch einige Nerven – gekostet, aber sehr viel Spaß gemacht und das Gruppengefühl innerhalb der IMPRS-CS sehr gestärkt. Das Ergebnis war ein rundherum gelungener Workshop, der allen Teilnehmern in besonderer Erinnerung bleiben wird. Dank der vielen positiven Rückmeldungen wird hoffentlich bald ein zweiter Workshop in Planung gehen; es wird gemunkelt, die Gelder dafür seien bereits in München beantragt...

● KATRIN DOMKE, PHILIPP SCHMIDT

Current PhD-Projects within the IMPRS:

Arndt, Sebastian: Investigation of metal catalysts with defect structures for the activation of small molecules.
IMPRS, Germany, TU/FHI: Prof. Schomäcker/Prof. Freund

Arrigo, Rosa: Large scale synthesis of Carbon nanotubes.
IMPRS, Italy, FHI: Prof. Schlögl/Prof. Horn

Baron, Martin: Characterization of vanadia clusters on well defined CeO_2 films.
IMPRS, Germany, FHI/HU: Prof. Freund/Prof. Winter

Benia, Hadj M.: Investigation of optical and electronic properties of pure and chemically modified metal clusters.
IMPRS, Algeria, FHI/HU: Prof. Freund/Prof. Winter

Blauth, David: Oxidation of NiAl: structure and effects of ion influence emission of electrons.
IMPRS, Germany, HU/FHI: Prof. Winter/Prof. Freund

Bdzoch, Juraj: Analysis and control of ultrafast reactions on metal surfaces.
IMPRS, Slovakia, FU/FHI: Prof. Wolf/Prof. Freund

Enderlein, Carsten: High resolution photoemission of low dimensional systems.
IMPRS, Germany, FHI/FU: Prof. Horn/Prof. Fumagalli

Farmer, Jason: Calorimetry of deposited metal particles.
IMPRS, USA, FHI/U Washington: Prof. Freund/Prof. Campbell

Gruber, Mathis: Interaction and reaction of hydrocarbons on oxides: DFT model investigations of electronic structure and spectroscopic properties.
IMPRS, Austria, FHI/FU: Prof. Hermann/Prof. Gross

Grüne, Philipp: Structure and Reactivity of late transition-metal clusters.
IMPRS, Germany, FHI/HU: Prof. Meijer/Prof. Rademann

Kirchmann, Patrick: Investigation of two-dimensional metal films and one-dimensional nano-wires on semiconductor surfaces.
FU, Germany, FU: Prof. Wolf/Prof. Horn

Kim, Ki Hyun: Photo-induced processes of molecules on metal nanoparticles.
IMPRS, Korea, FHI/FU: Prof. Freund/Prof. Wolf

Kumanova Todorova, Tanya: Structure, stability and reactivity of vanadia supported catalysts.
IMPRS, Romania, HU/FHI: Prof. Sauer/Prof. Freund

Li, Bo: Density functional theory studies of water adsorption at surfaces.
IMPRS, PR China, TU/FHI: Prof. Schöll/Prof. Scheffler

Li, Xinzheng: All-electron GW approximation based on FLAPW with the application to Transition Metal Oxides.
IMPRS, PR China, FHI/FU: Prof. Scheffler/Prof. Gross

Lian, Jichun: EPR spectroscopic characterization of defect centers on oxides.
IMPRS, PR China, FHI/FU: Prof. Freund/ Prof. Wolf

McNellis, Erik: First principles studies of molecular switches at surfaces.
IMPRS, Sweden, FHI/FU: Dr. Reuter/Prof. Wolf

Lloyd, Rhys: Investigations into Sulfated Zirconia Catalysis Using Model Thin Films.
IMPRS, United Kingdom, FHI/FU: Prof. Schlögl/Prof. Christmann

Rieger, Michael: CO oxidation on oxidized Pd surfaces: a combined DFT and kinetic Monte-Carlo study.
IMPRS, Germany, FHI/FU: Dr. Reuter/Prof. Wolf

Romanyshyn, Yuriy: Reactivity studies of ordered vanadium oxide surfaces.
IMPRS, Ukraine, FHI/HU: Prof. Freund/Prof. Manzke

Sarfraz, Adnan: Deposition of Amino Acids and Derivates on surfaces.
IMPRS, Pakistan, HU: Prof. Rademann/Prof. Freund

Sanchez Bodega, Pablo: Control of chemical systems on surfaces.
IMPRS, Spain, FHI/FU: Prof. Rotermund/Prof. Christmann

Scherf, Viktor: Adsorption of Ag on the Re(10-10) surface.
IMPRS, Kazakhstan, FU/FHI: Prof. Christmann/Prof. Freund

Schmidt-Weber, Philipp: Electronic and geometric structure of molecular aggregates on vincinal single crystal surfaces.
IMPRS, Germany, FHI/FU: Prof. Horn/Prof. Wolf

Schüller, Andreas: Investigation of interaction processes during grazing incidence ion scattering.
IMPRS, Germany, HU/FHI: Prof. Winter/Prof. Freund

von Volkmann, Konrad: Steering of photoinduced surface reactions using optimized femto second laser pulses.
IMPRS, Germany, FU: Prof. Wolf/Prof. Christmann

Zhang, Yongsheng: Oxide formation and oxidation catalysis at transition metal surface.
IMPRS, VR China, FHI/FU: Prof. Scheffler/Prof. Wolf

Typical schedules of a basic block course:

	9:30 – 11:00	11:30 – 13:00
Wednesday; 04/10/06	*K. Hermann: Quantum Chemical Methods and their Application to Model Systems for Heterogenous Catalysis*	*H.-J. Freund: Introduction to Surface Spectroscopies (Part I)*
Thursday, 05/10/06	*T. Risse: Introduction to Surface Spectroscopies (Part II)*	*K. Christmann: Adsorption on and Desorption from Surfaces - Thermodynamics*
Friday, 06/10/06	*K. Christmann: Kinetics of Adsorption and Desorption*	*K. Hermann: Quantum Chemical Methods and their Application to Model Systems for Heterogenous Catalysis*
Monday, 09/10/06	*K. Rademann: Electronic and Dielectric Properties of Nanoclusters*	*F. Jentoft: Acid-Base Properties of Surfaces*
Tuesday, 10/10/06	*K. Rademann: Electronic and Dielectric Properties of Nanoclusters*	*F. Jentoft: Supported Metal and Metal Oxide Species*
Wednesday, 11/10/06	*P. Fumagalli: Magnetism I: Basic Principles*	*J. Sauer: A Chemists View of Electronic Structure*
Thursday, 12/10/06	*J. Sauer: A Chemists View of Electronic Structure*	*C. Rüdt: Magnetism II: Introduction to Thin-Film Magnetism*

Schedule of a block course focussing on an advanced topic: nanoparticles: from gas phase to surfaces:

	9:00 – 10:30	11:00 – 12:30
Monday, 16/04/07	*K. Rademann: Metals in Atomic Rays and Cluster Beams and on Surfaces: Silver and Gold*	*G. von Helden: Shape analysis of gas-phase clusters*
Tuesday, 17/04/07	*H. Winter: Interactions of molecules and clusters with surfaces*	*A. Fielicke: Vibrational spectroscopy of clusters*
Wednesday, 18/04/07	*K. Rademann: Metals in Atomic Rays and Cluster Beams and on Surfaces: Silver and Gold*	*M. Beyer: Gas phase ion chemistry of clusters*
Thursday, 19/04/07	*H. Winter: Interactions of molecules and clusters with surfaces*	*S. Shaikhutdinov: Model catalysts: Characterization and Reactivity*
Monday, 23/04/07	*F. Jentoft: Supported Nanoparticles: Catalysis and Characterization*	*S. Shaikhutdinov: Model catalysts: Characterization and Reactivity*
Tuesday, 24/04/07	*F. Jentoft: Supported Nanoparticles: Catalysis and Characterization*	*M. Beyer: Gas phase ion chemistry of clusters*
Wednesday, 25/04/07	*K. Reuter: Theoretical approaches to bonding and reaction at solid surfaces*	*R. Schomäcker: Kinetic studies of surface reactions with real catalysts*
Thursday, 26/04/07	*K. Reuter: Theoretical approaches to bonding and reaction at solid surfaces*	*R. Schomäcker: Kinetic studies of surface reactions with real catalysts*

Lectures courses 2005 - 2007:

WS 05/06:

„Selected problems of interface science: thermodynamics and kinetics of interface processes“
(Prof. Dr. K. Christmann)
„Modern Methods in Heterogeneous Catalysis Research“
(Prof. Dr. R. Schlögl and Dr. F. Jentoft)
„Structural and Electronic Properties of Metal Oxides and their Surfaces “
(Prof. Dr. K. Hermann)
„Ultrafast Dynamics at Interfaces“
(Prof. Dr. M. Wolf)
„Selected problems of magneto optics and near field microscopy“
(Prof. Dr. P. Fumagalli)

SS 06:

„Experimental and theoretical problems of surface physics “
(Prof. Dr. K. Christmann)
“Experimental techniques of Surface Science - and how a theorist understands them”
(Dr. K. Reuter)
„Ultrafast Dynamics at Interfaces“
(Prof. Dr. M. Wolf)
„Magneto-Optics: Basic Concepts and Applications “
(Prof. Dr. P. Fumagalli)

WS 06/07:

„Selected problems of interface science: surface reactions and heterogeneous catalysis“
(Prof. Dr. K. Christmann)
„Basics of Theoretical Crystallography for Surface Scientists “
(Prof. Dr. K. Hermann)
„Modern Methods in Heterogeneous Catalysis Research“
(Prof. Dr. R. Schlögl and Dr. F. Jentoft)
„Ultrafast Dynamics at Interfaces“
(Prof. Dr. M. Wolf)
„Selected problems of magneto optics and near field microscopy“
(Prof. Dr. P. Fumagalli)

SS 07:

„Introduction into the chemistry at surfaces and interfaces “
(Prof. Dr. K. Christmann)
„Selected problems of magneto optics and near field microscopy “
(Prof. Dr. P. Fumagalli)
„Ultrafast Dynamics at Interfaces“
(Prof. Dr. M. Wolf)

Department of Inorganic Chemistry   Director: Robert Schlögl

Staff scientists:

Friederike Jentoft (Habilitation)
Axel Knop-Gericke
Frank Girgsdies
Bernd Kubias
Dirk Rosenthal
Olaf Timpe (FHI Safety Officer)
Annette Trunschke
Sabine Wrabetz
Hermann Sauer Service-Group EM (Electron Microscopy)
Dangsheng Su Service-Group EM (Electron Microscopy)

Elmar Zeitler (Emeritus)

Emmy-Noether Group:
Christian Hess (+ 2 graduate students)

Guest scientists, staying for at least six months:

Kristina Chakarova
Xiaowei Chen until 02/28/2007
Juan José Delgado Jaen until 02/28/2007
Karin Föttinger
Thomas Hansen
Zoltan Hlavathy until 07/31/2007
Yuri Kolen’ko
Kirill Kovnir
Katrin Pelzer
Ayyanperumal Sakthivel until 06/30/2007
Zi-Rong Tang
Genka Tzolova-Müller
Tzvetomir Valeriev Venkov until 03/31/2007
Yi-Jun Xu

Scientists (temporary) paid from external funds:

Malte Behrens
André Breuer
Andreas Furche
Michael Haevecker
Qiang Fu until 05/31/2006
Raimund Horn
Igor Kasatkin
Ming Hoong Looi
Jens-Oliver Müller
Oksana Storceva
Detre Teschner
Jean-Philippe Tessonnier
Elaine Vass until 07/31/2007
Di Wang
Marc Willinger until 11/15/2006
Sprios Zafeiratos
Aihua Zhang
Jian Zhang
Zaoli Zhang until 03/31/2006
Bo Zhug

Graduate students: 18 (9 from external funds)
+ 2 IMPRS
+ 6 students from University of Malaya, Kuala Lumpur

Technicians: 8 (+3 Service Group EM)
Trainees: 2

Recent developments in the Department of Inorganic Chemistry

Director: Robert Schlögl

1. General
   - 1.1 Project
   - 1.2 Understanding catalysis
2. Scientific Progress

2.1 Zirconia in hydrocarbon activation
   - 2.1.1 Defect chemistry
   - 2.1.2 Structure and reactivity
   - 2.1.3 Catalyst deactivation

2.2 Vanadia in selective oxidation
   - 2.2.1 n-Butane dehydrogenation over alumina supported vanadia
   - 2.2.2 Structure and dispersion of silica SBA-15 supported model catalysts

2.3 Molybdenum oxide based catalysts in C3 selective oxidation
   - 2.3.1 System of intermediate complexity: $(Mo,V,W)_5O_{14}$
   - 2.3.2 System of high complexity: MoVTeNb oxides

2.4 Copper in C1 chemistry
   - 2.4.1 Precursor chemistry
   - 2.4.2 Effect of the calcination atmosphere
   - 2.4.3.Microstructure of $Cu/ZnO/Al_2O_3$ catalysts

2.5 Palladium in model reactions
   - 2.5.1 Hydrogenation reactions
   - 2.5.2 Oxidation reactions

2.6 Nanostructured carbons as model and practical catalysts
   - 2.6.1 Synthesis and functionalization of carbon nanotubes
   - 2.6.2 Nanocarbons as catalyst for gas phase reactions
   - 2.6.3 Carbon as catalyst support:

2.7 Silver as catalyst for selective oxidation and hydrogenation
   - 2.7.1 Ag in epoxidation reactions
   - 2.7.2 Ag in selective hydrogenation

2.8 In situ molecular beam mass spectrometry

3. Service facilities provided by the department
   - 3.1 Library
   - 3.2. Service group Electron Microscopy

Publications of the Department of Inorganic Chemistry
Invited talks of the members of the Department of Inorganic Chemistry
Patents

1. General

The department AC has continued its activities centred on heterogeneous catalysis at the interface between fundamental studies of model systems and applied catalysis involving technical systems, practical catalyst synthesis and „real“ reaction conditions. In this large field of scientific activity the department concentrates on in-situ functional analysis and defined material synthesis. The department contributes actively in research and teaching to regional activities such as the SFB 546, the IMPRS “Complex Surfaces in Material Science” and the application for the COE initiative “Unifying concepts in catalysis”. The completion of the dedicated beam line at BESSY for high-pressure photoemission experiments (ISIS) in April 2007 was a major event resulting already in a multitude of fruitful insights. The department will be brought together in October 2007 in its dedicated building 12 years after its foundation allowing for the first time to fully exploit the collaborative efforts in its projects, and to operate all of its instruments under optimal conditions. Further information on departmental activities can be found on our web site at *www.fhi-berlin.mpg.de*.

1.1 Projects

The iron oxide project was completed with a conclusive kinetic study linking the mechanistic insights of 10 years of work on single crystalline thin oxide films to well-defined macrokinetic observations of the dehydrogenation (DH) of ethylbenzene to styrene. A consistent picture emerged containing a wealth of insight into structures and dynamics of the active phase. The investigation of the spin-off process of oxidative dehydrogenation (ODH) of ethylbenzene over nanocarbon materials will be continued until the emerging kinetic differences between DH over iron oxide and ODH over carbon are either substantiated or resolved. A functional picture of the industrial DH process was developed; the addition of a large excess of steam supported by the reactivity of the iron oxide may create the same active sites on deposited carbon as occurring under ODH conditions over nanocarbons.

The other projects are in full operation and have led in a broader perspective to a working hypothesis suitable to explain the material gap in heterogeneous catalysis.

1.2 Understanding catalysis

A concept of heterogeneous catalysts is developed linking the surface chemistry of the substrate (the desired process) with the material chemistry of the catalyst (an „invisible“ process). The key feature in the concept is the acknowledgement of the essential role of structural dynamics of an active catalyst under high performance operation conditions. The existence of structural dynamics has been evidenced by numerous phenomena studied in surface science. Their role in explaining the catalytic function was, however, seen as additive and not as critical allowing thus to justify the static description of catalyst surfaces.

The essential role of structural dynamics is scientific justification for the use of in-situ methods and for the enormous experimental resources required for this kind of catalysis research. The aims of this research are a generic definition of structural dynamics as well as the evolution of synthesis concepts for suitable materials (inorganic target synthesis). A core point is the confirmation of the observation that the optimal function of a catalyst is linked to one well-defined material as opposed to intended or unintentional mixtures of systems.

Going from a static low-performing state with weak feedback of the reaction onto the structure to high performance activates the dynamic regime of a catalyst in which the reaction products actively alter the structure of the operating catalyst. The working catalyst depicted in Figure 1.1 is characterized by the conversion of a low-active precursor phase into a highly active metastable active state through processes of restructuring. These processes are driven by sub-surface chemistry of reactant fragments being incorporated into the catalyst material, a process fuelled by the excess energy liberated during substantial transformation of the educts. The metastability induced by operation in the active mode is expression of the fact that highly reactive systems are far apart from their thermodynamic equilibrium. The price for this evolution is the propensity of the active phase to deactivate through phase transformations (redox processes, segregation or sintering). It is the “art” of catalyst synthesis to select composition and real structure such, that the transformation of the pre-catalyst into the active phase is as facile as possible during the process of “activation“ and that the subsequent equilibration into the thermodynamically stable situation through „deactivation“ occurs as slowly as possible.

The extent to which surface science at low conversion and high structural definition can describe a catalytic reaction depends on the strength of coupling of the feedback loops into structure and stability of the material. A strong coupling will be the more needed, the more demanding the catalytic reaction is, i.e. the more other elementary steps than sorption of molecules control the reaction. Highly specific catalysts of complex chemical composition or delicate geometric structure (such as mixed oxides or nanoparticles) will react strongly on the changes in energy throughput and modification of the reactants chemical potential and thus exhibit strong coupling constants in the feedback loops shown in Figure 1.1

The future work of the department is dedicated to the substantiation of this concept in several kinetically demanding processes mainly from the field of selective oxidation. Metals, oxides and supported systems (for the latter of which analogous structural modifications in terms of ligation hold instead of the solid state chemistry shown in Figure 1.1) will be study materials and various methods of modifying the strength of the feedback coupling constants will be employed. The qualitative confirmation of the concept of Figure 1.1 could provide the missing link between model and high performance systems in complex catalytic transformations. In a longer term perspective the quantitative form of the concept may be incorporated into multi-scale theoretical models of catalytic processes.

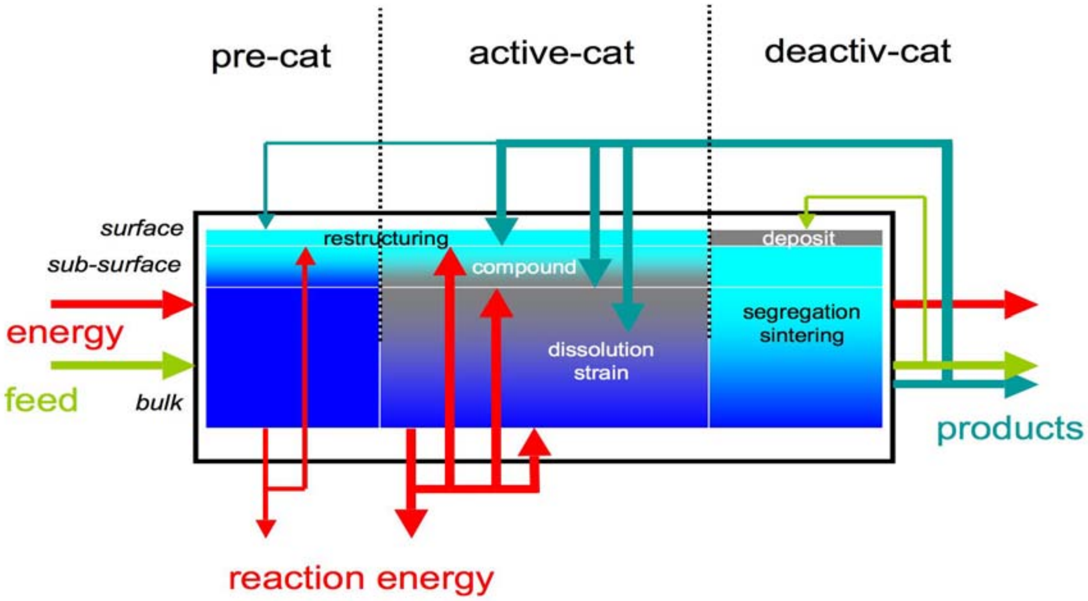


Figure 1.1 Schematic representation of a catalyst operating at low performance (model) conditions (pre-cat), at high performance conditions and in deactivated forms. The arrows indicate feedback processes to different compartments of the catalyst. The scheme applies to bulk systems. Similar feedback structures can be constructed for supported systems.

2. Scientific progress

2.1 Zirconia in hydrocarbon activation

Sulfated zirconia (SZ) is one of three types of materials that are suitable as active components of catalysts for the skeletal isomerization of alkanes. SZ can be operated at lower temperature than zeolitic catalysts, shifting the thermodynamic equilibrium towards the desired branched hydrocarbons, and without the problems inherent to the alumina system (water sensitivity, continuous Cl replacement) [1]. Previously, we had revealed that the promotional effect of cations such as Fe or Mn is most likely related to the formation of a solid solution with the zirconia [2]. The concurring loss in activity with the facile transformation of tetragonal into monoclinic zirconia supports the role of a metastable bulk structure in the formation of the active sites [3-5]. Research on the materials side in the past two years thus targeted the defect structure of sulfated zirconia materials. On the mechanistic side, the ability of the SZ catalysts to dehydrogenate and oxidize alkanes was in focus [6]. These reactions may be important for the isomerization but may also be responsible for the loss in activity with time.

2.1.1 Defect chemistry

Based on the previous experiences with the “glow phenomenon” [7,8], the defect chemistry can be varied via the calcination procedure, and by addition of promoters [2]. If the promoter cations with their valence < 4 are replacing Zr^{4+} ions in the lattice, oxygen vacancies will have to be formed for charge compensation. Depending on their charge, such sites can be detected by EPR or UV–vis spectroscopy. Ga is thus being used as a promoter now because it does not cause any interfering signals such as Mn and Fe. In cooperation with the group of Prof. Klaus Köhler within the framework of IDECAT, an in situ EPR experiment with on-line GC analysis has been set up at TU München. Several types of paramagnetic species, namely superoxide (O_2^-), Zr^{3+}, and F^+ centers (e^- in O vacancy) can be identified. Zr^{3+} ions do not seem to play a role for catalysis. Surface F^+ centers are formed during activation (723 K) in inert gas, and UV–vis data also reveal an increased defect density after activation. The concentration of superoxide species changes during alkane isomerization. In the future, we shall seek correlations between performance and the abundance of the individual species.

2.1.2 Structure and reactivity

At high temperatures (573 K), alkanes are completely oxidized to CO_2 by SZ, while sulfate is reduced to H_2S [6]. At moderate temperatures, alkanes are partially oxidized. A disulfate species ($S_2O_7^{2-}$) was recently identified as being active for oxidative dehydrogenation (ODH) of alkanes, which is thought to be followed by protonation of the resulting alkene to give a carbenium ion, which then acts as a chain carrier in the isomerization cycle [9]. Dehydrogenation is confirmed by C K edge NEXAFS on a nanocrystalline SZ thin film (used in the frame of a now terminated DFG priority program) [9]. For promoted catalysts, the maximum butane isomerization rate is proportional to the intensity of a disulfate S=O vibration, indicating the same active species and mechanism as for SZ [5]. The oxidizing power of the sulfate is enhanced in the presence of promoters [6,10]. We hypothesize that the reactivity of the sulfate (or other oxo anions) is tuned by the geometric and electronic alterations that the promoters inflict upon the support.

2.1.3 Catalyst deactivation

Deactivation proceeds on different time scales, requiring more than one type of phenomenon. UV–vis–NIR spectra recorded during catalysis show formation of water and bands attributable to mono and polyenic allylic cations [11]. Water, the product of ODH but also a poison for Lewis acid sites, is formed during the initial period of the reaction. Unsaturated deposits, however, accumulate continuously on the surface and may ultimately block sites but are apparently not the primary reason for deactivation. Comparison with zeolitic systems (collaboration with Prof. Murzin’s group at Åbo Akademi), reveals essentially the same, discrete surface species as on SZ, indicating a similar chemistry. This type of experiments will allow us to understand the roles of Pt and H_2 for the isomerization and specifically for the prevention of side reactions on these catalysts.

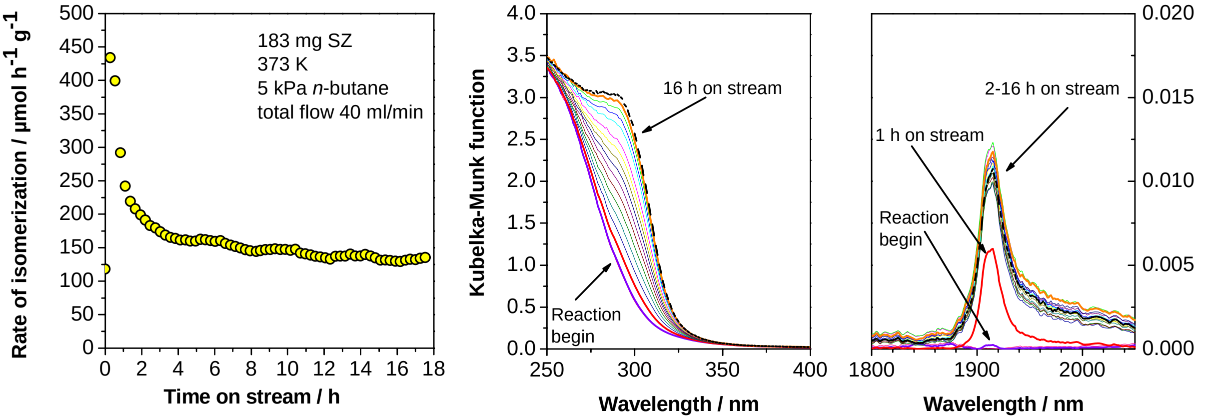


Fig. 2.1.2 In situ spectroscopy during n-butane (5 kPa) isomerization catalyzed by sulfated zirconia at 373 K. Left: isobutane formation rate, center: UV–vis spectra, right: NIR spectra.

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2.2 Vanadia in Selective Oxidation

2.2.1 n-Butane dehydrogenation over alumina supported vanadia

A series of V_xO_y/alumina (1-8 wt% V) catalysts were investigated for the selective dehydrogenation of *n*-butane. These experiments were part of the ATHENA collaboration in which other groups invstgated the same catalysts for various other aspects of their function. High-pressure *in situ* XPS provided several insights into the nature of vanadium species under reaction conditions. As shown in Figuure 2.2.1 for 3.5 wt% V/Al_2O_3, the major vanadium species present on the catalysts at 0.5 mbar oxygen and 673 K was V^{5+} (spectrum A). However, immediately after introduction of 0.4 mbar *n*-butane, reduction of the vanadium species was observed (spectrum D). In the case of catalysts where deactivation and carbon deposition were observed, the oxidation state of vanadium tended towards V^{3+}. On addition of 1-2% oxygen to the butane feed the V^{5+} component was greatly maintained (2% O_2 spectrum B, 1% O_2 spectrum C). However, a negative effect was observed with respect to the catalytic activity as a greater proportion of oxygen-containing products were observed.

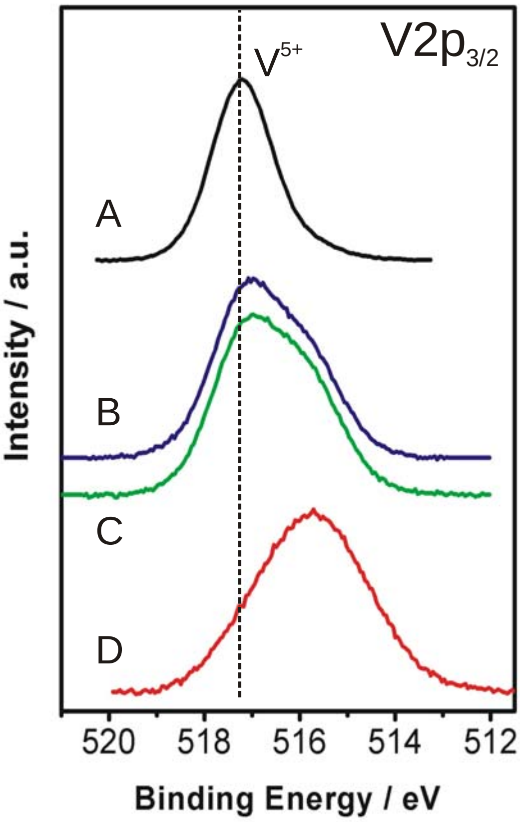

Fig. 2.2.1 In situ XPS spectra of V-alumina for butane dehydrogenation

Ex situ investigations of catalysts that had been reacted in *n*-butane at high pressure, yielded several additional insights. Firstly, carbon NEXAFS was able to distinguish differences in the deposited carbon depending on the initial vanadium loading. At higher loadings (3.5-8 wt% V), one main feature was observed relating to the presence of unsaturated hydrocarbons. Absence of features in the higher energy region suggests that the carbon is mainly amorphous [1]. On 1 wt% V/alumina, additional features were present in the 1s-π* region, which hint towards the formation of styrene-like compounds. Investigation of a catalyst still active prior to removal from reactor was shown by TEM to be completely encapsulated by carbon. However, the NEXAF spectrum showed a change in nature of the carbon when compared with the deactivated samples. There appeared to be an increase in the hydrogen content as well as strong features in the 1s-σ* region suggesting that there was an increase in the graphite-like nature of the coke.

The active vanadium component during *n*-butane dehydrogenation contains a mixture of oxidation states, however is greatly reduced from its initial 5+ state. Future investigations require balancing the oxygen content of the feed to reduce deactivation without reducing catalyst selectivity. Carbon NEXAFS has provided useful information regarding changes in the nature of the carbon laid down during reaction under different conditions. The results support the suggested mechanism of butane dehydrogenation over V/alumina catalysts [2], i.e.

dehydrogenation, cyclisation, polymerisation, followed by further cyclisation and condensation to form 1D and 2D polyaromatic coke.

The results further point towards an active involvement of carbon deposits in a special geometric structure at high operation temperatures. This result is consistent with observation of the dehydrogenation and oxidative dehydrogenation activity of oxygen-modified nanocarbons (see section 2.6) and may explain the beneficial role of traces of oxygen that are insufficient to oxidize the primary product hydrogen and shifting the equilibrium towards the product.

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2.2.2 Structure and dispersion of silica SBA-15 supported model catalysts

The synthesis, structure and reactivity behavior of silica SBA-15 supported vanadium oxide model catalysts for propane partial oxidation has been studied. Using a novel synthesis approach based on controlled grafting/ion exchange, highly dispersed vanadium oxide can be deposited homogeneously within the pores of mesoporous SBA-15 [1]. The reactivity behavior of the synthesized vanadia catalysts was tested in the selective oxidation of propane to acrylic acid in the presence of 30% water steam. At 400°C, a high selectivity of 84% (at 8% conversion) for acrylic acid formation was observed demonstrating that our model can successfully mimic active sites of more complex mixed metal oxide catalysts such as Mo-V-Te-Nb oxides [2].

To gain a deeper understanding of the role of steam on the selective oxidation of propane, the influence of water on the structure and dispersion of highly dispersed vanadia was investigated. A new multiple *in situ* spectroscopic experiment was set up, which for the first time combines Raman, UV-Vis and X-ray photoelectron spectroscopy (XPS) [3]. The UV-Vis and XP spectra show that the fully hydrated vanadia catalyst is slightly reduced but consists mainly of V^{5+} species. The corresponding Raman spectra are in excellent agreement with those of the water containing V_2O_5 gel $V_2O_5 \cdot 1.2H_2O$, which consists of polymerized pyramidal VO_5 units similar as in V_2O_5. Upon catalyst dehydration a highly dispersed V^{5+} species is formed, which consists of tetrahedrally coordinated vanadium with significantly smaller ensemble size (XPS). Therefore, it was shown that changes in the structure and dispersion of highly dispersed vanadia during the interaction with water are correlated [3].

As shown in Figure 2.2.2 additional transmission IR experiments using NO as probe molecule give evidence for the presence of mostly polymerized (at least dimeric) vanadia in the dehydrated state even at low V loadings (0.7 V/nm^2) [4].

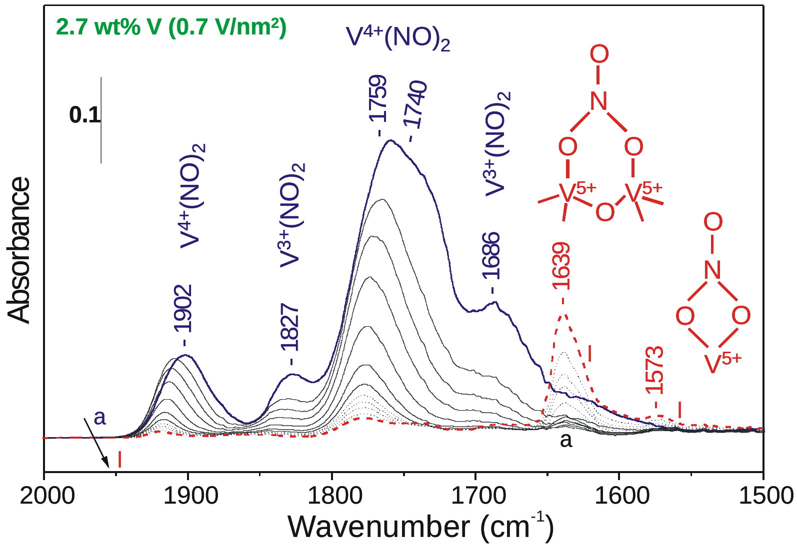

Figure 2.2.2 FTIR spectra of NO adsorbed at 298 K on reduced 2.7wt% V/SBA-15 after addition of oxygen (a) and subsequent temporal evolution (b-l).

As first application of our new setup vanadyl Raman cross-sections of crystalline V_2O_5 and highly dispersed vanadia species were correlated using the corresponding XPS V2p features [5]. The ongoing deeper structural elucidation of this-thought-to-be well defined model system involves theoretical studies in collaboration with the TH department and in-situ studies at BESSY plus high-precision EXAFS experiments in collaboration with T.Ressler (TU Berlin). The hydration state of the vanadia and a possible dynamics of the extent of oligomerisation below the formation of a crystal are currently studied. Initial experiments using microcalorimetry provide boundary values for heats of chemisorption of reactants. The dynamic nature of the sites will require in situ reaction-adsorption experiments.

The vanadium project benefits as a whole from the reference experiments carried out in the CP department. These studies provide spectroscopic data as well a functional model explaining the relevance of a defective vanadyl-terminated vanadium oxide. All circumstantial evidence in our project is consistent with the notion that an active site of vanadia must contain both V-O single bonds and V=O groups both playing essential roles in binding and activation C-H groups of adsorbed substrates. With respect to an extension of the studies to other supports and to the application of catalyst concepts derived from model studies, there is an increasing need to develop strategies for target synthesis of pre-determined vanadium species on oxides. Such strategies have to take fully into account the significantly varying surface chemical reactivity of various oxides under conditions of adsorption of vanadium precursor species. This complex issue will be addressed with a strategy similar to that developed in the copper project.

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2.3 Molybdenum oxide based catalysts in C3 selective oxidation

Selective oxidation of light alkanes with molecular oxygen to aldehydes or acids provides alternative access to chemical intermediates by utilization of natural gas or renewable feedstock as a replacement for olefin-based petrochemistry. However, the catalytic activation of C-H bonds in alkanes requires higher temperatures or more active catalysts. Furthermore, the increased reactivity of partially oxidized reaction intermediates is particularly challenging and accounts for high chemical and structural complexity of the catalytically active oxides. The direct oxidation of propane to acrylic acid proceeds with exceptional performance over crystalline MoVTeNb mixed oxides. Propane activation and high selectivity are attributed to the presence of an orthorhombic phase denominated as M1 (ICSD 55097). The bronze-like structure is similar to that of $Cs_{0.7}(Nb_{2.7}W_{2.3})O_{14}$ [1]. It is composed of octahedral MO_6 and pentagonal bi-pyramidal MO_7 units, (M=Mo,V,Nb), forming six- and seven-sided channels stabilized by built-in tellurium. The pentagonal bi-pyramidal motif is also found in the related tetragonal M_5O_{14}-type structure, (M=Mo,V,Nb,W,Ti,Ta), formed in MoV(W) oxides, which are active in propylene and acrolein oxidation.

The high degree of long-range order with respect to the metal constituents seems to be an important requirement for the development of active and selective metal-oxygen arrangements on the surface of the crystalline material under reaction conditions. With regard to the chemical complexity the synthesis of phase-pure complex mixed oxides is a challenging pre-requisite for understanding the mode of operation of the catalyst.

2.3.1 System of intermediate complexity: $(Mo,V,W)_5O_{14}$

$Mo_{0.91}V_{0.09}$ and $Mo_{0.68}V_{0.23}W_{0.09}$ oxides have been prepared by spray-drying mixed metal salt solutions followed by thermal treatment in air and/or helium at temperatures between 623 K and 713 K. XRD analysis confirmed phase purity and high crystallinity of the oxides obtained. The structural analysis of $(Mo,V)_5O_{14}$ indicated a homogeneous distribution of molybdenum and vanadium on all sites. Conversely, for $(Mo,V,W)_5O_{14}$, a preferred site occupancy of tungsten in the pentagonal bi-pyramidal unit and its neighboring octahedral sites was found. Vanadium preferentially occupies metal positions in corner-linked octahedrons not edge-sharing to the pentagonal block unit. In-situ XRD investigation of the thermal treatment showed that phase purity and crystallinity of the resulting $(Mo,V,W)_5O_{14}$ oxide are mainly achieved in the calcination process controlled by the redox potential of the gas atmosphere at a given temperature and by kinetic parameters that influence the removal of gaseous decomposition products from the precursor (i.e. gas flow rate and dwell time).

A structure stabilizing effect of tungsten in $(Mo,V,W)_5O_{14}$ under oxidizing conditions was found that can be assigned to its site preference in the M_5O_{14}-type structure [2]. The crystalline materials show catalytic activity in oxidation of propylene. A non-destructive depth-profiling performed by varying the excitation energy in in-situ X-ray photoelectron spectroscopic experiments in the presence of reactants at a total pressure of 0.5 mbar revealed a reversible enrichment of vanadium on the surface of the catalysts that is more pronounced after addition of steam to the feed. The crystalline bulk structure remains intact under these conditions indicating that the dynamic response of the oxide to the gas phase is a true surface phenomenon. The observation may point to the function of such a complex architecture of a catalysts namely as to provide the stability of a storage phase allowing to accommodate major compositional responses of its surface in a reversible way.

2.3.2 System of high complexity: MoVTeNb oxides

The hydrothermal synthesis and catalytic properties of MoVTeNb oxides in selective oxidation of propane to acrylic acid have been investigated. In contrast to phase cooperation

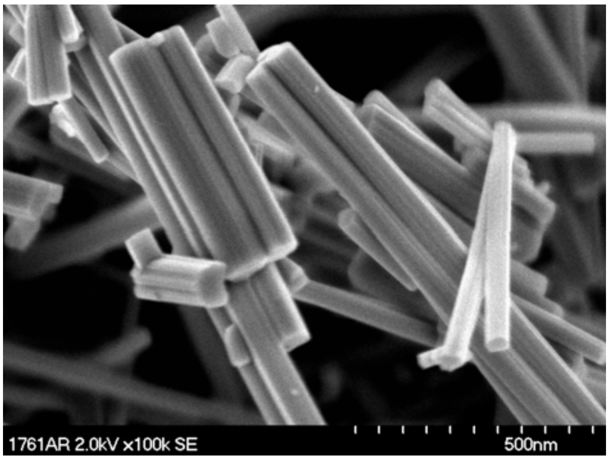

Fig. 2.3.1 SEM image of phase-pure M1

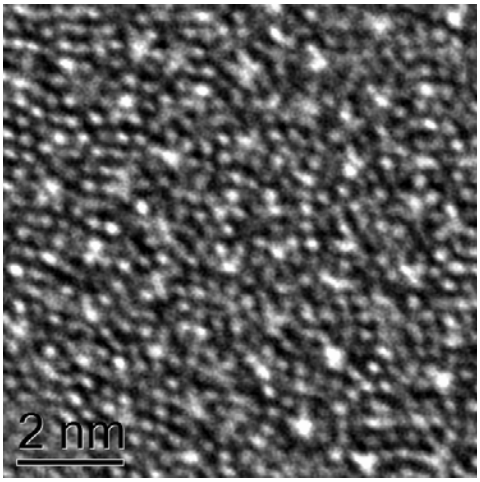

Fig. 2.3.2 HRTEM image of a M1 needle viewed along the <001>zone axis

concepts [3], propane conversion and formation rate of acrylic acid normalized to the total surface area of the mixed oxide increase with increasing content of the M1 phase in the crystalline catalyst. Phase-pure M1 converts propane to acrylic acid with a selectivity of about 80%, whereas the propane conversion is mainly dependent on the specific surface area. This finding supports the basic assumption in this project that the function of the catalyst in the complex transformation of propane to acrylic acid may be understood on the basis of the analysis of a single phase and stable active material. A reproducible synthesis and a suitable specific surface area of the material are pre-requisites for in-depth physicochemical investigations.

In contrast to the established route of precipitation and drying [4], hydrothermal synthesis enables the preparation of highly crystalline single-phase M1 without the necessity of further product purification by chemical treatment. However, the synthesis requires precise control of the reaction conditions especially with respect to temperature and time, and has to be optimized taking into account the technical parameters of the autoclave used. Raman spectroscopy and SEM-EDX analysis indicate an inhomogeneous distribution of the metals in the reaction mixture introduced into the autoclave. Under hydrothermal conditions, complete reorganization of the molecular building blocks occurs resulting in formation of nano-structured M1 that crystallizes in inert atmosphere at high temperatures (873-923 K) into phase-pure M1 with needle-shape morphology (Figure 2.3.1 and 2.3.2). SEM-based shape analysis of a series of phase-pure M1 catalysts reveals that the diameter of the needle-like crystals depends on the conditions of the thermal treatment. However, such studies have not shown a clear correlation between the catalytic activity and the occurrence of a certain crystal plane, e.g., the {001} plane. Independent of the crystal facet, the M1 surface is terminated by a structurally disordered surface layer roughly 0.7 nm thick, as evidenced by

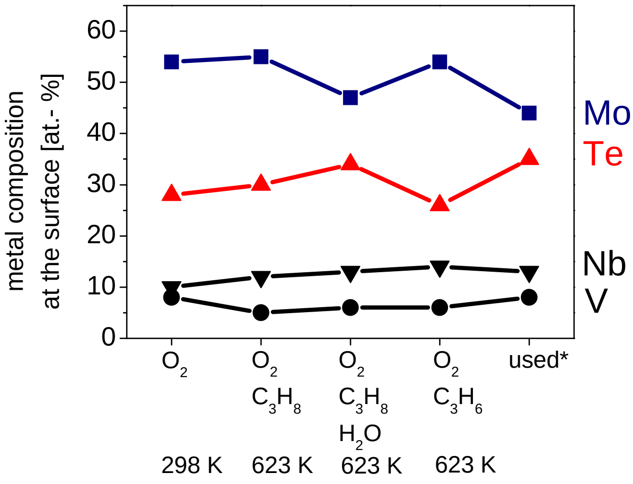

Fig. 2.3.3 Surface composition of M1 (catalyst ID 1761) measured by in-situ XPS (information depth approx. 1 nm) in the presence of O_2 (p=0.3mbar, T=298K) or feed (p=0.25 mbar, T=623K).
**catalyst tested in a fixed bed reactor at p=1 bar, 673 K.*

HRTEM [5]. This observation is in accordance with the reversible tellurium enrichment of the M1 surface to an extent incompatible with the M1 stoichiometry, as found by in-situ photoelectron spectroscopy in the presence of propane and oxygen and even more pronounced in the presence of steam at reaction temperature (Figure 2.3.3). The open channel structure of M1 is, apparently, responsible for considerable dynamics observed in the topmost surface layers that reversibly respond to the gas phase in agreement with the structural and morphological stability of phase-pure M1 catalysts under the reaction conditions of propane oxidation.

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2.4 Copper in C1 chemistry

Cu catalysts such as Cu/ZnO/(Al_2O_3) are active, e.g., in methanol synthesis and methanol steam reforming (MSR). A knowledge-based catalyst design requires understanding of the catalyst’s “real” structure and its relation to catalytic activity. This is tackled by detailed characterisation of active catalysts and their precursors. Furthermore, synthetic tools have to be optimised or newly developed to tailor the structural properties in the desired way in order to prepare highly active catalysts as well as suitable 2^{nd}-generation model systems [1].

2.4.1. Precursor chemistry

The optical absorption spectra of the Cu,(Zn)-hydroxycarbonates malachite, rosasite and aurichalcite, which are typical components of the co-precipitated precursor mass in course of Cu/ZnO catalyst preparation (Figure 2.4.1), were recorded in the UV-vis-NIR range for phase pure co-precipitated samples and for well crystalline mineral samples. Theoretical calculations can successfully model the experimental spectra by assuming that Cu^{2+} is preferentially located on crystallographic sites exhibiting strong Jahn-Teller distortion of their octahedral coordination environment. Understanding the spectra of these reference compounds is a pre-requisite to use in situ optical spectroscopy for characterisation of complex precursor mixtures.

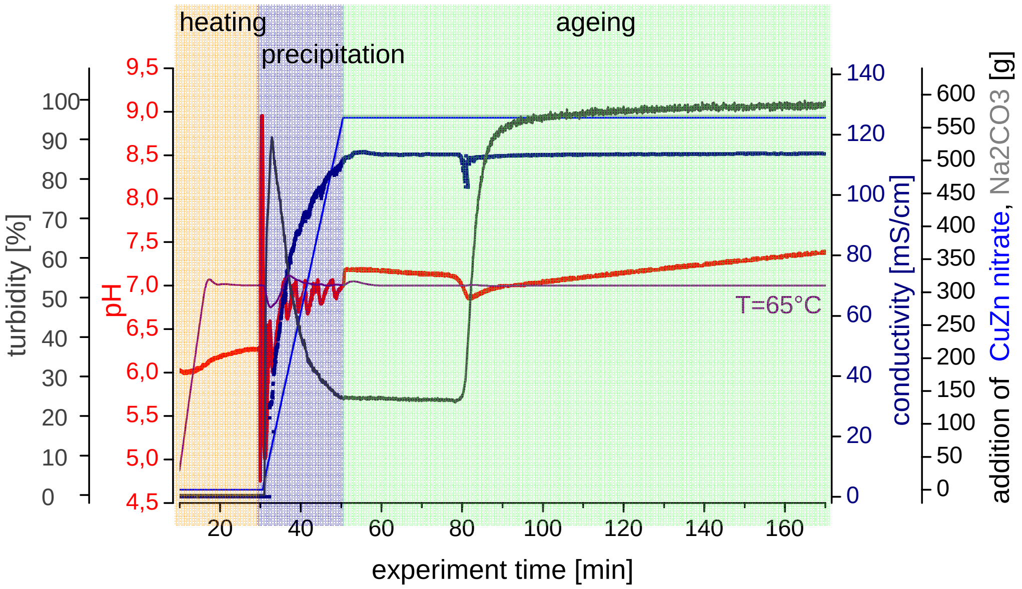

Fig. 2.4.1 Precipitation and ageing of a Cu,Zn hydroxycarbonate in a fully automated and computer-controlled precipiation reactor.

Ternary Cu/Zn/Al precursors usually contain mixed layered double hydroxides (LDH) after co-precipitation. Cu-rich LDHs have been prepared in phase-pure form and were characterised as a function of composition and calcination temperature [2]. After calcination at 330 °C an amorphous material is obtained. Due to the initially perfect distribution of the metals in one precursor phase, reduction yields small Cu particles of around 5 nm in size. These particles exhibit extended interfacial contacts to an amorphous $ZnAl_2O_4$-like matrix.

2.4.2 Effect of the calcination atmosphere

The effect of different calcination atmospheres on the MSR activity of Cu/ZnO catalysts was investigated by means of decomposing a Cu,Zn-

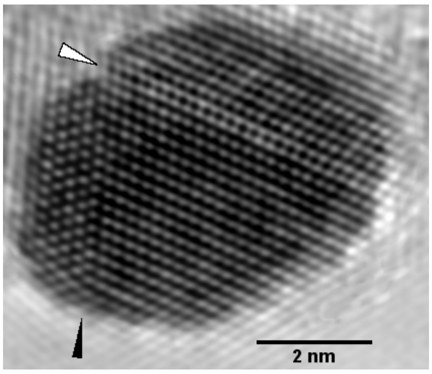

Fig. 2.4.2 HRTEM image of a copper particle in a $Cu/ZnO/Al_2O_3$ catalyst

hydroxycarbonate in 20% O_2, CO_2 and O_2/CO_2 (1:1) in 80% N_2, respectively. The activities were not affected significantly, whereas the samples calcined in presence of CO_2 exhibit a lower production of CO, i.e. a superior selectivity. Further characterisation of these samples by TG-MS and *in situ* XAS revealed not only a higher residual carbonate content after calcination, but also increased structural disorder of the Cu particles after reduction. These results indicate that the calcination atmosphere is a suitable parameter to influence the quality of the active sites. The data further suggest the importance of non-equilibrated Cu surfaces for catalytic performance and the necessity to control the Cu-support interfacial contact (by carbonate buffer layers).

2.4.3.Microstructure of $Cu/ZnO/Al_2O_3$ catalysts

The effect of different preparation routes on the properties of $Cu/ZnO/Al_2O_3$ catalyst was investigated by a combined *in situ* XRD, *in situ* XAS, TPR and TEM study [3]. Five samples prepared according to different patented procedures were tested in MSR and compared to a commercial catalyst. The variation of activities could not be explained by different Cu surface areas alone. The commercial sample was most active and the only one to exhibit a measurable Cu lattice strain, probably induced by an advanced Cu/ZnO interface. The microstructure of this sample was also most homogenous as indicated by a narrow and symmetric TPR profile and particle size distribution curve. Similar to the binary system [4], the presence of a suitable microstructure seems to greatly enhance the catalytic performance.

This also holds for the methanol synthesis reaction as was revealed in a detailed TEM, HRTEM (Figure 2.4.2) and *in situ* XRD study of a series of “real” ternary catalysts [5]. Earlier experiments on this topic from the literature utilized supports and loadings remote from technical examples leading to a completely different microstructure of the system namely an oxide support with dispersed Cu particles instead of the practical catalysts being a porous agglomerate of Cu with oxide spacers. A statistical meaningful number of Cu particles (5000 – 24000) were analysed by TEM and the resulting size distribution data were implemented in the analysis of the microstructure based on profile fitting of XRD patterns. With this approach a correlation of the defect concentration as well as the lattice strain and the activity could clearly be identified (Fig. 2.4.3). Defects such as twin boundaries and stacking faults can be visualised with HRTEM (Figure 2.4.2, arrows) and, according to these results, might contribute to the active state of Cu. Such an analysis is one of the few examples where a structure-function correlation was established substantiating the real structure as a descriptor for the active sites. The analysis further shows that no correlation exists between activity and the basic structural properties of the system accessible from standard XRD analysis. This result further puts into a direct perspective the synthesis efforts described in the previous two sections with the catalyst performance; it offers explanations for the "black magic" how details of precipitation and calcination affect the final performance of a system that is not the direct result of the synthesis unit operation investigated.

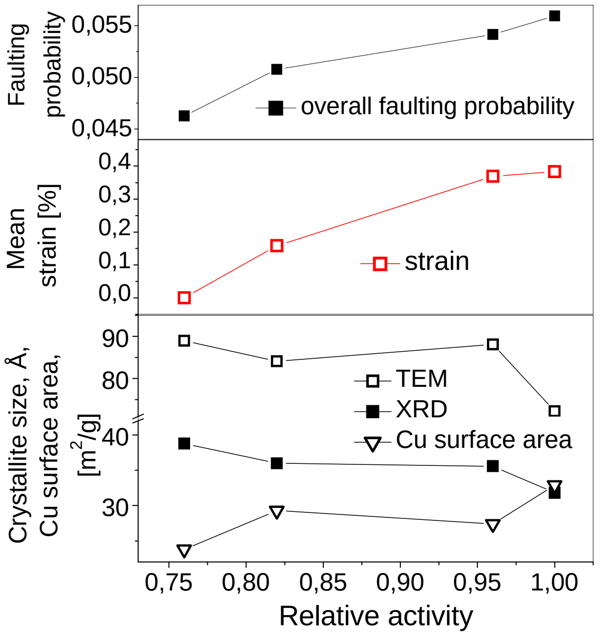

Fig. 2.4.3 Microstructural parameters obtained with TEM and XRD as a function of relative catalytic

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2.5 Palladium in model reactions

2.5.1 Hydrogenation reactions

Palladium particles are able to add one hydrogen molecule to both alkenes and alkynes. To achieve selectivity in semi-hydrogenation the surface-near region of Pd has to undergo strong modifications in which a significant amount of carbon from cracked feed molecules penetrates into the palladium surface, modifying its geometric as well as its electronic structure (see Figure 2.5.1.).

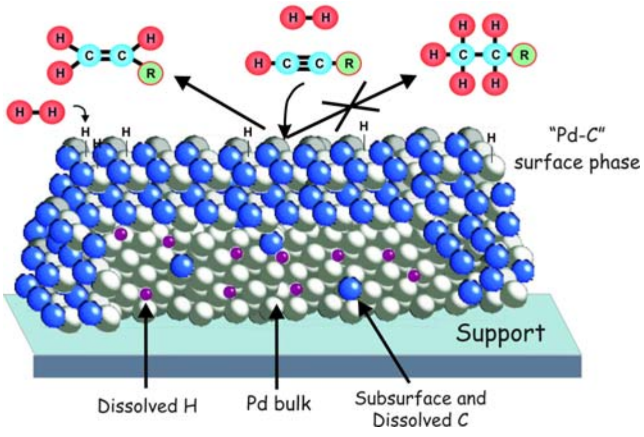

Fig. 2.5.1: Rough model of selective alkyne hydrogenation on palladium

In situ XPS experiments proved the presence of a surface Pd-C phase, as established previously [1]. Pd-C formation was found to be a general process in every selective alkyne hydrogenation reaction we studied, while it was always absent with alkene feed. Its role, in line with the hydrogenation model suggested by the CP department [2], is to inhibit the emergence of bulk-dissolved hydrogen to the surface, or even hinder its population. Bulk-dissolved / subsurface hydrogen was shown to be a very reactive but unselective species. The population of subsurface hydrogen is becoming possible above a critical H_2/alkyne ratio, since the initial alkyne hydrogenolysis decreases, shifting the equilibrium of hydrogen vs. carbon penetration towards hydrogen diffusion. High-pressure XPS experiments have clearly shown the correlation between diminishing Pd-C and changing hydrogenation selectivity favouring alkane formation.

Total hydrogenation can be avoided by tuning the alkyne-to-hydrogen ratio. However, e.g. in the semi-hydrogenation of small amounts of acetylene in a large excess of ethylene, the reaction has to be prevented from running into the oligo- and polymerization path by other means as the feed ratio is fixed. Both requirements can be met by using palladium intermetallic compounds, IMCs (PdGa, Pd_3Ga_7, $Pd_{15}Cu_{85}$, PdZn. These compounds became available in high quality through collaboration with the MPI Dresden (Y. Grin). These compounds exhibit well-ordered crystal structures with Pd atoms solely coordinating to the second metal atoms in the first shell. Analysis of the chemical bonding by quantum chemical calculation of the electron localization function (ELF) reveals pronounced directed (covalent) bonding in PdGa and Pd_3Ga_7. The catalytic function was analyzed by FT-IR of CO and in situ XPS, and the site isolation concept as well as the modified electronic state was validated. The samples are catalytically highly active, are long-term stable and exhibit superior selectivity towards ethene than the presently used supported alloy $Pd_{20}Ag_{80}$ catalysts.

2.5.2 Oxidation reactions

This part of the project is concerned with the characterization of the active state of Pd during oxidation of ethene on polycrystalline Pd and during the total oxidation of methane on the well-defined Pd(111) single crystal surface in the pressure range between 10^{-6} and 1 mbar. These studies were performed in collaboration with the University of Innsbruck, Austria and the University of Limerick, Ireland, using in-situ XPS at BESSY, temperature-programmed thermal desorption TPD, LEED and AES.

An investigation of the interaction of the Pd (111) surface with clean oxygen allowed the identification of several oxygen surface species of different activity, while the interaction with carbon from ethene decomposition induces the formation of a Pd-C phase even in the presence of oxygen with similar spectroscopic feature like the Pd-C phase observed in the selective hydrogenation of pentyne [3,4]. Pd is also well-known for a high selectivity in partial oxidation reactions, e.g. of ethene to acetic acid and vinyl acetate, whereby a carbon-modified state of the Pd catalyst is active under rather reducing conditions.

Studies under UHV conditions concerned the activity of chemisorbed oxygen and of the surface oxide Pd_5O_4 towards CO oxidation and the decomposition of ethene followed by carbon incorporation at an atomic scale. In-situ XPS allowed to obtain a detailed picture of the modification of the surface under close-to-real conditions in the oxidation of methane and ethene at pressures up to 1 mbar[5]. In ethene oxidation, the most active state is a highly reduced Pd surface with a surface-near Pd_xC_y phase, while methane oxidation is favoured on the Pd_5O_4 surface-oxide covered surface, which acts as a precursor for formation of active bulk PdO[6]. The complex interplay of surface oxides with bulk metal and bulk oxide gives rise to kinetic hysteresis phenomena that were analyzed by in situ XPS and assigned to respective phase transformations. The most active state was found to be a transient state of sub-surface-oxygen in Pd occurring either during oxidation of metal or during reduction of oxide. It should be noted that analogous behaviour was found in a study looking at the reactivity of Ru in CO oxidation and methanol oxidation. The correlation of the reactivity of the two elements in the same reaction will be the subject of ongoing studies with the working hypothesis that the same states of activity are reached at different reaction conditions reflecting the differences in electronic structure of the elements.

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2.6 Nanostructured carbons as model and practical catalysts

Nanostructured carbons as catalysts offer the unique opportunity to study active sites in oxidation without any interference from structural oxygen or from sub-surface oxygen species. Nanocarbons are electron-transparent supports for studying clusters of single-phase metal oxides in selective oxidation. The project benefits in both areas from extensive collaboration with the TH department where studies of local structures of active sites, their reactivity and their catalytic function are conducted at an extent that would be prohibitive in effort for metals or metal oxide systems. Theory has made predictions about reactivity of oxygen on flat and curved structures that will be verified in our department using high-pressure studies that only are amenable to the reactivity of carbon being inert under UHV-type conditions.

2.6.1 Synthesis and functionalization of carbon nanotubes

Nanocarbon as catalyst for the oxidative dehydrogenation (ODH) reaction requires a material allowing solving the formulation issue and withstanding corrosion problems in oxygen at elevated temperatures. Activated carbon (AC) produced from biomass was chosen as support. Chemical modifications were developed to reduce diffusion problems in the micropores and to physically anchor the nanotubes to prevent detachment during reaction. The CNT synthesis is investigated *in situ* in an ongoing work using a high-pressure DSC equipped with an online mass spectrometer to identify the influence of several parameters such as reduction conditions, growth conditions, and effect of contaminant. Other natural support materials such as Etna lava or betonite are used for the immobilization of CNTs. All the supported CNTs are active in the tested ODH reactions.

Nitrogen-containing CNFs/CNTs show enhanced catalytic performance in several catalytic applications of carbon-based material. Our interest is focused on the synthesis of hierarchical structured N-CNFs/AC by CVD of hydrocarbon over a transition metal supported on AC. Both C_2H_4 - NH_3 in mixture or CH_3CN have been used as C and N source. Characterizations prove that using CH_3CN is more promising way for the N functionalization. In addition, we show that post-synthesis treatment of CNTs with nitrogen-containing molecules such as NH_3 is also a suitable route for incorporating N functionalities on the surface of CNTs.

2.6.2 Nanocarbons as catalyst for gas phase reactions

The work has focused on the kinetic analysis, scale-up and long-term testing of ODH of ethyl benzene to styrene, and on the activation of alkane (butane) and alkene (1-butene) molecules over CNTs. The kinetic analysis on sp^3-nanodiamond and sp^2-nanotube gives the same reaction order and activation energies revealing that the reaction pathway and the nature of the active sites are the same over both sp^2– and sp^3–carbon [1]. The reaction follows the Langmuir-Hinshelwood mechanism, in which breaking of C–H bonds is kinetically relevant. Our mechanistic findings differ in nature from those over metal or metal oxide catalysts involving lattice oxygen as kinetically limiting. In this way it is possible to prove that ODH can also occur as surface-only reaction and does not require bulk lattice oxygen as it is still frequently stated in review articles on selective oxidation. From scale-up (10 g) and long-term testing (500 h) of the reaction in a mini-plant reactor, we found that the microstructure of the carbon material essentially determines its long-time performance and stability and only nanocarbon (and not activated carbon as in contrast to literature) robustly catalyze the ODH reaction. In Fig. 2.6.1, we present the microstructure of three different types of nanocarbons used in our tests. No noticeable change in morphology of the used nanocarbon was observed even after long-time testing. CNTs can exhibit a performance as good as the conventional DH process with advanced catalyst systems but at a temperature 300°C lower than that of the current industrial process and without use of steam. The figure of merit is the productivity in mmol styrene/g cat/h being now equal for DH and ODH. This promises practical applicability when the transport limitations can be overcome limiting current selectivity.

We tested for the first time the use of CNTs as catalysts for the ODH of n-butane and 1-butene. For the ODH of n-butane, both CNTs and activated carbon display a remarkable and stable catalytic activity. Addition of P_2O_5 as promoter suppresses the total oxidation and significantly increases the yield of butadiene. Further it was shown that carbon catalysts are superior to carbon-supported $FePO_4$ catalysts. For the ODH of 1-butene, CNTs are active and superior to activated carbons. Characterizations of CNTs before and after reaction reveal that oxygen functional groups are the active sites for the ODH reaction. Their detailed speciation is now under way.

2.6.3. Carbon as catalyst support

Our work reveals that commercially available CNTs containing metal particles are highly active catalysts for NH_3 decomposition [2]. Fe, Co, and Ni are typical active phases used to catalyze the growth of CNTs. They remain as highly dispersed impurities on the CNTs after the CVD process. We use the as-synthesized CNTs as catalysts without any additional chemical pretreatment. The catalytic performance is comparable to or higher than that of commercially available catalysts for NH_3 decomposition. The decomposition is selective to N_2, H_2; no signals of CH_4 due to methanation of carbon could be detected. In addition, we have used bimetallic nanoparticles (Fe, Co, Ni, Mo) supported over CNTs to replace Ru for NH_3 decomposition.

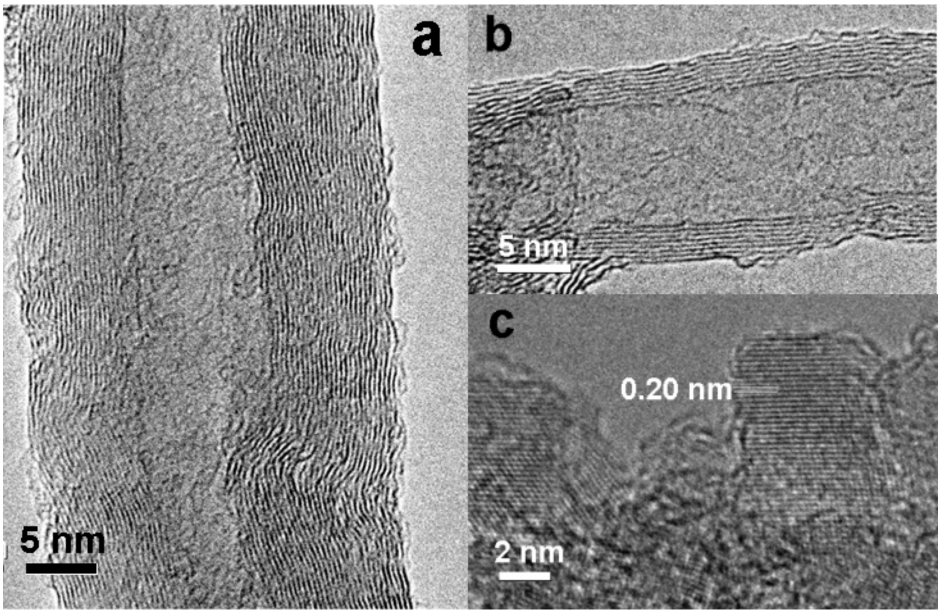

Fig. 2.6.1 HRTEM images of used nanocarbons: (a) long (3–14 μm) and thick-wall (15±10 walls) nanotube; (b) long (1–10 μm) and thin-wall (8±4 walls) nanotube; (c) nanodiamond.

We developed a microreactor designed and optimized for sub-milligram quantities of catalyst directly deposited on a TEM grid, which allows a direct structure-performance correlation of the tested catalyst. The catalytic activity of V_xO_y/CNTs was probed for ODH of propane to propylene. The catalyst showed high activity in the early stages of the reaction, but then undergoes a deactivation. TEM analysis has shown the crystallization of initially present hydrated V^{3+} species into nanorods of an oxide of higher formal valence during the reaction, thus proving that the dispersion of V_xO_y plays a dramatic role on its catalytic activity.

The catalytic activity of highly dispersed Mo_xO_y on CNTs is tested for selective oxidation of *n*-butane. Mo_xO_y/CNTs exhibits a stable activity towards selective oxidation products, i.e. maleic anhydride, acrylic acid, acetic acid and methacrolein, at temperatures as low as 300°C. These results reveal clearly that structural dynamics of a single-phase oxide is a necessary and sufficient pre-requisite for catalytic function that may be realized in other ways than through chemical complexity of mixed metal bulk oxides.

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2.7 Silver as catalyst for selective oxidation and hydrogenation

2.7.1 Ag in epoxidation reactions

Different unsupported silver catalysts have been investigated by HP-XPS under reaction conditions of the epoxidation of propene using molecular oxygen ($T \leq 520$ K, $p = 0.5$ mbar). The study was focused on the surface characterization of the operating catalysts. Two different families of oxygen species were identified. A nucleophilic oxygen species embedded into the silver substrate was observed. It is characterized by low binding energy (ca. 529 eV). It may co-exist with and emerge from an oxide species characterized by the formation of ionic silver. A second electrophilic oxygen species at higher binding energies was identified. This species does not form ionic silver and is located onto silver atoms. It co-exists and is the precursor to a ubiquitous bulk-dissolved atomic oxygen species. The presence of oxygen forms in both families that interact only weakly with the electronic structure of silver leads to a considerable variability of the positions of the respective XPS peaks caused both by variations of ground and final states of the oxygen with its relative abundance. As surface and sub-surface species co-exist in both

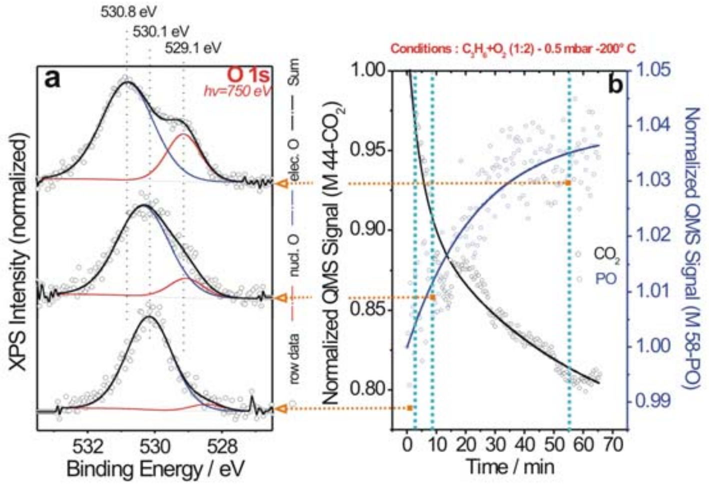

*Figure 2.7.1. **a** In situ XPS and **b** QMS data, showing the relation of adsorbed oxygen species with propene oxide selectivity.*

families, only a moderated structure-function correlation is expected as oxygen in substantial depth from the surface still contributes to XPS but not to the catalytic function.

Comparison of mass spectrometry and photoelectron spectroscopy data during in-situ observation revealed that the selectivity of the catalysts to propene epoxide depends strongly on the binding energy of the electrophilic oxygen, which is influenced by the presence of the nucleophilic species. The chemical shift of the electrophilic oxygen is an indicator for the reactivity being correlated with the deficit of electron density at the silver site where the oxygen is adsorbed. This concept unifies the multiple species reported in the literature designated as "δ+ oxygen" or as "super-electrophilic" species.

2.7.2 Ag in selective hydrogenation

The hydrogenation of acrolein over various forms of silver, also supported on SiO_2 or ZnO, has been investigated in the frame of a (now terminated) DFG priority program in collaboration with Prof. Peter Claus' group at TU Darmstadt [1]. Catalytic tests, conducted over a wide pressure range (mbar to 20 bar), showed an onset of formation of allyl alcohol beyond 100 mbar (at 523 K). This system provides an excellent example of an experimentally described pressure gap as below that critical pressure only total hydrogenation occurs. Following angle resolved NEXAFS measurements, the onset is ascribed to a change in the adsorption geometry of the substrate upon increasing coverage [2]. H_2 is activated by Ag and exists in mobile form, because support hydroxyl groups can be isotopically exchanged. Advantageous for allyl alcohol formation are further smaller silver particles (in the nanometer range) and the proximity of a reducible oxide component. More specifically, the presence of defects in Ag and the presence of oxygen, most likely subsurface oxygen, seem to be important for the catalytic behavior. The nature of the silver particles (size and oxygen content) depends not only on support, preparation and pretreatments; the dispersion was affected considerably by the reaction. The dynamic material's properties and the strong pressure dependence of the performance make this hydrogenation reaction a perfect example to underline the necessity of situ experiments under typical reaction conditions.

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2.8 In situ molecular beam mass spectrometry

Oxidative alkane activations proceed at high temperatures, making coupled homogeneous-heterogeneous reaction pathways a plausible option besides pure surface reactions. The catalyst may produce and release reactive intermediates, e.g. radicals [1,2], and substantial excess energy into the homogeneously heated gas phase, so that surface and gas phase steps can occur simultaneously [2].

During the last Beirat meeting, we introduced the design of a molecular beam mass spectrometer setup. A catalytic wall reactor is placed inside a vacuum chamber, and a fraction of the reacting gases expands through a nozzle in the wall forming a molecular beam. This adiabatic expansion quenches reactive intermediates. An appearance-potential quadrupole mass spectrometer allows identifying the molecular beam constituents in a 2—D analysis by their mass numbers and their ionization and appearance potentials. On-line GC to observe the equilibrated net reaction products analyzes the reactor effluent. A scanning pyrometer measures axial temperature profiles. A gas mixture of CH_4, O_2 and He (C/O: 0.6) is fed to Pt or Pt/10%Rh tubes, which are heated resistively until ignition occurs. The reaction can be run at temperatures up to 1300 °C.

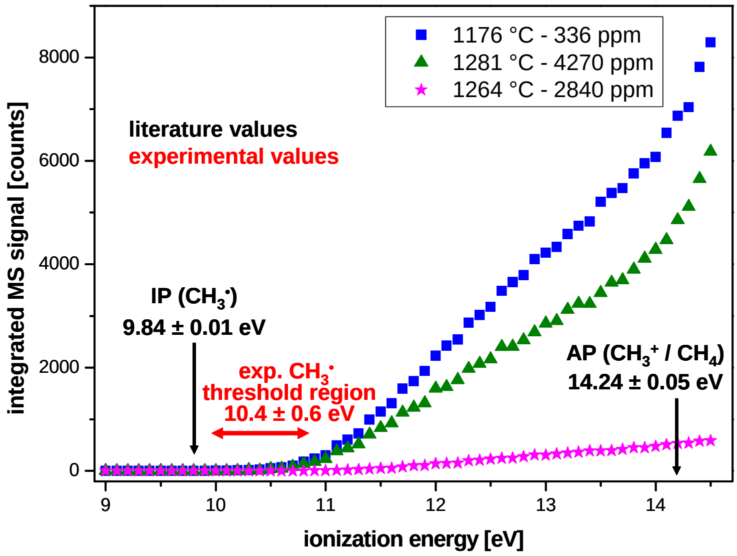

Fig. 2.8.1 Variation of methyl radical concentration with reaction temperature during methane CPO.

At 1120°C over Pt, the effluent stream contains H_2O, CH_4, CO, O_2, H_2, CO_2 and traces of C_2H_6 and C_2H_4 [3]. Upon further heating, the gas phase reaction starts, as indicated by the formation of a hot zone (1280 °C) within the axial temperature profile. Product analysis by on line GC also evidences a change in reaction mechanism, namely the complete consumption of O_2, a strong increase in H_2 production, and significant amounts of C_2H_2. Simultaneously, methyl radicals with an ionization energy of 9.81 eV have been extracted from the reaction zone via the molecular beam interface and distinguished from methane fragments (CH_3^+, appearance potential 14 eV). Methods to estimate radical concentrations have been developed, and their concentration increases with temperature as do those of C_2 species. It was thus confirmed by in-situ detection that the radicals are involved in the conversion of CH_4 to higher hydrocarbons in the gas phase reaction mode as it was strongly suggested from quenching experiments. Catalyst surfaces have been analyzed after use, they undergo significant restructuring, carbonaceous deposits are formed, and catalyst material is transported.

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3. Service facilities provided by the department

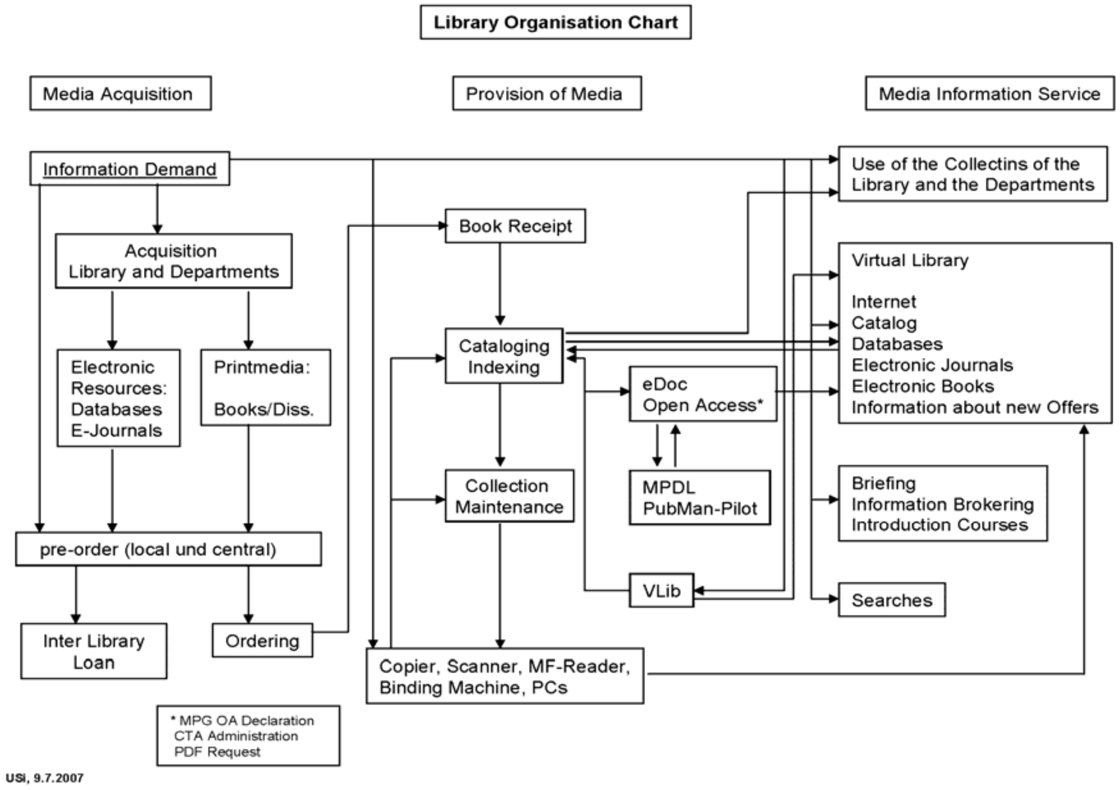
3.1 Library

The Library is constantly monitoring the publication market, with regard to new trends, e.g. Open Access. The FHI is practicing open access to scientific results in two ways: Publication in Open Access Journals and institutional self-archiving on the eDoc Server. The library assists the scientists by offering seminars and regular training courses on how to make best use of the eDoc Server.

Presently the Max Planck Digital Library (MPDL) is preparing a new publication management system with additional tools. The FHI is one of the pilot institutes in the eSciDoc Project and the library operates for further development in close cooperation with the MPDL.

Furthermore, the Library participates in the development and maintenance of the Max Planck Virtual Library (VLib).

The range of electronic services of the FHI Library includes various database descriptions, access terms and conditions for e-journals as well as catalogues. Printed scientific information is still an important resource in the forms of the exhaustive topical collection and of increasingly important monographs that need to be made accessible for the whole FHI and the MPG. Therefore, the qualified library personnel will remain indispensable also in the new age of electronic „libraries without walls“.



3.2. Service group Electron Microscopy

In the report period, the Service Group Electron Microscopy has worked in the following three areas: i) Routine TEM/SEM investigation of samples from the Department AC and other departments of FHI; ii) TEM/SEM studies in the frame of Max-Planck Project House Enerchem; iii) Investigation of external samples from the cooperation partners of FHI. Some works are reported in the following.

FHI internal works: The Service Group is active in all the projects of the department AC and provides basic service to other Departments of FHI. Typical examples of extended service comprise SEM of single crystal Mo, Au-foil, W-tip for STM from the Department **CP**; or microstructural investigations of ceramic, silver and glass fibres from the Department **PC**. ***Enerchem and MPG**:* Carbon, mesoporous metal nitrides, carbon from HTC were provided by the **MPI-Golm**. The routine and advanced TEM/SEM/EELS characterizations were done to determine the morphology, structure, composition of all samples. For metal nitrides the pore structure was studied. Image simulation and image analysis were performed. Electronic structure was deduced from EELS with sp^2/sp^3 quantification. Samples for Li-Ion batteries

(Si/SiO/C and Ru/C) from **MPI-Mainz** were characterized with the respect of morphology, structure, composition and for the correlation between microstructure with electronic properties. Nano-structured metal oxides for hydrogen production from **MPI-Mülheim** were studied with TEM/SEM. In addition to the Enerchem partners, the Service Group has investigated samples from other Max-Planck Institutes, among them, for instance, **MPI Dresden** (PdGa, Ga/polyvinylpyrrolidon).

External service work: The external service work is carried out based on the multi-cooperation of the Institute. Service work was done in the frame of EU-Projects CANAPE, ELCAT, AuriCat, Athena; in the frame of DFG-Projects (among them SFB-546), in the frame of ELCASS, in the frame of MPG-CAS partner groups program, in the frame of DAAD projects. Samples studied in bi-lateral cooperation of FHI include those from Universität Bochum, Hahn-Meitner Institut GmbH, Technische Universität Wien, Humboldt Universität zu Berlin, Freie Universität Berlin, University of Malaysia, Unviersität Innsbruck, Technische Universität Berlin, University of Milano. In the cooperative research network SFB 546 several groups from TU Berlin and from LICAT are supported with substantial efforts in nanostructural analysis of vanadium oxide catalysts. With the AG Rühl from FU Berlin a service contract has been set up involving the training of a dedicated user from FU for cluster analysis.

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Teschner, D., A. Wootsch, O. Pozdnyakova-Tellinger, J. Kröhnert, E. Vass, M. Hävecker, S. Zafeiratos, P. Schnörch, F. C. Jentoft, A. Knop-Gericke and R. Schlögl: Partial pressure dependent in-situ spectroscopic study on the preferential CO oxidation in hydrogen (PROX) over Pt/ceria catalysts. Journal of Catalysis **249**, 316–325 (2007).

Venkov, T. V., C. Hess and F. C. Jentoft: Redox Properties of Vanadium Ions in SBA-15 Supported Vanadium Oxide: an FTIR Spectroscopic Study. Langmuir **23** (4), 1768-1777 (2007).

Virnovskaia, A., S. Jørgensen, J. Hafizovic, Ø. Prytz, E. Kleimenov, M. Hävecker, H. Bluhm, A. Knop-Gericke, R. Schlögl and U. Olsbye: In situ XPS investigation of Pt(Sn)/Mg(Al)O catalyst during ethane dehydrogenation experiments. Surface Science **601** (1), 30-43 (2007).

Wang, L., J. Zhang, D. S. Su, Y. Ji, X. Cao and F.-S. Xiao: Simple Preparation of Honeycomb-like Macrostructured and Microporous Carbons with High Performance in Oxidative Dehydrogenation of Ethylbenzene. Chemistry of Materials **19** (11), 2894-2897 (2007).

Wu, Y., H.-M. Liu, B.-Q. Xu, Z.-L. Zhang and D. S. Su: Single-Phase Titania Nano-crystallites and Nano-fibres from Titanium Tetrachloride in Acetone and other Ketones. Inorganic Chemistry **46** (12), 5093-5099 (2007).

Zenkovets, G. A., G. N. Kryukova, V. Y. Gavrilov, S. V. Tsybulya, V. A. Anufrienko, T. A. Larina, D. F. Khabibulin, O. B. Lapina, E. Rödel, A. Trunschke, T. Ressler and R. Schlögl: The structural genesis of a complex $(MoVW)_5O_{14}$ oxide during thermal treatments and its redox behavior at elevated temperatures. Materials Chemistry and Physics **103** (2-3), 295-304 (2007).

Zhang, J., D. S. Su, A. Zhang, D. Wang, R. Schlögl and C. Hébert: Nanocarbon as Robust Catalyst: Novel Mechanistic Insight into Carbon-mediated Catalysis. Angew. Chem. Int. Ed. **46**, 1-6 (2007).

Zhang, J., M. Comotti, F. Schüth, R. Schlögl and D. S. Su: Commercial Fe- or Co-Containing Carbon Nanotubes as Catalysts for NH_3 Decomposition.
Chemical Communications **19**, 1916-1918 (2007).

Doctoral Thesis:

Aburous, S. A.: Highly Oriented Pyrolytic Graphite (HOPG) as a Model catalyst for the Oxidative Dehydrogenation of Ethylbenzene over Carbon Materials. Freie Universität Berlin 2007.

Invited Talks of the Members of the Department of Inorganic Chemistry

Michael Hävecker

2007 Russian-German Seminar on Catalysis, 2007-07-10, Altai Mountains, Russia:
Methanol oxidation on Ru catalysts: Reaction pathways and catalytically active sites.

Christian Hess

2006 Center for Catalysis and Surface Science, 2006-11-30, Northwestern University, USA:
Nanostructured vanadia model catalysts for partial oxidation reactions.

2007 Bundesanstalt für Materialforschung und –prüfung (BAM), 2007-05-11, Berlin, Germany:
Synthesis, characterization and application of nanostructured vanadia model catalysts for partial oxidation reactions.

Friederike Jentoft

2005 Catalysis Seminar, 2005-10-07, University of California, Berkeley, USA:
Reactivity of Promoted Sulfated Zirconia Isomerization Catalysts.

2006 Seminar Fakultät für Chemie und Mineralogie, 2006-01-10, Universität Leipzig, Germany:
Analyse eines variablen Katalysators: Reaktivität von promotiertem Zirconiumoxid.

Workshop Microelectronics meets Catalysis: Innovative Oxide Materials, 2006-07-20 to 2006-07-21, Hanse Wissenschaftskolleg HWK at Delmenhorst, Germany:
Zirconium Oxide – a Variable Catalyst Component.

Mitteldeutscher Katalyseverbund, 2006-10-30, Universität Leipzig, Germany:
Physicochemical Characterization: IR and UV-vis Spectroscopy.

Seminar Laboratory of Industrial Chemistry, 2006-11-23, Åbo Akademi University Turku, Finland:
Modern Alkane Isomerization Catalysts: Complex Materials for a Simple Reaction?

2007 Seminar Süd-Chemie AG, 2007-02-23, Bruckmühl, Germany:
Sulfated Zirconia as a Starting Point in the Quest for New Alkane Isomerization Catalysts.

Seminar Department of Chemistry, 2007-06-04, University of Reading, UK:
A Fundamental Approach to the Development of Novel Alkane Isomerization Catalysts.

Seminar Chemical, Biological, and Materials Engineering, 2007-06-15, University of Oklahoma, Norman, USA:
The Chemistry of Low Temperature Alkane Isomerization Catalysts.

Axel Knop-Gericke

2006 BESSY Scientific Advisory Committee Meeting, 2006-04-23 to 2006-04-24, Berlin, Germany:
The influence of subsurface carbon on the selectivity in the hydrogenation reaction of 1-pentyne over Pd catalysts.

Workshop Catalysis @ 4th generation light sources, 2006-06-19, University College London, United Kingdom:
In situ XPS – A Tool to bridge the Pressure Gap in Heterogeneous Catalysis. (

Workshop on the Reactivity and Stability of Surfaces and Nano Particles at Elevated Pressures, 2006-09-27 to 2006-09-30, Irsee, Germany:
High pressure X-ray photoelectron spectroscopy: A surface sensitive tool for the investigation of working catalysts.

Institute Seminar, 2007-02-14, Strasbourg, France:
Subsurface Species in Heterogeneous Catalytic Reactions: Insights by in situ Photoelectron Spectroscopy.

Russian-German-Seminar on Catalysis, 2007-07-09 to 2007-07-12, Novosibirsk-Altai Mountains, Russia:
The role of subsurface species in heterogeneous catalytic reactions. Bridging the Gap Between Model And Real Catalysis.

Katrin Pelzer

2006 Max-Planck Institut für Chemische Physik fester Stoffe - Department Seminar, 2006-06-16, Dresden, Germany:
Ruthenium nanoparticles stabilized by ligands grafted on the surface.

LCOMS - Department Seminar, 2006-11-21, Lyon, France:
In situ molecular beam mass spectrometry for high temperature catalysis research.

2007 UNAXIS, 2007-02-25 to 2007-02-27, Balzers, Liechtenstein:
Heterogeneous Photocatalysis on Transparent Semiconducting Oxides.

Wolfgang Ranke

2006 International Workshop on Nanostructured Materials, NANOMAT 2006, 2006-06-21 to 2006-06-23, Antalya, Turkey:
Surface science meets catalysis research: epitaxial iron oxide films for in-situ model catalysis.

Robert Schlögl

2005 CJS National Meeting, 2005-03-28 Yokohama, Japan:
Nanostructured Heterogeneous Catalysts.

Irsee Symposium on the Role of Vacancies, Disorder and the Relationship between Surface and Bulk Structure in Selective Oxidation Catalysis (Robert K. Grasselli Foundation), 2005-05-11, Irsee, Germany:
The Potential of MoVTe Catalysts for Propane Oxidation: The Role of Defects for the Catalytic Function.

Gordon Conference on Catalysis, 2005-06-27, Colby-Sawyer College, New London, NH, USA:
The impact of in-situ spectroscopies on complex oxides for the synthesis of novel selective oxidation catalysts.

Seventh European Congress on Catalysis, EuropaCat-VII, 2005-08-27, Sofia, Bulgaria:
Why should we study heterogeneous catalysis by in-situ methods?

Südchemie AG, 2005-09-28, München, Germany:
CuZn in alternativen Trägermaterialien mittels innovativer Synthesemethoden.

DGMK/SCI Session: “Oxidation and Functionalization: Classical and Alternative Routes and Sources”, 2005-10-12, Milano, Italy:
Material oxides for selective oxidation. How essential is chemical complexity?

4th ECLASS Meeting, 2005-10-22, Roscoff, France:
ECLASS 2005: From a concept to an integrated project at work.

e-Science Forum Wissensvernetzung. Digitale Dienstleistungen für die Wissenschaft, 2005-10-25, Berlin, Germany:
Entwicklungen in Deutschland. Resümee und Ausblick.

Lecture in honour of Prof. Knözinger, Ludwig-Maximilians-Universität, 2005-10-27, München, Germany:
In-Situ Untersuchungen zur Funktion polykristalliner Oxidationskatalysatoren.

GDCh Lecture, Universität Essen, 2005-11-02, Duisburg, Germany:
Die Bedeutung der Synthese anorganischer Festkörper für die moderne heterogene Katalyse.

Bayer Kammergespräche, “Kamingespräche” of the winners of the Otto Bayer and Familie Hansen awards, 2005-11-04, Leverkusen, Germany:
Technology transfer for nanostructured carbon materials: public/private partnership.

2006 GDCh-Vortrag, Universität Marburg, 2006-01-18, Marburg, Germany:
Nanokatalyse: Etwas inhaltlich Begründetes oder nur ein schöner Begriff?

49. Sitzung DECHEMA-Ausschuss C “Katalyse“, 2006-01-19, Fankfurt a.M., Germany:
Nanotechnologie und hererogene Katalyse: gibt es eine funktionale Begründung?

2nd CONCORDE Conference, 2006-01-26 to 2006-01-28, Thessaloniki, Greece:
The relevance of structural disorder for catalytic functionally.

Seminar at Dow Chemical Corporation, 2006-02-27, Charleston, WA, USA:
In-situ photoemission of catalytic silver and copper systems.

XXth International Winterschool on Electronic Properties of Novel Materials: Molecular Nanostructures, 2006-03-03 to 2006-03-10, Kirchberg/Tirol, Austria:
Surface chemistry & heterogeneous catalysis of carbon nanostructures.

Leibniz-Institut für Katalyse e.V., 2006-03-19, Rostock, Germany:
Wie statisch sind heterogene Katalysatoren?

Seminarvortrag Süd-Chemie AG, 2006-03-27, Louisville, USA:
Nanostructured carbons as a toolbox for chemical applications.

Seminar at University of Minnesota, 2006-05-05, Minneapolis/Minnesota, USA:
Synthesis and Dynamics of Mixed Metal Catalysts (MMO) for Propane Oxidation.

Achema 2006, 2006-05-18, Frankfurt a.M., Germany:
NanoC – A research and technology provider for nanostructured catalysis and adsorbents.

GdCH-Vortrag, 2006-05-23, München, Germany:
Wie statisch sind heterogene Katalysatoren?

Bunsentagung, 2006-05-27, Erlangen, Germany:
Mechanical and chemical strain in copper as essential effects for its activity in selective oxidation of methanol.

80th ACS Colloid and Surface Science Symposium, 2006-06-18, Boulder/Colorado, USA:
Nano-catalysis: Why is small critical for the function of gas-solid reaction.

Festvortrag Carl v. Ossietzky Universität, 2006-06-20, Oldenburg, Germany:
Warum ist "nano" gut für die Katalyse?

8th Pannonian International Symposium on Catalysis, 2006-07-04 to 2006-07-07, Szeged, Hungary:
Solid State Dynamics of Heterogeneous Catalysts.

TOCAT 5, 2006-07-23 to 2006-07-28, Tokyo, Japan:
Copper in Hydrogen Catalysis.

1st European Chemistry Congress, 2006-07-27 to 2006-07-29, Budapest, Hungary:
Dynamics of Oxide Catalysts: What can Heterogeneous Catalysis Learn from Molecular Catalysis.

E-MRS Fall Meeting, 2006-09-04 to 2006-09-08, Warsaw, Poland:
The Relevance of Nanostructuring for the Function of Heterogeneous Catalysts.

14. Workshop Applied Surface Analysis, 2006-09-20, Kaiserslautern, Germany:
Synchrotron Excited High Pressure Photoemission – a novel method for material characterization.

ASEVA Summerschool, Workshop on Nanotechnologies, 2006-09-26, Avila, Spain:
Why is Nanostructuring Essential for Catalysis: Morphological and Electronic Structural Aspects.

2007 GDCh-Vortrag, Technische Universität, 2007-01-23, Ilmenau, Germany:
Heterogene Katalyse mit Kohlenstoff-Nanostrukturen.

Gordon research Conference on Chemical Reactions, 2007-02-11 to 2007-02-15, Ventura, Cal. USA:
The constitution of reacting surfaces under realistic partial pressures.

Dow Chemical Corporation, 2007-04-11, Midland MI, USA:
Selective oxidation of small alkane molecules.

IDECAT Conference on Catalysis Concepts: complexity and diversity in catalysis, 2007-05-12 to 2007-05-17, Porquerolles, France:
Understanding heterogeneous catalysis of demanding processes: how essential is complexity?

NAM/North American Catalysis Society 20th Conference, 2007-06-15 to 2007-6-18, Houston, Texas, USA:
Bringing together in-situ Spectroscopy and Electron Microscopy to Study the Function of Complex Oxide Catalysts.

14. Tagung Festkörperanalytik, 2007-07-18, Vienna, Austria:
Surface analysis under gas pressure.

15th International Conference on Vacuum Ultraviolet Radiation Physics. 2007-07-29 to 2007-08-03, Berlin, Germany:
High Pressure Photoemission: A versatile tool for functional material science.

Int. Conference on Synthesis of Complex Oxides, 2007-08-18 to 2007-08-23, Santa Barbara, CA, USA:
Dynamics of oxide catalysts: Synthesis and analytics.

Uta Siebeky

2006 Workshop: E-Journals in der Praxis, 2006-06-20 to 2006-06-21, Zentralbibliothek Forschungszentrum Jülich, Germany:
E-Journal Verwaltung im Fritz-Haber-Institut: Bericht aus einer Spezialbibliothek.

eDoc Nutzer-Workshop, 2006-11-23, Garching, Germany:
Publikationsdatenmanagement mit eDoc im Fritz-Haber-Institut.

2007 Integrität wissenschaftlicher Publikationen, 2007-03-23 to 2007-03-24, Berlin, Germany:
Auf der Green Road to Open Access. Ein Praxisbericht aus dem Fritz-Haber-Institut der MPG.

Dangsheng Su

2005 International symposium on air pollution abatement catalysis, 2005-09-21 to 2005-09-24, Cracow, Poland:
Euro IV Diesel Engine Soot: Microstructure and Oxidation Behaviour.

Universidad de Alicante, 2005-10-27, Alicante, Spain:
Manipulating carbon nanotube to carbon nanobulb and carbon tube-in-tube assembly.

2006 Seminar Dept. of Industrial Chemistry and Engineering of Materials, Univ. Messina, 2006-01-16, Italy:
Electron Microscopy and its Application in Heterogeneous Catalysis.

Seminar Max-Planck-Institut für Chemie, 2006-01-26, Mainz, Germany:
Microstructure and Oxidative Behaviour of Euro-IV Diesel Engine Soot Particulate.

2nd Croatian Congress on Microscopy with International Participation, 2006-05-17 to 2006-05-19, Topusko, Croatia:
Application of electron energy-loss spectroscopy in material sciences.

Institute Seminar, Utrecht University, Department of Chemistry, Inorganic Chemistry and Catalysis, 2006-05-23, Utrecht, The Netherlands:
TEM and EELS of Carbon Materials.

Seminar Institute for Ceramic, 2006-06-09, Chinese Academy of Science, Shanghai, China:
The Beautiful World of Carbon.

Seminar Institute of Neurobiology and Molecular Medicine, 2006-07-04, CNR, Rome, Italy:
Carbon nanoparticles: microstructure and morphology.

The 13th Chinese National Congress of Catalysis, 2006-10-18 to 2006-10-21, Lanzhou, China:
Understanding the Activity-Structure Correlation of Catalysts: Contribution of Electron Microscopy to Heterogeneous Catalysis.

Seminar Department of Chemistry, 2006-11-03, Tsing Hua University, Beijing, China:
Hierarchically structured Nanocarbon: Synthesis and Applications.

4th China-Japan-Korea Joint Symposium on"Carbon Materials to Save the Earth", 2006-11-09 to 2006-11-11, Tsinghua, China:
Carbon-Supported Catalysts: A TEM Study.

Seminar Dalian Institute for Chemical Physics, 2006-11-17, Dalian, China:
Catalyst for Electrocatalysis: Problem and Challenge.

Institutskolloquium, 2006-11-23, Leibniz-Institut für Katalyse e.V., Berlin, Adlershof, Germany:
Soot particulates.

2007 3rd NTNU Seminar on Synthesis and Applications of Carbon Nanofibers/Nanotubes, 2007-02-14, Trondheim, Norway:
TEM study of nanocarbon supported catalysts.

Symposium on Nanocatalysis, 2007-03-04, Dalian, China:
Catalysis over nanocarbon: Concept, Problems, Challenges and New Developments.

Lee Hsun Lecture Series on Material Science, Institute for Metal Research, 2007-04-06, Shenyang, China:
Transmission Electron Microscopy and Nanoscience.

International Symposium on Air and Water Pollution Abatement AWPA 2007, 2007-06-21, Zakopane, Poland:
How Cytotoxici are the Soot Particles of Low-Emission Diesel Engines?

ElCryst2007 - New Possibilities through New Instruments & Advanced Methods, European Electron Crystallography Workshop, 2007-09-16, Aachen, Germany:
The role of transmission electron microscopy in catalysis.

Detre Teschner

2007 Symposium on Applied Catalysis, 2007-07-18 to 2007-07-20, Glasgow, UK:
Pd-C surface phase as an essential parameter of selective alkyne hydrogenation.

Annette Trunschke

2005 5th World Congress on Oxidation Catalysis, 2005-09-25 to 2005-09-30, Sapporo, Japan:
Propane Oxidation over Nanostructured Molybdenum-Vanadium Mixed Oxides: In-situ Studies of the Geometric and Electronic Structure.

5th World Congress on Oxidation Catalysis, 2005-09-25 to 2005-09-30, Sapporo, Japan:
Incorporation of Ru into MO_x *catalysts for partial oxidation of light alkanes -The use of HPA-Ru adducts as metastable precursor materials.*

4th ELCASS Meeting, 2005-10-22 to 2005-10-26, ROSCOFF, France:
Nanostructured Molybdenum Oxide Catalysts for the Selective Oxidation of C3 Hydrocarbons.

2006 232nd ACS National Meeting, 2006-09-10 to 2006-09-14, San Francisco, CA, USA:
Surface analysis of the ab-plane of MoVTeNbOx catalysts for propane (amm) oxidation by low energy ion scattering (LEIS).

2007 Symposium on Advances in Selective Heterogeneous Oxidation Catalysis, 2007-06-07 to 2007-06-10, Irsee, Germany:
Dynamics of Surface Structures of Complex Oxides.

North American Catalysis Society, 20th North American Meeting, 2007-06-17 to 2007-06-22, Houston, TX, USA:
Novel mesostructured Mo-V-Te-Nb mixed oxide catalysts for selective oxidation of propane to acrylic acid.

Other activities

Jentoft, F. C.: Invited to become Associate Editor of Advances in Catalysis (2007, accepted).

Knop-Gericke, A.: Member of the ESRF Chemistry Review Committee 2004-2006.

Trunschke, A.: Appointed as a member of the examination board of the defence of the doctoral thesis of Johan Holmberg (A study of propane and propene ammoxidation over the Mo-V-Nb-Te-oxide system), 2006-10-20, University Lund, Sweden.

Department of Chemical Physics — Director: H-J. Freund

Staff Scientists:

Dr. M. Heyde		from 01.03.2007
Dr. H. Kuhlenbeck	(Habilitation)	
Dr. N. Nilius		
Dr. T. Risse	(Habilitation)	
Dr. G. Rupprechter	(Habilitation)	until 31.08.2006
Dr. H.-P. Rust		until 28.02.2007
Dr. S. Schauermann		
Dr. S. K. Shaikhutdinov		
Dr. M. Sterrer		from 01.05.2006
Dr. K. Watanabe		

Guest scientists, staying for at least six months, paid by FHI:

Dr. Oleksandr Bondarchuk
Dr. Esther Carrasco Burgos
Prof. Dietrich Menzel
Dr. Zhihui Qin
Dr. Emile Rienks

Guest scientists, staying for at least six months, paid from external funds:

Dr. Heather Abbott	*AvH Fellow*
Dr. Athula Bandara	*AvH Fellow*
Dr. Marcella Passos Felicissimo	*AvH Fellow*
Dr. Pierre Lévesque	
Dr. Maxim Yulikov	
Dr. Xiao Lin	
Prof. Gianfranco Pacchioni	*AvH Awardee*
Dr. Jani Sainio	
Dr. Joaquin Silvestre-Albero	*AvH Fellow*
Dr. Violeta Simić-Milošević	
Dr. Thomáš Skála	
Dr. Dario Stacchiola	*AvH Fellow*
Dr. Martin Sterrer	
Dr. Marko Sturm	
Prof. Francisco Zaera	*AvH Awardee*

Graduate Students: 23 (6 IMPRS students,
9 students paid from external funds)

Technicians: 9
Technicians of Crystallab: 2

Associated Research Group : Phil Woodruff (group leader)
1 graduate student
1 postdoc

PP&B Group: H. Junkes (group leader)
1 Trainee
4 Technicians

AvH= Alexander von Humboldt Foundation

Recent Developments in the Department of Chemical Physics

Director: H.-J. Freund

General Remarks

Since the last visit of the Fachbeirat the following changes occurred among the staff members of the department.

Dr. Norbert Ernst retired from his position in February 2006.

Anton Rahm left the Institute effective in September 2007 to take on a position with the company SPECS.

Dr. Risse received his Habilitation in June 2007, and he was promoted to a permanent staff member.

Dr. Günther Rupprechters group leader position has been filled with Dr. Martin Sterrer, who was before a postdoctoral fellow in Dr. Thomas Risse's group.

Dr. Hans-Peter Rust retired from his position March 2007. He still is on a part time contract (1 day per week) to consult with Dr. Markus Heyde who replaced him.

Dr. Swetlana Schauermann returned from her postdoctoral stay (financed by the DFG) in Cambridge with Professor Richard Lambert, and at the University of Washington, Seattle, with Professor Charles Campbell.

A Max-Planck partner group at Hefei University in China with Professor Weixin Huang has been established.

Within the Department of Chemical Physics there are at present eight working groups:

1. Spectroscopy and Spectro-Microscopy
   Helmut Kuhlenbeck

2. Structure and Reactivity
   Shamil Shaikhutdinov

3. Atomic Force Microscopy
   Markus Heyde

4. Scanning Probe Spectroscopy
   Niklas Nilius

5. Magnetic Resonance
   Thomas Risse

6. Catalysis/Laser Spectroscopy
   Martin Sterrer

7. Molecular Beam
   Swetlana Schauermann

8. Photon-Induced Processes
   Kazuo Watanabe

Associated Research Group: Scanned-energy Mode Photoelectron Diffraction
Phil Woodruff
University of Warwick, Coventry, U.K.

In the Department of Chemical Physics we have continued to concentrate in the last two years on the study of oxide surfaces, in particular thin film systems and its interaction with deposited metal atoms and clusters. The results from our research activities are first highlighted and then more in detail described as they were associated with different working groups. The Department has also participated in a number of projects funded from outside sources which are listed below:

Collaboration H.-J. Freund, A. Fortunelli:
„Growth and Supra-Organization of Transition and Noble Metal Nanoclusters (GSOMEN)“

Collaboration H.-J. Freund, G. J. Hutchings:
„Catalysis by Gold (Auricat)“

Collaboration H.-J. Freund, Th. Klüner: DFG, SPP 1093
“Dynamik von Elektronentransferprozessen an Grenzflächen”

Collaboration H.-J. Freund, J. Libuda: DFG, SPP 1091
“Projekt: Synthese und Partialoxidation von Methanol an wohldefinierten Modellträgerkatalysatoren – Teilprojekt: Molekularstrahluntersuchungen zur Wechselwirkung und Partialoxidation von Methanol an wohldefinierten Modellträgerkatalysatoren”

Collaboration H.-J. Freund, G. Rupprechter: DFG, SPP 1091
“Projekt: Synthese und Partialoxidation von Methanol an wohldefinierten Modellträgerkatalysatoren – Teilprojekt: Spektroskopie an Modell-katalysatoren unter Reaktionsbedingungen mittels Summenfrequenz-Erzeugung (SFG)”
Collaboration N. Nilius: DFG, SPP 1234
“Quantum transport at the molecular scale”

Collaboration H.-J. Freund, Th. Risse: ESF COST Action D41
“Inorganic Oxides: Surfaces and Interfaces“

Collaboration H.-J. Freund, S. K. Shaikhutdinov:
SFB 546 Struktur, Dynamik und Reaktivität von Übergangsmetalloxid-Aggregaten, Teilprojekt B1
„Struktur-Reaktivitäts-Beziehung von Vanadiumoxid-Aggregaten auf geordneten Übergangsmetalloxidoberflächen“

Collaboration H.-J. Freund, H. Kuhlenbeck:
SFB 546 Struktur, Dynamik und Reaktivität von Übergangsmetalloxid-Aggregaten, Teilprojekt C1
„Elektronenstruktur und Adsorptionsverhalten von geordneten Vanadium-, Molybdän- und Nioboxidoberflächen“

Collaboration von D. P. Woodruff (Warwick), J. Sauer:
SFB 546 Struktur, Dynamik und Reaktivität von Übergangsmetalloxid-Aggregaten, Teilprojekt C8
„Structure determination of VO_x surfaces, thin films and interfaces based on scanned-energy mode photoelectron diffraction”

Collaboration H.-J. Freund, S. K. Shaikhutdinov, S. D. Jackson (Glasgow):
EPSRC, U.K.
„Advanced Technology in Catalytic Chemistry and Engineering for Novel Application (Athena)“

Collaboration H.-J. Freund, G. Centi (Messina):
Network of Excellence, E.U.
„Integrated Design of Catalytic Nanomaterials for a Sustainable Production (IDECAT)“

Collaboration H.-J. Freund, M. Asscher (Jerusalem):
G.I.F.
„Dynamics of Electronic Processes in Confined Environment“

Collaboration H.-J. Freund, E. Umbach (Würzburg):
BMBF
BESSY „SMART- ein hochauflösendes Elektronen-Spektro-Mikroskop für die Oberflächenforschung“

Further collaborations include:

Collaboration on oxide surfaces: H.-J. Freund and Prof. Carlos Alberto Achete, Instituto Nacional de Metrologia, Rio de Janeiro, Brazil.

Collaboration H.-J. Freund with a partner group in China: Prof. Weixin Huang, University of Science and Technology, Chinese Academy of Sciences, Hefei, China.

Collaboration on solid-liquid interfacial STM: H.-J. Freund and Prof. Klaus Wandelt, Institute of Physical and Theoretical Chemistry, University of Bonn, Bonn, Germany.

Collaboration on Ni_2P single crystal surfaces: H.-J. Freund and Prof. Kiyotaka Asakura, Catalysis Research Center, Hokkaido University, Sapporo, Japan.

Collaboration on spin labelling and EPR of proteins: Th. Risse and Prof. Wayne Hubbell, Jules Stein Eye Institute, School of Medicine, UCLA, Los Angeles, California, USA.

The department has associated with the PP&B group.

The following highlights include results of research projects as well as on instrumental developments:

- The SMART project, carried out in collaboration with Eberhard Umbach's group reached a resolution of 3.1 nm in the LEEM mode with spherical and chromatic aberration corrected optics and thus a new world record. Thomas Schmidt was awarded the Innovation-Award on Synchrotron Radiation 2006.

- The mechanism of methanol oxidation was investigated in detail both on flat V_2O_3 surfaces and on supported vanadium oxide clusters. Methoxy formation was observed with STM and XPS and a model for the transformation to formaldehyde has been developed with theoretical support from Joachim Sauer's group.

- For the first time a thin well ordered alumosilicate film has been prepared and characterized. This opens up possibilities to study "zeolite chemistry", i.e. acid-base catalysis on a flat surface.

- Atomically resolved AFM images of MgO(100) and a thin alumina film on NiAl(110) at low temperature (4-5 K), confirming earlier STM investigations have been obtained. Also, atomically resolved dynamic force spectroscopy measurements were performed.

- Deposited metal atoms and clusters on MgO(100) and on alumina/NiAl(110) have been studied. Results on the manipulation of metal atoms into the formation of clusters and the self organisation of Au chains as well as their spectroscopy have been investigated, partly in collaboration with the groups of Gianfranco Pacchioni and Joachim Sauer.

- EPR spectra of metal atoms (Au) on oxide surfaces were obtained as reported before and the correlation of their electronic properties with their adsorption behaviour has been studied via infrared spectroscopy during the last two years.

- In a series of studies, the influence of thickness of oxide films towards the properties (i.e. adsorption site and charge state) of deposited metal nanoparticles have been investigated. In collaboration with Gianfranco Pacchioni's group this has led to a new concept to control the electronic properties and concomitantly the chemical reactivity of metal atoms, metal clusters and islands deposited on such thickness designed materials.

- Several major milestones have been reached in building a multi-technique integrated w-band EPR spectrometer for single crystal surface studies under UHV conditions.

- It was demonstrated how EPR spectroscopy may provide information on structure and dynamical changes of proteins interacting with flat surfaces, i.e. model lipid membranes for example.

- Molecular beam experiments in conjunction with synchrotron based XPS studies have revealed a new route for oxide formation on supported Pd nanoparticles. Oxide formation is favoured at the Pd-support interface rather than the Pd vacuum interface, thus indicating that single crystals would not exhibit the necessary complexity of the material to provide useful information on technical catalysts.

- Investigations on the kinetics of hydrogenation (in collaboration with Francisco Zaera) and dehydrogenation reactions have let us gain insight into the influence of carbonaceous species deposited during the reaction on the selectivity of such reactions.

- In collaboration with Charles Campbells group a micro calorimeter for measurements of adsorption enthalpies on supported nanoparticles is being developed and built.

- Adsorption studies and kinetic measurements on a variety of systems have been carried out under ambient conditions allowing us to compare directly with results gained from molecular beam studies.

- The impact of plasmon excitation in small supported Ag particles on the photochemistry of adsorbed species (NO, Xe) has been studied. New phenomena in plasmon assisted rare gas desorption from Ag particles have been observed and possible mechanism have been suggested. The participation of Dietrich Menzel has been essential in those studies.

Progress Reports

In the following, results from the various groups obtained during the last two years are summarized:

Spectroscopy and Spectro-Microscopy

The studies in the past two years mainly dealt with ordered V_2O_3(0001), V_2O_5(001), and MoO_3(010) layers grown on Au(111). Preparation, surface characterization, and adsorption/reaction studies were in the foreground of the investigations with a certain focus put onto microscopic details of the reactivity of the surfaces. These studies were performed in the framework of the Sonderforschungsbereich 546 of the Deutsche Forschungsgemeinschaft.

Structure of vanadyl terminated and vanadium terminated V_2O_3(0001)

Well ordered V_2O_3(0001) films with a thickness of about 100 Å were prepared by evaporation of vanadium onto Au(111) in an oxygen ambient followed by further oxidation and annealing. These layers are terminated by a layer of vanadyl groups under typical UHV conditions. The oxygen atoms of the vanadyl groups may be removed by electron irradiation which leads to a chemically highly active ordered surface terminated by vanadium atoms. In addition to structural studies with STM these surfaces were also investigated with IV-LEED employing a LEED system equipped with a channelplate in order to minimize surface damage due to the electron beam. With this the atomic positions of the atoms in the surface regions could be determined. Layer distances significantly different from distances in the bulk as well as modified lateral atomic distances were found in both cases, reminiscent of the case of the Cr_2O_3(0001) surface which was studied a number of years before.

NEXAFS studies of V_2O_3(0001), V_2O_5(001) and MoO_3(010) thin films

Similar to the case of V_2O_3(0001), V_2O_5(001) and MoO_3(010) were prepared as thin films on Au(111). However, in the latter cases higher oxygen pressures than suitable for UHV systems are required so that a high-pressure cell was constructed and used for the preparation of these oxides. In both cases the oxidation of the respective metal layer was carried out with a pressure of 50 mbar which leads to well ordered layers with a low density of defects.

These surfaces were characterized in detail with O1s NEXAFS using synchrotron radiation from the BESSY II storage ring in Berlin. Angular dependent spectra were recorded and modelled with DFT by the group of K. Hermann in the theory department, leading to an assignment of the spectral features to the different types of oxygen in the surface region.

Methanol adsorption on V_2O_3(0001) and V_2O_5(001)

Methanol adsorbs molecularly onto vanadyl terminated V_2O_3(0001) at low temperature and warming up leads to molecular desorption only. Removal of all or part of the vanadyl oxygen atoms leads to a surface which can produce formaldehyde from methanol with the additional formation of methane and water. Neither hydrogen evolution nor methanol combustion, as would be indicated by CO or CO_2 formation, was found. With STM it could be shown that methoxy only forms on those surface areas where the vanadyl oxygen atoms have been removed prior to methanol adsorption indicating the importance of the surface vanadium atoms for the reaction. As indicated by vibrational spectroscopy the remaining vanadyl groups on a partially reduced surface take place in the reaction; probably via formation of hydroxyl groups at low temperature followed by desorption as water in the course of the formaldehyde formation reaction at elevated temperature.

The situation for $V_2O_5(001)$ is similar to some extent in that the natural vanadyl terminated surface is inactive. Removal of part of the vanadyl oxygen atoms leads to some reactivity towards formaldehyde formation, but the reactivity is much smaller than in the case of the reduced $V_2O_3(0001)$ surface. It appears that only certain types of defects are active for formaldehyde formation which are probably double defects according to STM.

SMART Project

Combining high-brilliance synchrotron radiation with a parallel imaging LEEM (low energy electron microscope) or PEEM (photoemission electron microscope) allows a comprehensive characterization of surfaces, adsorbates, and ultrathin films. One of the most challenging projects in this field is the SMART (Spectro-Microscope with Aberration correction for many Relevant Techniques) installed at BESSY. The goals of a lateral resolution of 2 nm and an energy resolution of 100 meV can only be achieved by aberration correction and energy filtering. The tetrode mirror in the SMART is the first and only working aberration corrector which simultaneously compensates for both, the spherical and chromatic aberrations of the electron lens system. Recently, the SMART could demonstrate a lateral resolution of 3.1 nm; up to now the best value achieved for this kind of microscope. Utilizing different sources (linearly or circularly polarized x-rays, UV-light, electron gun, etc.) the SMART excels as a versatile instrument with a variety of contrast mechanisms by imaging photo-emitted (XPEEM, UV-PEEM) and reflected electrons (LEEM, MEM). Thus it enables the spatially resolved study of morphology, chemical distribution, electronic state, molecular orientation, magnetization, work function, structural properties, atomic steps, etc. Within seconds the instrument can be switched from microscopy to two further modes: (a) laterally resolved spectroscopy from small object areas (nano-XPS, nano-AES, nano-NEXAFS, etc.) and (b) laterally resolved and energy filtered imaging of angular distributions: nano-PED (photoelectron diffraction), Fermi surface/valence band mapping, LEED (low energy electron diffraction), etc.

Structure and Reactivity

The group has a long standing interest in studying (i) the atomic structure of various well ordered oxide films (ii) structure and catalytic behaviour of gold nanoparticles; (iii) preparation and reactivity of oxide supported vanadia clusters. In addition, the use of thin ice films in the preparation of model catalytic systems has been studied in attempts to mimic a “wet chemistry” preparation of the real catalysts.

Silica and aluminosilicate thin films.

Atomically flat, crystalline SiO_2 films are grown on a Mo(112) single crystal using reactive Si deposition onto the O/Mo surface followed by vacuum annealing at ~1200 K. Combining scanning tunneling microscopy (STM), infrared reflection absorption spectroscopy (IRAS), X-ray photoelectron spectroscopy (XPS) data and density functional theory (DFT) calculations (performed by Prof. J. Sauer and coworkers at the Humboldt University, Berlin), it is unambiguously shown that the film consists of a two dimensional network (monolayer) of corner sharing [SiO_4] tetrahedra, with one oxygen of each tetrahedra binding to the protruding Mo atoms of the Mo(112) surface. High temperature annealing in oxygen or using mildly pre-oxidized Mo substrates irreversibly leads to the films, containing additional oxygen atoms adsorbed directly onto the Mo(112) surface, referred to as “O-rich” films in contrast to the “O-poor” films formed in UHV. The presence of the “extra”-oxygen atoms in the structure, as predicted by DFT, has been confirmed by XPS and IRAS studies. Interestingly, the formation of one-dimensional silica stripes of 0.5 nm in width has been observed at sub-monolayer silica coverage. The structure has been assigned to paired rows of corner sharing [SiO_4] tetrahedra chemisorbed on a Mo substrate. Combined experimental and theoretical results allowed us to build a phase diagram for 1D- and 2D- silica structures formed on Mo(112). Following this approach, well-ordered aluminosilicate films have been synthesized for the first time using Si and Al co-deposition onto Mo(112). Again, the atomic structure has been determined by combination of high-resolution experimental results and density functional theory. It is found that at low Al:Si ratio, the structure is formed by Al replacing the Si atoms in the silica film and consists of a two-dimensional layer of corner sharing [SiO_4] and [AlO_3] units.

In the course of studies of the film thickness effects on the structure and reactivity of supported metal particles, a new method to grow sub-nm, stoichiometric SiO_2 films has been developed. Based on photoelectron and infrared spectroscopy studies, it has been concluded that the ~0.9 nm-thick silica films grown on Mo(112) exhibit characteristics observed for >2.0 nm-thick films grown on conventional Si substrates. Therefore, these results may also have strong implications on the further miniaturization of the metal oxide semiconductor gate technology.

Structure of environmental effects on gold/ceria system.

Gold has recently received much attention in catalysis owing to the unique catalytic properties of Au nanoparticles. Previously, gold particles supported on different oxide (Al_2O_3, FeO, Fe_3O_4, Fe_2O_3) and carbon films have been studied in the group. In the last two years, our research activity has been shifted towards the Au/ceria system. This is basically driven by the high catalytic activity observed for this system in many reactions and also by intensive debates in the literature concerning the presence and the role of charged (cationic) Au species, first reported on the Au/ceria catalysts.

The morphology of ceria films grown on a Ru(0001) substrate has been studied by STM in combination with low-energy electron diffraction and Auger electron spectroscopy. By modifying the recipe suggested in the literature the preparation conditions were determined for the growth of nm-thick, well-ordered $CeO_2(111)$ films covering the entire surface, with a low density of the point defects assigned to oxygen vacancies. A circular shape of terraces observed by STM suggests a large variety of undercoordinated sites at the step edges.

Gold preferentially nucleates on point defects present on the terraces of fully oxidized films only to a low density. The nucleation expands to the terrace step edges, providing a large variety of low-coordinated sites. Only at high coverage, the Au particles grow homogeneously on the $CeO_2(111)$ terraces. The morphology of Au particles has been further examined by STM in situ and ex situ at elevated (up to 20 mbar) pressures of O_2, CO, and CO + O_2 at 300 K. The particles are found to be stable in O_2 ambient up to 10 mbar, meanwhile gold sintering emerges at CO pressures above ~ 1 mbar. Sintering of the Au particles, which mainly proceeds along the step edges of the $CeO_2(111)$ support, is observed in CO + O_2 (1:1) mixture at much lower pressure (~10^{-3} mbar), thus indicating that the structural stability of the Au/ceria catalysts is intimately connected with its reactivity in the CO oxidation reaction.

These results are in line with the those observed for the Au particles deposited on ultra-thin FeO(111) films. The Au particles are found to be quite stable in O_2 and H_2 environments at pressures up to 2 mbar. However, in CO and CO+O_2 atmospheres, the destabilization of Au particles located at the step edges occurs leading to the formation of mobile Au species, which migrate across the oxide surface.

Vanadia surfaces: from bulk V_2O_5(010) to vanadia clusters.

Vanadia based systems have been studied in the framework of the SFB 546 project including also the group of Dr. H. Kuhlenbeck in the Department, which basically studied the structure and reactivity of the vanadia thin films. To complement the studies, the S&R group has been focused on the supported vanadia clusters, and also studied surface reconstruction of a V_2O_5(001) single crystal, for comparison.

Restructuring of the V_2O_5(001) surface was monitored by scanning tunneling microscopy and spectroscopy at elevated temperatures. In situ band gap mapping of the crystal surface revealed a reversible metal-to-insulator transition at 350-400 K, which occurs inhomogeneously across the surface and expands preferentially in the direction of the vanadyl (V=O) double rows of V_2O_5(001). Supported by DFT and Monte-Carlo simulations, the results are rationalized on the basis of the anisotropic growth of vanadyl oxygen vacancies and a concomitant metal-to-insulator transition at the surface. Heating to elevated temperatures leads to irreversible surface reduction which proceeds sequentially as $V_2O_5(001) \rightarrow V_6O_{13}(001) \rightarrow V_2O_3(0001)$, as observed by high-resolution STM.

Vanadium oxide particles were prepared by physical vapor deposition of vanadium in oxygen ambient onto ice precovered well-ordered silica thin films. Morphology, electronic structure, and vibrational properties of the vanadia deposits were studied by STM, XPS, IRAS and temperature programmed desorption. The results show that the ice behaves as an oxidative agent, that favors vanadium oxidation up to V^{4+}, and as a buffer layer that precludes strong interaction of the V ad-atoms with the silica film. At room temperature, upon desorption of the unreacted water, nanosized particles of vanadia hydroxide like gel, containing V-OH and, to a lesser extent, vanadyl (V=O) species, are formed. Vacuum annealing at 550 K leads to the total dehydration and partial reduction of the particles to V_2O_3, which expose the V-terminated surface. Subsequent re-oxidation in O_2 irreversibly transforms the surface to the V=O terminated one, i.e. the same as for the reactive deposition onto the clean silica surface. The results suggest that the structure of silica supported vanadia catalysts is determined by a calcination step and should be considered under low oxygen pressure conditions as vanadium sesquioxide nanoparticles with the V=O terminated surface.

Atomic Force Microscopy

In the last few years it has been demonstrated that atomic force microscopy (AFM) can be the bridge to nanoscale science on oxide surfaces and insulating surfaces in general. Atomic resolution of oxide surfaces allows insights into the physics behind surface reactivity – essential for model catalysis. This knowledge then provides a nano-toolkit to study reaction mechanisms and dynamics on oxide surfaces. Further, the development of functionalized tips and defined oxide surfaces would offer complete freedom to study any surface reaction process. However, providing the ultimate level of understanding requires developments in AFM itself, particularly, chemical sensitivity in atomically resolved images. The overall goals of the ongoing AFM project in our group are to:

> develop chemical specificity in atomic resolution AFM,
>
> establish AFM as the pre-eminent tool for nanoscale studies of oxide surfaces,
>
> demonstrate the ability of AFM to aid in the understanding and design of catalytic agents.

Atomic resolution has been a “holy grail” of scanning probe methods for the last two decades.

With our scanning probe microscope setup we have achieved atomic resolution in both operating modes, in scanning tunnelling microscopy (STM) as well as in AFM. The microscope is operated in ultrahigh vacuum at low temperature to ensure defined imaging conditions, high stability and drift reduction. The unique breakthrough experiments demonstrated the enormous potential of local imaging for our understanding of the mechanisms of surface processes. Here we have measured for the first time clear atomically resolved images of the thin alumina film on NiAl(110) by AFM operated in a dynamic mode. Resolving such large and complex unit meshes is not only the acid test for the resolution capability of our machine, but also a useful confirmation of the currently accepted model for the films atomic structure. For the mapping of complex oxide surface structures an extreme stability and high sensitivity are needed for true atomic resolution in order to map even very small differences in the lateral arrangement of a few pm.

Similar work is currently performed on the surface of the hydrodesulphurisation catalyst Ni_2P. This system is fairly new to surface science and only very few high resolution microscopy results are available. Here, a (0001) cut single crystal has been studied with STM. Resulting images show an interesting hexagonal superlattice with characteristic defects and anti-phase domain boundaries. AFM work on this system is on the way. It is worth to be mentioned that the different coordination of the two species might shed light on the ongoing question of the origin of atomic contrast in force microscopy. The work on this crystal is done in collaboration with Prof. Asakura's group at Hokkaido University in Japan.

Over the last two years lots of measurements have been performed in close collaboration with M. Sterrer, T. Risse and N. Nilius on thin MgO(001) films deposited on Ag(001).

This type of oxide film has been investigated by our low-temperature STM and scanning tunnelling spectroscopy (STS) by analysing localized electronic defects. Depending on the location of the defect, for the first time different defect energy levels have been observed in the band gap of MgO. The charge state of defects was manipulated by interactions with the scanning tunnelling microscope tip. Comparison with ground state energy levels of color centers on the MgO surface has been obtained from embedded cluster calculations supporting the assignment of the defects to singly and doubly charged color centers.

Furthermore, adsorption properties of single gold and palladium atoms have been explored with respect to the thickness of supported MgO films. For Au on different MgO film thicknesses (3 ML and 8 ML), significant differences in the distribution of Au adsorption sites and in the Au cluster geometry have been found, which are in line with recent calculations and electron paramagnetic resonance experiments. On the surface of thick MgO films or unsupported MgO, Au adsorbs on O sites, and the equilibrium cluster geometry is three-dimensional. In contrast, the calculations predicted on thin MgO films a change of the preferred Au nucleation site and a stabilization of two-dimensional Au cluster geometries.

While Pd atoms are arranged in a random fashion, Au atoms form an ordered array on the surface. The long-range ordering as well as the STM appearance of single Au atoms on a 3 monolayer thin MgO film can be explained through partial charge transfer from the substrate to Au atoms as predicted recently by density functional theory calculations. In contrast with that, Au atoms on a thick film were found to be essentially neutral.

The intensive measurements by STM and STS are currently followed by site specific atomically resolved dynamic force spectroscopy measurements on the same model system. Atomically resolved AFM images have been combined with site specific frequency shift versus distance measurements. The frequency shift has been measured as a function of z and the lateral displacement. With these measurement characteristics we have probed inequivalent surface sites on thin MgO films to extract atomic-scale information on surface chemical reactivity and possible adsorption sites for metal atoms and small clusters.

For the detailed interpretation of interaction forces and energy we have spent many efforts in the precise recalculation of experimental frequency shift measurements. Therefore, we have developed methods for cantilever parameter determination in dynamic force spectroscopy concerning spring constant and amplitude, which are essential for further interpretation of the obtained site specific measurements by AFM.

Our setup allows direct observation of the adsorption properties of single atoms and molecules. The tendencies to adsorb at first on step edges or kink sites rather than on terraces, directly measured diffusion coefficients of adsorbed species, and the observation of the sites of electron-stimulated surface desorption, can be derived from atomically resolved dynamic force spectroscopy data. Such measurements will make enormous qualitative difference to our understanding of the mechanisms of the surface processes.

We are currently starting to characterize the chemical composition of oxide surfaces of binary and more complex compounds and to identify and probe chemical activity of various surface sites and defects with respect to chemical species adsorbed on an AFM tip, such as hydroxyl, metal particles and organic groups.

More importantly, it will help to transform atomic resolution AFM from a “magic box” into a powerful tool for chemical surface analysis well-integrated with other surface science methods.

Scanning Probe Spectroscopy

The activities of the SPS group focused on the implementation and application of local spectroscopic techniques into the framework of STM, in particular on combining optical, electronic and vibrational spectroscopy with the topographic abilities of the technique. To achieve this goal, several instrumental developments have been realized during the last two years. The Photon-STM, used for local optical characterization of the sample surface, has been equipped with a photo-multiplier tube, which enables acquisition of optical maps simultaneously with topographic images in order to identify emission centers on the surface. Furthermore, a deuterium lamp has been attached to the STM chamber to record spatially averaged photoluminescence and reflectance spectra that can be compared with the local emission response induced by electron injection from the STM tip. The SPEC-STM has finally left its construction stage and is now routinely used to perform measurements at 10 K sample temperature. The possibility of the instrument to couple photons and electrons into or out of the tunnel junction makes it an extremely versatile tool to study the interaction of individual objects, e.g. atoms, molecules and metal particles, with light and charged carriers.

Four different metal-oxide systems have been in the experimental focus during the last two years. (i) As a prototype oxide material showing optical activity, MgO thin films have been prepared on a Mo(001) surface and investigated by means of LEED, grazing incidence X-ray diffraction, STM and local light emission spectroscopy. The 5% mismatch between the MgO and the Mo lattice constant induce a complex relaxation behavior in the oxide film as a function of thickness. The MgO forms a coincidence lattice with the Mo support first, which breaks open into small mosaics separated by dislocation lines with increasing thickness. Further release of the misfit strain is achieved by the formation of large rectangular islands interrupted by deep [001] oriented grooves, as expected for a Stranski-Krastanov like growth mode. Electro-luminescence spectroscopy with the STM revealed a crossover in the MgO emission characteristics as a function of excitation bias. At electron energies above 25 eV, two emission peaks at 3.1 and 4.4 eV are observed, which are compatible with an exciton-mediated mechanism involving oxide corner and step sites. This emission is efficiently quenched when dosing small amounts of Au onto the surface (<0.1 ML), manifesting the identity of optically active centers and Au nucleation sites on the oxide surface. With decreasing electron energy, a new emission peak at much lower energy (1.7-2.0 eV) is detected, whose intensity strongly varies across the MgO surface. This spatially inhomogeneous emission signal is associated to the radiative decay of electrons between image potential states in front of the MgO film. As the energy position of those states sensitively depends on the sample work function, the technique is used to probe this quantity across the surface with nm spatial resolution, revealing a general work function decrease with increasing oxide thickness. The photon emission data produced by electron injection from the STM tip into the MgO surface have been verified by conventional photo-luminescence spectroscopy.

(ii) Increasing efforts have been taken to explore the special properties of polar oxide materials, specifically of FeO(111) where a surface dipole builds up between adjacent $Fe^{\delta+}$ and $O^{\delta-}$ planes. Already the FeO bilayer on Pt(111) has revealed a number of unexpected properties, such as regular modulations in the surface potential, self-organization effects of ad-material and the occurrence of Kondo physics. The evolution of these properties has now been studied as a function of thickness. Already for the second FeO layer, the oxide film reconstructs and forms a large number of competing surface structures, all of them characterized by large unit cells and complex arrangements of the surface atoms. For some of them, a considerable drop in the surface potential with respect to the bilayer has been detected via tunneling spectroscopy (STS), indicating an efficient reduction of the surface dipole due to structural reorganization. The possibility to fabricate patterned oxide surfaces has also been explored for ultra-thin alumina films grown on vicinal NiAl(16,14,1).

(iii) Thin V_2O_3 films on Au(111) have been investigated as a model system for a strongly correlated oxide material that shows fascinating surface chemistry in addition. Employing STS, the opening of a correlation band gap at temperatures below the Mott transition of V_2O_3 has been detected. The size of the gap was found to depend on the preparation conditions of the oxide, e.g. the oxygen pressure during oxidation and the annealing temperature, and exhibits short-ranged spatial variations across the surface. The partial opening/closing of the V_2O_3 gap has been attributed to slight variations in the concentration of V vacancies and/or interstitials in the oxide bulk that are partly neutralized by electron exchange with the Au support. The bulk electronic structure clearly affects the spatial arrangement of adsorbates on the vanadia surface, as probed for single Au and Pd adatoms. On the vanadyl-terminated (V=O) surface, preferential adsorption is observed at sites with smaller band gap and higher DOS close to the Fermi level. While binding at regular oxide site does not introduce new states in the gap region, adsorption on defects (here missing V=O groups) results in a new resonance level close to E_F.

(iv) Single adatom adsorption experiments have also been performed on SiO_2 films on Mo(211). The monolayer thick film is characterized by six-membered Si-O rings that leave a cavity of 4.5 Å diameter in their center. According to theoretical prediction, this hole is sufficiently large to incorporate single Pd atoms but too small for the slightly larger Au monomers. A corresponding behavior has been experimentally verified by low-temperature STM/STS. The Pd atoms completely immerse in the Si-O hexagons, thereby inducing strong alterations in the electronic structure of the surrounding oxide material. Single Au atoms, on the other hand, do not bind to defect-free oxide terraces and exclusively occupy dislocation lines between two regular oxide patches.

More recently, the interaction of large organic molecules (e.g. metal porphorins) with various oxide surfaces has moved into the focus of the group. The experiments aim for a better understanding of how a molecular electronic system is affected by bond formation to a weakly (e.g. a wide gap insulator) and a strongly interacting support (e.g. a metallic oxide). The molecule-support interactions are hereby investigated via electronic, vibrational as well as optical spectroscopy with the STM.

Magnetic Resonance

The magnetic resonance group has worked on four different topics. The first topic is a collaborative effort with the low temperature STM group and is concerned with the impact of defects on the electronic properties of metal particles which was explored using Au particles on single crystalline MgO films. The second project is a collaborative effort with the catalysis group and aims at a characterization of bimetallic Fe/Pd particles as a model system for Fischer-Tropsch catalysts. The group has also worked on the installation of an ultrahigh vacuum compatible high-field electron paramagnetic resonance (EPR) experiment operating at 95 GHz. Finally, the group has made efforts to develop the characterization of proteins on surfaces using a technique called site directed spin labeling.

Au/MgO

The first project focuses on point defects and their impact on the properties of metal particles adsorbed to them. As a prototype system Au particles deposited on single crystalline MgO(001) films grown on Mo(001) were chosen. It was shown previously that EPR spectroscopy is capable to characterize paramagnetic color centers (oxygen vacancies) on MgO(001). The impact of the color centers on the electronic properties of Au clusters was probed by means of IR spectroscopy using CO as a probe molecule. The nucleation at color centers results in a red shift of the CO streching frequency by 50-120 cm^{-1} with respect to Au clusters on the unperturbed surface. The amount of red shift depends strongly on the size of the particles. The red shift can be understood by a transfer of electrons from the color center to the Au cluster. The negatively charged Au particles have the ability to donate more electrons into the π*-orbitals of the CO molecules as compared to their neutral counterparts which leads to the observed red shift. The amount of red shift depends rather critically on the size of the particles. When the particles grow in size the extra charge gets more and more delocalized over the cluster giving rise to a decrease of the effect with increasing size. The very same behavior was also observed for negatively charged Au clusters in the gas phase studied in the Department of Molecular Physics. These investigations were among the first showing the impact of color centers on the electronic properties of metal particles and the observed red shifts compare favorably with values of the CO streching frequency reported for catalytic systems.

Pd/Fe bimetallic particles

Bimetallic Pd-Fe particles supported on a thin well ordered alumina film grown on NiAl(110) crystal were studied with respect to the geometric, electronic, magnetic, and adsorption properties. The properties of the particles depend not only on the overall composition and their size, but also on the distribution of the constituents within the clusters. For the model systems prepared under ultrahigh vacuum conditions these properties can be tuned by variation of the preparation conditions. Effects of the cluster size as well as the surface composition on the properties were investigated by combining STM, TPD and IRAS using e.g. CO as a probe molecule for the latter experiments. Pd and Fe show a similar growth behavior on the alumina film at 300 K. Both metals nucleate and grow preferentially at line defects of the support. For both deposition orders STM reveals that the particle density remains almost constant indicating that the second metal is predominately nucleating on the existing particles. However, the surface composition is strongly different for the two deposition orders due to the strong tendency of Pd to segregate to the surface of the particle. From these measurements a core shell growth mode is inferred for Pd subsequently deposited on Fe particles, while the opposite deposition order leads to a substantial intermixing of the metals. Apart from this characterization of the bimetallic particles under UHV conditions these systems were tested with respect to their catalytic properties under ambient conditions. The hydrogenation of butadiene, which has previously been studied for pure Pd particles on the same surface, shows that the addition of Fe does lower the activity of the catalyst if present on the surface, but it can help to increase the selectivity towards the primary hydrogenation products.

W- Band EPR machine

The group has build up a high field (95 GHz) EPR machine operating under UHV conditions and combines this technique with STM and IR to allow for a comprehensive characterization of the surfaces. As compared to the existing EPR setup operating at 10 GHz this offers an enhanced spectral resolution combined with an improved intrinsic sensitivity. To accommodate the specific needs of a UHV surface science experiment it is not possible to use a monomodal resonator, instead we decided to use a semi-convex Farby-Perot interferometer as the resonator structure. Here, the single crystal metal surface in UHV serves as the planar mirror of the Fabry-Perot interferometer while the concave mirror is located in fine vacuum and sealed against the UHV by a 150 μm thick microwave transparent quartz window. The requirements in terms of long term stability both against drift as well as vibrations have been improved by now, such that accumulation of data over long periods of time is possible. Measurements on stable radicals in air show that the setup has the sensitivity to detect submonolayer amounts of paramagnetic defects. Currently the first measurements on color centers on MgO(001) films are under way.

Proteins on surfaces

The goal of this project is to develop the methodology know as site directed spin labeling to gain insight into the structure and dynamics of proteins on planar surfaces and correlate this information with physical and chemical properties of surfaces. We could already show that EPR spectroscopy can provide information on structure as well as structural changes of proteins on surfaces. The use of oriented protein ensembles on planar surfaces allows to exploit the tensorial nature of the interaction between the spin label and the static magnetic field. It was previously shown that the angular dependent spectra measured for an oriented array of protein molecules can be used to deduce their orientation using T4 lysozyme vectorially adsorbed to a planar, zwitter-ionic lipid bilayer as a model system. The main problem that hampers the analysis of such data is the lack of microscopic understanding of the molecular dynamics of the spin labels. To this end two strategies were explored. The first approach was a theoretical one where molecular dynamics simulations were used to calculate the line shape of spectra of T4 lysozme. These MD calculations provide additional molecular understanding of the dynamics of the spin label and provide means to rationalize the assumptions made within the previously used line shape analysis mentioned above. The second approach was to investigate single crystals of these molecules and correlate X-ray crystallography and EPR spectroscopy on the very same protein single crystal to elucidate the structure and dynamics of the spin labeled side chains in detail. These investigations were done in collaboration with the group of Wayne Hubbell at UCLA. In addition, dipolar interaction between two spin labels, which is currently used to deduce the distance between certain positions within the protein, was studied with the particular focus to elucidate the possibility to extract its vectorial properties namely the orientation of the inter residue direction with respect to the surface.

Catalysis/Laser Spectroscopy

In the last two years we have pursued our studies on metal single crystals and oxide-supported metal clusters using linear (polarization-modulation IRAS) and non-linear (sum-frequency generation) in-situ vibrational spectroscopies in high-pressure environment as well as catalytic reactor studies using gas-chromatographic detection on various systems: Pd(111), Pd/Fe_3O_4/Pt(111), Au/Fe_3O_4/Pt(111), Fe-Pd/alumina/NiAl(110), and Au/MgO/Ag(100). Furthermore, preparations are under way for our future experimental field of interest, i.e. the investigation of metal precipitation from the liquid phase onto single-crystalline oxide substrates using in-situ spectroscopic and microscopic techniques. These activities comprise the installation of a scanning tunneling microscope operating under liquid environment and the adoption of the SFG set-up, including the construction of a new sample compartment for studies of solid-liquid interfaces. To meet the requirements for those experiments, a partial reconstruction of the laser laboratory has become necessary.

In addition, the PM-IRAS experiment has been replaced by a completely new set-up (PM-IRAS 2), the installation of which is now completed.

Surface vibrational sum-frequency generation (SFG) spectroscopy

SFG spectroscopy using CO as a probe molecule combined with TDS analysis was used to study the growth and stability of Pd and Au clusters on a 10 nm thick Fe_3O_4 film grown on Pt(111). The SFG spectra of CO adsorbed on stabilized Pd particles with a nominal thickness of 6 Å and 3 Å, respectively, give characteristic CO resonances for on-top and bridgebounded CO, comparable to IRAS results. However, CO adsorption on as-prepared Pd particles that have subsequently been annealed to various temperatures show remarkable differences. Whereas for 6 Å Pd particles primarily on-top CO is detected for annealing temperatures up to 600 K, both bridge and on-top species are present on the 3 Å Pd particles. Furthermore, for the 3 Å particles a phase change in the SFG signal occurs between 300 and 400 K. This may directly be related to the different morphology of the Pd particles after deposition and the stronger sintering of 3 Å particles as compared to the 6 Å particles, underlining the importance of the stabilization of Pd particles in order to obtain reproducible results. Gold clusters of different size (0.25 Å - 6 Å) are also subject to sintering as revealed by both SFG and TDS results after several annealing steps.

Apart from Fe_3O_4, we have also used MgO thin films as a substrate to study the adsorption properties of CO on gold clusters using SFG. These experiments are based on previous STM observations from our low-temperature STM group, where differences in the Au cluster growth depending on the thickness of the MgO layer were found: two-dimensional on thin films (3 ML) and three-dimensional on thick films (8 ML). Our SFG results for 1 Å gold deposited at 90 K on MgO films of 20 ML, 10 ML, 7ML, and 4 ML thickness, respectively, indicate the presence of two CO adsorption states, with one associated to CO adsorbed on three-dimensional Au clusters and the other one due to CO adsorption on small or flat Au aggregates. The relative intensities of the corresponding SFG signals change in favor of the second adsorption state with decreasing MgO layer thickness, confirming the results of the STM experiments.

With the intention to bridge experiments currently performed under UHV conditions with the forthcoming studies in aqueous media, first SFG experiments of water adsorption at 90 K on a 20 ML thin MgO film supported by Ag(100) have been performed. A characteristic band due to the symmetric stretch vibration of hydrogen-bonded water in ice is observed to grow with increasing water coverage, indicating a polar ordering of the ice layer. This effect strongly depends on the deposition conditions, in particular the H_2O deposition rate. H_2O adsorption experiments at higher deposition temperature and pressure, respectively, are planned in order to investigate the stages of surface hydroxylation of thin MgO films using SFG and to study the influence of a hydroxylated surface on the properties of deposited metal clusters and their catalytic activity.

Kinetic measurements

After exhaustive kinetic studies of the selective hydrogenation of 1,3-butadiene on Pd single crystals and alumina-supported Pd nanoparticles using our batch reactor working at a pressure of 1 bar with gas-chromatographic detection, this model reaction has also been applied to bimetallic Fe-Pd particles supported by alumina, a joint project with the ESR group (see report of the ESR group). Preparations to test these bimetallic model catalysts in the Fischer-Tropsch synthesis are currently in progress.

Polarization-modulation infrared reflection-absorption spectroscopy (PM-IRAS)

PM-IRAS experiments have been mainly devoted to obtain supporting spectroscopic information for the hydrogenation of 1,3-butadiene over Pd catalysts, which has previously been studied extensively with respect to catalytic activity. Accordingly, infrared studies under hydrogenation reaction conditions and post-reaction XPS measurements have been performed on Pd(111). Due to the flat adsorption geometry of 1,3-butadiene and the reaction products, no surface species could be detected with IRAS. However, the reaction could be followed by analyzing the gas-phase spectra that were acquired simultaneously and contain fingerprint information of the respective reaction products. The obtained results are perfectly in line with the reaction mechanism proposed from the kinetic studies, i.e. in the early stages 1,3-butadiene is hydrogenated to 1-butene through 1,2-hydrogen addition, while after complete consumption of 1,3-butadiene, readsorbed 1-butene yields n-butane through hydrogenation and cis/trans-2-butane through isomerization. A post-reaction surface analysis by XPS revealed a rather small amount (0.3 ML) of carbon deposits, showing that poisoning of the Pd surface by carbonaceous species plays, under the given reaction conditions, only a minor role.

Molecular Beam

The activities of the molecular beam group focused on the establishing the correlations between the structural and electronic properties of the complex nanoparticle supported model catalysts and their catalytic activity in chemical reactions. The application of molecular beam techniques in combination with the time-resolved RAIR spectroscopy provides very detailed information on the reaction mechanisms and kinetics under well-controlled conditions. Previously, this approach has been successfully applied to several relatively simple reaction systems such as CO oxidation, dissociation of NO and decomposition and oxidation of methanol on Pd particles supported on a chemically inert Al_2O_3/NiAl(110) film. In the last two years we extended the range of reaction systems towards more complex organic reactions exhibiting several competing reaction pathways and/or involving elementary reaction steps proceeding on a chemically active support. Particularly, the group has been focusing on two new fields: (i) the investigation of cis- and trans-2-butene conversions in the presence of deuterium on Pd/Fe_3O_4/Pt(111) model catalyst and determining the factors governing the stereo- and chemoselectivity towards different reaction pathways (cooperation with F. Zaera, University of California, Riverside, USA); (ii) the elucidation of the role of metal-support interaction in the kinetics of methanol decomposition on Pd nanoparticles supported on a chemically active Fe_3O_4/Pt(111) oxide film. Additionally, the group has been engaged in the planning and construction of the new single crystal adsorption microcalorimeter operating under UHV conditions for measuring heats of adsorption and reaction (cooperation with C.T. Campbell, University of Washington, Seattle, USA).

cis- and trans-2-butene conversions on Pd/Fe_3O_4/Pt(111)

The promotion of olefin conversions is one of the most studied processes in heterogeneous catalysis. Recently, it has been shown in our department that the formation of weakly bound "subsurface" hydrogen species is a key factor for hydrogenation to occur efficiently on Pd nanoparticles. There are, however, a number of issues unresolved still. Specifically, it has been determined that olefin conversions under ambient conditions do not take place on clean metal surfaces, but rather on metals covered by the carbonaceous deposits that result from an early decomposition of the reactants. The exact role that those strongly adsorbed species play in the catalytic mechanism is still not known. We investigated the conversions of cis- and trans-2-butene on the clean and carbon-precovered Pd nanoparticles of various sizes (4-65 nm) supported on Fe_3O_4/Pt(111) film by means of TPD, IRAS and isothermal pulsed molecular beam experiments aiming at a deeper understanding of the role of those strongly bound carbonaceous deposits in the heterogeneously catalyzed organic reactions.

Three different reaction pathways have been identified for this reaction system: *dehydrogenation* proceeding through several consecutive steps and resulting in the formation of carbonaceous species on the surface; *cis-trans isomerization* accompanied by the H-D exchange as well as *hydrogenation* with formation of butane. On the initially clean surface all those competing reaction pathways were found to proceed. However, accumulation of the spacious partly dehydrogenated hydrocarbon species at low temperatures (190 – 210 K) results in the fast contamination of the metal particles and the vanishing catalytic activity towards isomerization and hydrogenation. At temperatures exceeding 250 K, dehydrogenation occurs more readily enabling a sustained catalytic activity towards isomerization/H-D exchange over a long period of time. However, no persisting catalytic activity for the competing hydrogenation has been observed on the initially clean surfaces. Carbon deposition on the Pd particles changes the catalytic behavior of this system dramatically. The presence of strongly adsorbed carbonaceous species induces the sustained catalytic activity for hydrogenation of 2-butenes, so that both isomerization and hydrogenation can proceed on the carbon-modified surfaces. The rate of hydrogenation was found to be limited by the amount of hydrogen atoms in a specific weakly bound state available in the system as determined from the transient kinetic behavior of the reaction. Performing TPD measurement for hydrogen desorption from the clean and carbon-modified Pd particles, we were able to prove that co-adsorbed carbon considerably increases the relative abundance of weakly bound subsurface hydrogen atoms, thus inducing hydrogenation and governing selectivity of 2-butene conversions.

Strongly bound carbonaceous deposits showed also a pronounced effect on the stereoselectivity in cis- and trans-2-butene conversions. Whereas the isomerization rates of cis-2-butene were found to be similar on the initially clean and carbon-precovered particles, the isomerization rate of trans-2-butene dropped by a factor of 2 in the presence of carbonaceous species.

Methanol decomposition on Pd/Fe_3O_4/Pt(111)

The role of the strong metal-support interaction in heterogeneously catalyzed reactions has been explored for methanol adsorption and decomposition on Pd/Fe_3O_4/Pt(111) model catalyst. Catalytic activity of the Pd/Fe_3O_4 catalyst with respect to methanol decomposition shows pronounced differences as compared to the previously studied Pd/Al_2O_3 system: whereas methanol adsorbs molecularly on the inert Al_2O_3 film, it undergoes decomposition on a chemically active Fe_3O_4 support. The formation of two types of methoxy surface species has been observed on the Fe_3O_4 film by IRAS. The methoxy groups on the oxide film exhibit exceptionally high thermal stability – up to 500 K – on the pristine Fe_3O_4 film, thus allowing the film to act as a reservoir for active surface species participating in the further reaction steps. On the Pd/Fe_3O_4 catalyst, the support-related methoxy species spill over to the metal particles, opening up a new reaction channel. Dissociation of the support-related methoxy groups involving C-O bond scission on Pd/Fe_3O_4 catalyst results in a considerably higher rate of carbon accumulation compared to Pd particles supported on a chemically inert Al_2O_3 film. We attribute the higher rate of carbon formation to the increasing effective flux of active methoxy groups to metal particles at elevated temperatures due to spillover from the Fe_3O_4 film. Formation of interface Pd oxides was found to hamper the spillover of methoxy species through the support-metal boundary and suppress the rate of carbon formation on the metal particles.

Photon-Induced Processes

The activities of the group are focused on the investigation of photoexcitation and photochemistry on metal nanoparticles deposited on thin oxide films. The electronic structures and the optical properties as well as the catalytic properties strongly depend on the particles size and the morphology, especially when the size is below tens of nanometers. The excitation of surface plasmon of metal nanoparticles (Mie plasmon) leads to a strong enhancement of the surface electric field. These factors offer possibilities to tune and enhance photochemistry on particulate surfaces. Experimental methods such as two-photon photoemission spectroscopy (2PPE), mass selected time-of-flight measurements (MS-TOF), resonance enhanced multiphoton ionization (REMPI), and temperature programmed desorption (TPD) are employed for the investigation.

The 2PPE spectra of silver nanoparticles (AgNPs) on thin alumina films on NiAl(110) have been measured as a function of photon energy. A clear resonance peak at 3.6 eV corresponding to the (1,0)-mode of Mie plasmon was observed. The photoelectron yields were larger by a factor of hundreds compared to Ag(111). The effects of plasmon excitation on surface photochemistry were then investigated in the systems of NO and Xe on AgNPs.

NO molecules adsorbed on 8-nm AgNPs below 75 K form dimers and monomers as in the case of Ag(111). Photodesorption cross sections were measured at photon energies between 2.3 eV and 4.7 eV with nanosecond laser pulses by analyzing the exponential decay of photodesorption signal which reflects the decrease of coverage of adsorbates. Desorption of NO from the dimer could be distinguished from that from the monomer as the photodesorption cross section of the former is about ten times larger than that of the latter. A large enhancement of photoreaction of the dimer (~6×10^{-17} cm^2) about 13 times larger than that on Ag(111) was observed at 3.5 eV in p-polarization which is close to the (1,0) mode of Mie plasmon of AgNPs at 3.6 eV. The translational energy distributions of NO measured by MS-TOF were about 600 K and 900 K for NO dimers and monomers, respectively, and did not depend on the photon energy, however. It is therefore concluded that the plasmon excitation enhances the photodesorption cross sections of NO on AgNPs but it does not change the photodesorption mechanisms. More detailed information about the photodesorption dynamics, i.e., energy partitioning into vibronic degrees of freedom will be investigated by REMPI. The photodesorption mechanism of NO on AgNPs can be explained in terms of MGR or Antoniewicz model in which desorption proceeds via the transiently negative ion (TNI) state (~2.5 eV for NO dimer) which is created by the attachment of a hot electron from the substrate.

For Xe physisorbed on AgNPs, on the other hand, the above desorption mechanism is not possible because there is no TNI state of Xe in the uv range. However, nonthermal desorption of Xe was observed only when the (1,0) mode of Mie plasmon was excited at 3.5 eV in p-polarization at low laser fluences (~1 mJ/cm^2). The translational temperature of desorbing Xe in this case was more than 300 K, which is much higher than the substrate temperatures (~40 K). At other photon energies only thermal desorption of Xe was observed at higher laser fluences. Moreover, on plasmon resonance, the photodesorption yield fluctuated erratically showing herds of spikes instead of the exponential decay. The power spectrum of desorption yield data is flat, which means that photodesorption of Xe on the plasmon resonance is random and/or chaotic. Such an erratic behavior disappears at higher laser fluences as thermal desorption becomes dominant. Both the nonthermal desorption and the erratic behavior can be explained in terms of plasmonic coupling among AgNPs which creates hot spots of enhanced surface electric field and also is predicted by theory to increase the decay time of plasmon from ~10 fs to more than ~200 fs. A new desorption mechanism was proposed for the nonthermal desorption of Xe based on plasmon-induced Pauli repulsion between Xe atoms and surface electrons of AgNPs. A simple molecular dynamics simulation showed that this is possible.

The next step is to control the plasmon resonance by changing the size, morphology, and/or composition (e.g., Au-Ag alloys) of nanoparticles. Preliminary measurements showed that photodesorption cross section of NO from AgNPs was increased as the particle size was reduced below 8 nm, which may reflect the change of decay channels of plasmon from radiation to electron-hole pairs creation (Landau damping). The combined studies of optical/electronic properties (2PPE) and photochemistry will thus shed light on unique photocatalytic properties of metal nanoparticles.

Scanned-energy mode photoelectron diffraction

This activity is based on a strong collaboration with Phil Woodruff at the University of Warwick and Christine Lamont at the University of Huddersfield and originally involved Alex Bradshaw in the Surface Physics Department. A postdoctoral researcher based at the FHI is funded through SFB 546 of the DFG, while a research student is jointly funded by CP and AC.

Scanned-energy mode photoelectron diffraction (PhD) is a novel synchrotron-radiation-based method to determine quantitatively the local structure at surfaces in an element-specific and chemical-state-specific fashion. While the group continues to exploit this method to investigate the structure of increasingly complex small molecules (most recently the nucleotide base, thymine) on metal surfaces, the focus of the FHI-based component of the collaboration is on transition metal oxide surfaces, and particularly VO_x. During the last 2 years work has focussed on and V_2O_3 on Pd(111), but with some continuing interest in adsorbates (notably water) on $TiO_2(110)$.

The work on V_2O_3 grown on Pd(111) (and most recently on Au(111)), for which one obtains high-quality films as judged by sharp LEED patterns, exploits prior characterisation work by the Electron Spectroscopy and Synchrotron Radiation group within CP on the preparation and reactivity. While the PhD technique is more naturally suited to studies of adsorbate structures than of clean surfaces (because it is generally not possible to distinguish between surface and sub-surface emitter atoms) significant amounts of PhD data have been collected from the clean, as-prepared, $V_2O_3(0001)$ surface. In order to determine the integrity of this approach, similar data from the $TiO_2(110)$ surface have also been analysed. The results yield optimised values of the surface relaxations in good agreement with the most recent results by other methods, notably in the relaxation of the bridging oxygen atoms that had been the subject of considerable controversy. Encouraged by these results we have performed a similar analysis on the $V_2O_3(0001)$ surface. The results clearly confirm the large relaxation of the outermost half-vanadium terminating layer, consistent with the theoretical results obtained within the TH Department by Klaus Hermann and colleagues. What has proved more challenging, however, is to establish whether or not this surface is terminated by a surface vanadyl, V=O, species. Theoretical calculations favour this termination, and vibrational spectroscopy obtained within the CP department also provides evidence for such a surface species, but our PhD results are unable to distinguish between models with and without the surface vanadyl. However, we have recently progressed to a detailed analysis of the local geometry of surface OH species formed by reaction with atomic H or molecular water. This study shows that the OH species are certainly not mainly or significantly in the V-atop sites associated with the vanadyl O atoms, and we are currently collaborating actively with Klaus Hermann in the TH department to make a detailed comparison of theoretical and experimental structural solutions.

PP&B (Personal Computers, Realtime & Image Processing)

Based on the data network infrastructure, provided by the Joint Network Center (GNZ), the PP&B group is responsible for the installation and maintenance of the desktop systems (including laptops), workstations, telephone system and the electronic building control system. The technical consulting service supports scientists of the institute in the configuration, modification, acquisition, and adaption of computer equipment to the experiments (in close cooperation with the service group for electronics). Some remarkable examples from the last two years are the installation of high resolution image system for SMART and the setup of a common acquisition system for the different experiments in the MP Department (cPCI based with VxWorks realtime system).

Several server systems perform services for data storage, mail, web, printing, number crunching and databases for different document archives. A Computer Cluster (50 Opteron CPU) was built up for the Theory Department and is supervised by the PP&B group. A new general computer server (fhix, 72 cores, 208 GByte Memory, Infiniband interconnect) for the Institue was setup end of 2005 and is well used by different groups.

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Invited Talks of the Members of the Department of Chemical Physics

Marcella Felicissimo

2006 *Pd-Fe Bimetallic Particles Supported on a Thin Al_2O_3 Film Grown on NiAl(110)*
Institute of Physics, University of Groningen
31.10.2006, Groningen, The Netherlands

Pd-Fe Bimetallic Particles Supported on a Thin Al_2O_3 Film Grown on NiAl(110)
MPI für Mikrostrukturphysik
20.11.2006, Halle, Germany

Hans-Joachim Freund

2005 *Investigation of Supported Nanoparticles at the Atomic Level*
Seminar, Physic Department, Helsinki Technical University
07.12.2005, Helsinki, Finland

Metal Cluster on Oxides: From a Few Atoms to Big Naked and Ligand Stabilized Clusters
Pacifichem Conference 2005
15.12.-20.12.2005, Hawaii, USA

Catalytic Control at the Atomic Level: Deposited Nanoparticles
Pacifichem Conference 2005
15.12.-20.12.2005, Hawaii, USA

2006 *Model Catalysts*
Lecture Series in Heterogeneous Catalysis
06.01.2006, Berlin, Germany

Nanoparticles on Oxides as Models for Heterogeneous Catalysts: An Atomic View
10th International Symposium on Catalyst Deactivation
05.02.-08.02.2006, Berlin, Germany

Investigation of Supported Nanoparticles at the Atomic Level
4th Annual University of California Symposium on Surface Science and Its Applications
09.02.-10.02.2006, Berkeley, USA

Modelle für die Heterogene Katalyse aus atomarer Sicht
Graduiertenkolleg 894
24.02.2006, Freyburg an der Unstrut, Germany

Electron Spin Resonance and Low Temperature-STM of Metal Atoms and Clusters on Single Crystal Surfaces
Symposium on Surface Science 2006
05.03.-11.03. 2006, St. Christoph am Arlberg, Austria

Defects on Magnesium Oxide Surfaces: An STM and ESR Study
APS March Meeting
13.03.-17.03. 2006, Baltimore, USA

Modelle für heterogene Katalysatoren auf atomarer Basis: Kohlenwasserstoffhydrierung an Palladium und Palladiumhydrierungsnanoteilchen
Kolloquium, BASF
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19.05.-20.05. 2006, Isparta, Turkey

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Model Catalysts: An Atomic View
Microscience 2006
27.06.-29.06.2006, London, U.K.

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Defects as Centres for Chemical Reactivity on Oxide Surfaces
EURODIM 2006,
10.07.-14.07.2006, Milano, Italy

From Atoms to Clusters as Models in Heterogeneous Catalysts
Fifth Tokyo Conference on Advanced Catalytic Science and Technology (TOCAT5)
23.07.-28.07.2006, Tokyo, Japan

Atomare Einblicke in die Katalyse: Oxidgetragene Nanopartikel
Geburtstagskolloquium Ibach-Lüth, FZ Jülich
11.08.06, Jülich, Germany

Catalysis at the atomic scale
Symposium to honor Bill Salaneck on the occasion of his 65th birthday
17.08.-19.08.2006, Linköping, Sweden

Oxide Supported Nanoparticles: Models in Catalysis at Atomic Resolution
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ECOSS 24, Plenary
04.09.-08.09.2006, Paris, France

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Oxide supported Nanoparticles: Models in Catalysis at Atomic Resolution
XX SICat
17.09.-22.09.2006, Gramado, Brazil

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15.10.-19.10.2006, Himeji, Japan

Die Entwicklung eines Europäischen Forschungsrats: Konzepte und Tendenzen
Dies Academicus
04.11.2006, Erlangen, Germany

Metal Atoms and Clusters on Oxide Surfaces: Recent Advances
GRI Symposium on Cluster Science; Breakthrough Advances in Cluster Science
07.11.-09.11.2006, Nagoya, Japan

Ultra-thin Film Oxides: Materials with Tailored Properties
IXCRI 2006
29.11.2006, Kuala Lumpur, Malaysia

Model Systems for Heterogeneous Catalysts Based on Thin Oxide Films
Workshop on Catalysis and Surface Science
13.12.-15.12.2006, Santa Barbara, USA

2007 *Models for Heterogeneous Catalysts at the Atomic Level*
Centenary Lecture Tour, University College London
15. 01.2007, London, U.K.

Models for Heterogeneous Catalysts at the Atomic Scale
Centenary Lecture Tour,
17.01.2007, Cardiff, U.K.

Oxide Supported Nanoclusters
Centenary Lecture Tour,
19.01.2007, Nottingham, U.K.

Oxide Supported Nanoclusters
Centenary Lecture Tour
22.01.2007, Aberdeen, U.K.

Oxide Supported Nanoclusters
Centenary Lecture Tour
24.01.2007, Manchester, U.K.

Modelle für heterogene Katalysatoren: Atomare Einblicke
GdCH-Kolloquium, Universität Köln
02.02.2007, Köln, Germany

Thin Oxide Films as Model Supports for Heterogeneous Catalysts: An Atomic View
Seminar, Chemistry Department, Lehigh University,
20.03.2007, Bethlehem, USA

Oxide Supported Nanoclusters
Spring Symposium of the Catalysis Society of New York
21.03.2007, ExxonMobile Research Facility, New York, USA

Model Systems in Heterogeneous Catalysis at the Atomic Level
Seminar, Physics Department, Rutgers University
22.03.2007, Piscataway, USA

Bulk and Supported Catalysts: Selectivity at the Atomic Scale
ACS Symposium „Nanoscale Inorganic Catalysis“
25.03.-29.03.2007, Chicago, USA

The Surface Science of Metal and Oxide Catalysts: Model Systems at the Atomic Level
ACS Gabor A. Somorjai Award Lecture
25.03.-29.03.2007, Chicago, USA

Atom-Scale Description and Control of Complex Surface Structures
Meeting in Honor of Prof. Francisco Nart
11.04.-13.04.2007, Sao Carlos, Brazil

Models for Heterogeneous Catalysts: Preparation and Characterization
4th San Luis Summer School on Surface, Interfaces and Catalysis
14.04.-16.04.2007, Cuernavaca, Mexico

From Atoms to Clusters: Models for Heterogeneous Catalysts
4th San Luis Conference on Surface, Interfaces and Catalysis
16.04.-21.04.2007, Cuernavaca, Mexico

Models for Heterogeneous Catalysts: Preparation and Characterization
4th San Luis Conference and Summer School on Surface, Interfaces and Catalysis
14.04.-23.04.2007, Cuernavaca, Mexico

Deposited Nanoparticles: Models for Heterogeneous Catalysts at the Atomic Dimension
Gastvortrag, Leopold-Franzens-Universität Innsbruck
30.04.2007, Innsbruck, Austria

Deposited Nanoparticles: Models for Heterogeneous Catalysts at the Atomic Dimension
Nanocatalysis Summer School
31.05.2007, Les Houches, France

Models for Heterogeneous Catalysts: Preparation and Characterization
Nanocatalysis Summer School
31.05.2007, Les Houches, France

Model Systems in Heterogeneous Catalysis: Selectivity Studied at the Atomic Level
Irsee IV
07.06.-10.06.2007, Irsee, Germany

Models for Heterogeneous Catalysts: Preparation and Characterization
NSF-PASI Workshop
Electronic States and Excitations on Nanostructures
11.06.-22.06.2007, Zacatecas, Mexico

Models in Heterogeneous Catalysis at the Atomic Level
NSF-PASI Workshop
Electronic States and Excitations on Nanostructures
11.06.-22.06.2007, Zacatecas, Mexico

Modelle für die Heterogene Katalyse: atomare Einblicke
Verleihung der Ehrendoktorwürde K. Wandelt, Universität Leipzig
Electronic States and Excitations on Nanostructures
15.06.2007, Leipzig, Germany

Modelsystems in Catalysis: An Atomic View at Deposited Atoms and Supported Clusters
International Bunsen Discussion Meeting
29.06.-30.06.2007, Heidelberg, Germany

Metal Atoms and Model Clusters on Oxide Surfaces: Electronic Structure and Reactivity
IVC17/ICSS13 and ICN+T 2007 Congress
02.07.-06.07.2007, Stockholm, Sweden

Model Systems in Heterogeneous Catalysis: Selectivity Studied at the Atomic Level
International Symposium on Relations Between Homogeneous and Heterogeneous Catalysis
16.07.-20.07.2007, Berkeley, USA

Model Systems in Catalysis: An Atomic View at Deposited Atoms and Supported Clusters
Colloquium, Department of Chemistry, UC Irvine
24.07.2007, Irvine, USA

Models for Heterogeneous Catalysts: Preparation and Characterization
Colloquium, Department of Chemistry, UC Irvine
03.08.07, Irvine, USA

Photochemistry at Metal Nanoparticles
Elementary Reactive Processes at Surfaces Conference, Donostia International Physics Center
Colloquium, Department of Chemistry, UC Irvine
09.08.07, Irvine, USA

Modelsystems in Catalysis: An Atomic View at Deposited Atoms and Supported Clusters
University of North Texas
27.07.2007, Denton, USA

Reactions on Oxide-supported Nanoparticles
Elementary Reactive Processes at Surfaces Conference, Donostia International Physics Center
31.08.-01.09.2007, Donostia-San Sebastian, Spain

Metal Atoms and Clusters on Oxide Surfaces: Electronic Structure and Reactivity
Jyvaskyla Nanoscience Days
25.10.-26.10.2007, Jyvaskyla, Finland

From Clusters to Catalysis – Transition Metals and Transition Metal Oxides
Sfb Symposium “From Clusters to Catalysts – Transition Metals and Transition Metal Oxides”
18.10.-21.10.2007, Erkner, Germany

Markus Heyde

2007 *Dynamic Force Microscopy Studies on Model Catalysts*
University of Ulm, Department of Chemistry
10.05.-11.05.2007, Ulm, Germany

Structure of the Aluminium Oxide Film on NiAl(110) by Dynamic Force Microscopy
IBM Research GmbH, Zurich Research Laboratory
22.05.-23.05.2007, Rüschlikon, Switzerland

Heinz Junkes

2006 *Software and Systems - Einsatz einer eigenen Datenbank als Benutzermanagementsystem [Datenbanken]*
iX Cebit Forum 2006
11.03.06, Hannover, Germany

2007 *Software and Systems - Aufbau und Betrieb einer dynamischen IT-Infrastruktur [Skalierung]*
iX Cebit Forum 2007
16.03.07, Hannover, Germany

Dietrich Menzel

2005 *Electronically Induced Surface Chemistry: Localised Bond Breaking Versus Delocalization*
ALS'05th International Symposium on Atomic Level Characterization for New Materials and Devices
04.12.05, Kona, Hawaii

2006 *Laserinduced Photodesorption from Nanoparticles: Plasmon Enhancement for* $NO/Ag/Al_2O_3$
Symposium on Surface Science 2006
10.03.06, St. Christoph am Arlberg, Austria

Photophysics and Photochemistry of Metal nanoparticles: Electronic Excitations and Photodesorption of NO on Supported Ag Particles
Colloquium of Physics Department, Dahlhousie University
13.07.06, Halifax, Canada

2007 *Photochemistry at Metal Nanoparticles*
International Bunsen Discussion Meeting
29.06.2007, Heidelberg, Germany

Niklas Nilius

2005 *Elektronische und Optische Eigenschaften von metallischen Nanoteilchen auf dünnen Oxidfilmen*
HU-Berlin, AG Prof. Winter: Grenzflächen und dünne Schichten,
17.11.2005, Berlin, Germany

2006 *Adsorption and Nucleation on thin Oxide Films*
RWTH-Aachen, Institutsseminar Festkörperphysik
18.01.06, Aachen, Germany

Eigenschaften dünner FeO und Al_2O_3 *Filme*
Universität Bremen
09.06.06, Bremen, Germany

Construction and Properties of One-dimensional Systems in the STM
Fokus-Studiengang, Universität Würzburg,
30.08.06, Würzburg, Germany

2007 *Light Emission Spectroscopy with the STM*
Keynote-Speaker IFF-Spring-school, FZ Jülich
15.03.07, Jülich, Germany

From Work Function Tuning to Kondo Physics: The Properties of Thin Oxide Films
CeNS-München, Colloquium
25.05.07, München, Germany

From Self-organization to Kondo Physics: The Properties of Thin FeO Films
University of Halle, Symposium: Oberflächen von 3d Übergangsmetalloxiden
13.06.07, Halle, Germany

Thomas Risse

2006 *A Combined EPR and STM/STS Approach to Investigate Color Centers and their Interaction with Metal Atoms on Thin MgO(001) Films*
NIS Colloquia: Nanostructured Oxide Surfaces II
23.02.-24.02.06, Torino, Italy

On the Interaction of Metal Atoms and Cluster with Color Centers on Oxide Surfaces
EUROCORES SONS Summer School on Metal Clusters and Surfaces
03.07.-6.07.06, Tirrenia, Italy

Properties of Metal Atoms and Clusters Adsorbed on Color Centers of Oxide Surfaces
CECAM Workshop “Catalysis from First Principles”
11.09.-14.09.06, Lyon, France

Point Defects on Oxide Surfaces and their Influence on the Properties of Deposited Metal Atoms and Clusters
SFB Colloquium TU-Darmstadt
23.10.06, Darmstadt, Germany

Point Defects on Oxide Surfaces and their Influence on the Properties of Deposited Metal Atoms and Clusters
COST Workshop
02.11.06, Vienna, Austria

2007 *A Combined EPR and STM/STS Approach to Investigate Color Centers and their Interaction with Metal Atoms on Thin MgO(001) Films*
IWOX V
07.01.-12.01.07, Lake Tahoe, USA

How Does EPR Spectroscopy Fits into Surface Science?
Seminar Jules Stein Eye Institute, University of California Los Angeles
17.01.07, Los Angeles, USA

Modification of the Electronic Structure of Au Atoms and Clusters by the Properties of MgO Films
Workshop on "Properties of metal particles on oxide surfaces"
12.04.-13.04.07, Erlangen, Germany

ESR Spektroskopie an wohl definierten planaren Oberflächen: vom Ultrahochvakuum zu physiologischen Bedingungen
Seminar im Rahmen der Besetzung einer W3-Professur für Physikalische Chemie, Universität Heidelberg
23.04.07, Heidelberg, Germany

The Effect of Film Thickness on the Properties Au Atoms and Clusters on the MgO(001) Films
Workshop on "Properties of thin oxide films"
10.05.-12.05.07, Barcelona, Spain

Günther Rupprechter

2005 *Spectroscopy on Model Catalysts Under Ambient Pressure*
Chemisches Institut, Otto-von-Guericke-Universität Magdeburg
01.12.2005, Magdeburg, Germany

2006 *IR Spectroscopy*
Lecture as part of the Lecture series "Modern Methods in Heterogeneous Catalysis Research", organized by the Fritz Haber Institute, Humboldt University Berlin and the Technical University Berlin
13.01.06, Berlin, Germany

Monitoring adsorbed molecules during catalytic reactions at mbar pressure"
Max Planck Institute of Carbon Research, Mühlheim an der Ruhr
24.01.06, Mühlheim an der Ruhr, Germany

A Surface Science Approach to Ambient Pressure Catalytic Reactions
Second International Congress on Operando Spectroscopy
26.04.06, Toledo, Spain

In situ SFG und IR Spektroskopie an Modellkatalysatoren im Ultrahochvakuum und unter Atmosphärendruck
Institute of Chemical Technologies and Analytics, Vienna University of Technology
28.04.06, Vienna, Austria

Monitoring Oxidation Reactions with PM-IRAS Spectroscopy
Workshop "Nanoscience on Surfaces", Burg Schlaining
30.05.2006, Stadtschlaining, Austria

Vibrational Spectroscopy in Catalysis
Summer School on "Surface reactivity and nanocatalysis”,
Interdisciplinary Nanoscience Center (iNANO), University of Aarhus Denmark
13.06.2006, Elbetoft, Denmark

Messing Around with Hydrogen
Institute of General Physics, Vienna University of Technology
27.06.2006, Vienna, Austria

Surface Science Studies of Ambient Pressure Catalytic Reactions
8th Pannonian International Symposium on Catalysis
06.07.2006, Szeged, Hungary

Vibrational Spectroscopy of Molecules on Catalytically Active Surfaces
ISIS series of seminars at the Rutherford Appleton Laboratory
25.07.2006, Didcot, U.K.

Swetlana Schauermann

2005 *Molecular Beam Experiments and Microkinetics on Model Catalysts*
Chemistry Department, Washington University
October 2005, Seattle, USA

2006 *Molecular Beam Experiments on Model Catalysts*
Chemistry Department, University of Cambridge
February 2006, Cambridge, UK

2007 *Selectivity in Hydrocarbon Conversion on Supported Model Catalysts*
Surface Science Seminar, Chemistry Department, Washington University
June 2007, Seattle, USA

Shamil Shaikhutdinov

2005 *Iron Oxide Thin Films: Preparation, Surface Structure and Use in Model Catalysts*
Seminar, Institute of Physics, Humboldt University Berlin
16.11.2005, Berlin, Germany

2006 *On the Role of Subsurface Hydrogen in Hydrogenation Reactions on Palladium*
SURCAT 2006
25.07.-28.07.2006, Cardiff, Wales

Thin Silica Films: Growth, Atomic Structure and Properties
Seminar, University College London
14.06.2006, London, UK

2007 *Oxide Nanoparticles on Ultrathin Oxide Films*
COST Meeting
10.05.-12.05.2007, Barcelona, Spain

Model Heterogeneous Catalysts at Atomic Resolution
1-st IDECAT Conference
12.05.-17.05.2007, Porquerolles, France

Model Studies for Understanding Structure-Reactivity Relationships in Catalysis
Seminar, Institute of Physics CAS,
22.05.2007, Beijing, China

Thin Films of Iron Oxides: Preparation, Surface Structure and Use in Model Catalysts
Seminar, Cardiff School of Chemistry
13.06.2007, Cardiff, Wales, UK

Towards Understanding Structure-Reactivity Relationships in Catalysis: Model Studies
Russian-German Seminar on Catalysis
09.07.-13.07.2007, Altai Mountains, Russia

Adsorption of Water on Well Defined Oxide Surfaces
XVII Intern. Conference “Horizons of Hydrogen Bond Research”
02.09.-8.09.2007, St-Petersburg, Russia

Martin Sterrer

2006 *Defects on Oxide Surfaces and their Interaction with Metal Atoms and Clusters*
Technische Universität Wien, Institut für Materialchemie
26.04.06, Vienna, Austria

Kazuo Watanabe

2006 *Photoexcitation and photochemistry on metal nanoparticles*
Hokkaido University
26.05.2006, Sapporo, Japan

2007 *Photoexcitation and photochemistry on metal nanoparticles: Towards plasmonic photocatalysts*
The University of Tokyo
09.04.2007, Chiba, Japan

Photoexcitation and photochemistry on metal nanoparticles
Technische Universität München
21.06.2007, München, Germany

Phil Woodruff

2006 *Getting quantitative structure information on molecular adsorbate systems*
University of Liverpool
26.01.2006, Liverpool, UK

Quantitative surface structure determination of model adsorption systems: what do we learn?
Microscience 2006
27.06-29.06.2006 London, UK

Getting atomic-scale information from complex surfaces using synchrotron radiation
AVS 53rd International Symposium
12.11.-17.11.2006 San Francisco, USA

2007 *Photoelectron Diffraction: from phenomenological demonstration to practical tool*
15th International Conference on Vacuum
Ultraviolet Radiation Physics,
29.07.-03.08.2007, Berlin, Germany

Department of Molecular Physics — Director: Gerard Meijer

Group leaders:

Knut Asmis	(Habilitation)
Uwe Becker	(Habilitation)
Hendrick Bethlem (part-time; also at Laser Centre, Vrije Universiteit Amsterdam)	
Horst Conrad	(Habilitation)
André Fielicke	
Bretislav Friedrich	(Habilitation)
Gert von Helden	
Karsten Horn	(Habilitation)
Jochen Küpper	
Bas van de Meerakker	
Andreas Osterwalder	
Melanie Schnell (Liebig stipend)	
Wieland Schöllkopf	

Guest scientists, staying for at least six months:

Marcin Frankowski	until 01/31/2007
Daniel Goebbert	
Steven Hoekstra	
Thorsten Kampen	until 02/28/2006
Arantzazu Mascaraque	until 10/31/2006
Taisuke Ohta	

Scientists, staying for at least six months, paid from external funds:

Markus Braune	
John Doyle	AvH Awardee
Sanja Korica	
Irena Labazan (until 12/31/2006)	AvH Fellow
Jonathan Lyon	AvH Fellow
Adela Marian (Marie Curie Fellowship since Oct 2007)	AvH Fellow
Markus Metsälä	
Axel Reinköster	
Jens Viefhaus	
Bum Suk Zhao	AvH Fellow

Guest scientists (temporary):

Philip R. Bunker	The Steacie Institute, Ottawa, Canada
Boris Sartakov	RAS, Moscow, Russia
Alec Wodtke	UCSB, Santa Barbara, USA
Achim Peters	Humboldt University Berlin
Nicolas Polfer	
Joost Bakker	

Graduate students:	19	(4 IMPRS students)
Diploma students:	10	
Technicians:	13	
Trainees:	8	

Recent Developments in the Department of Molecular Physics

Director: Gerard Meijer

The research projects in the Department of Molecular Physics are described below in different sections. The first section deals with "Molecular physics studies with infrared radiation". These experiments are largely performed at the Free Electron Laser for Infrared eXperiments (FELIX) facility, at the FOM Institute for Plasmaphysics "Rijnhuizen" in Nieuwegein, The Netherlands. In these research projects, the IR optical properties and dynamics of molecules, clusters and cluster-adsorbate complexes are studied in the gas-phase. Highlights during the last two years have been the measurement of the stepwise solvation of an amino-acid and the appearance of the zwitterionic structure, the measurement of the far-infrared vibrational spectra for a variety of transition metal clusters, and the spectroscopic identification of unexpected structures for gas phase aluminum-oxide clusters. To be able to perform complementary studies to those at the FELIX facility, commercially available table-top IR laser systems with the associated molecular beam machines have been installed at the FHI. A detailed presentation of the progress in this research area is given on the posters MP 1 through MP 5.

A large experimental effort is devoted to research under the theme of "Cold Molecules". The aim of these research projects is to develop experimental schemes to achieve full control over both the internal and external degrees of freedom of neutral molecules, and to exploit these schemes in investigations of the properties of (samples of) cold molecules. In various experiments, time-varying electric fields are used to slow down and trap neutral polar molecules. Alternative methods to produce samples of cold molecules as well as a variety of schemes to achieve further cooling of trapped samples of molecules are actively being pursued. Highlights of this research have been the proof-of-principle demonstration of collision studies as a function of collision energy, the demonstration of a "molecular synchrotron", and, most recently, the demonstration of guiding and deceleration of molecules above a microstructured electrode array, *i.e.*, the controlled manipulation of "molecules on a chip". The progress in this research area, together with a description of future research plans, is presented on the posters MP 6 through MP 16.

Apart from these research activities that were introduced at the FHI with the appointment of Gerard Meijer, the ongoing research activity originating from the former Department of

Surface Science is described in the sections on “VUV photoionization studies” and on “Electronic structure of surfaces and interfaces”. This work is presented in more detail on the posters MP 17 through MP 20.

Molecular physics studies with infrared radiation

FELIX is ideally suited for a large variety of experiments in gas phase molecular physics. On the one hand this is due to the available wavelength tuning range, extending from 2.5 to 250 μm and thereby covering the full “molecular fingerprint” region, and the possibility of user-controlled wavelength scanning. The feature which really distinguishes FELIX from other FELs for applications in this research area is that it has the highest output energy per microsecond throughout the relevant wavelength range, which is the crucial factor when one wants to be able to resonantly pump as much energy as possible into an isolated molecule. The only other FEL facility world-wide, which can somewhat compete with FELIX in this respect, is the CLIO facility in Orsay, France.

In some experiments, FELIX is used to excite neutral or charged gas phase molecules or molecular complexes. The change in quantum state or the dissociation of complexes can be monitored as a function of excitation wavelength. These experiments require the absorption of only one or two photons and can then lead to, for example, the unravelling of the IR spectral properties of important gas phase molecules and ions or to an enhanced understanding of energy transfer in molecular systems. On the other hand, FELIX can also be used to resonantly pump several hundred photons into a single gas phase molecule. The internal energy can then become very high with temperatures reaching several thousand Kelvin. Most molecules will now dissociate by evaporating off small atomic or molecular fragments. Very tightly bound species, however, will undergo thermionic emission, *i.e.,* they choose to evaporate off an electron instead. The resulting charged species can be easily detected, and monitoring them as a function of wavelength yields information on the IR spectrum of the neutral molecule.

The light output of FELIX comes in macropulses of 5 μs duration at a repetition rate of 10 Hz. Each macropulse contains micropulses which are 300 fs to 5 ps long and spaced by 1 ns. The bandwidth is Fourier transform limited, implying a typical spectral resolution of several cm^{-1} at a central frequency of 1000 cm^{-1}. FELIX is therefore mainly restricted to studies in which a vibrational resolution suffices. The available energies of about 100 mJ per macropulse make a variety of multiple photon excitation and double-resonance detection schemes possible. In all our experiments we rely on mass-selective ion detection in the end, and the IR spectral information is obtained via the FELIX induced change in ion signal.

In February 2006, a fire destroyed the modulator room at the FELIX facility. This not only led to the destruction of essential, custom-made components for FELIX, but also left the whole laser system together with the experimental machines in the user stations covered under a thick layer of soot. Fortunately, several new components for a planned upgrade of FELIX had already arrived at the facility and could be used to get FELIX up and running again in August 2006, a true *tour-de-force* of the responsible technical personnel. Directly after the start-up, however, FELIX was not running as stably and reliably as it used to, and, in addition, it was only running for a reduced number of hours per week. Earlier this year, FELIX has come back to its original performance characteristics and to the standard mode of operation; overall, we probably lost almost a year of FELIX beam-time due to this accident.

The fire accident has also considerably delayed the installation and commissioning of FELICE, the Free Electron Laser for IntraCavity Experiments (FELICE). In August of this year, however, this new beam-line at the facility has produced its first laser light. We have designed and installed a molecular beam machine as an integral part of FELICE. In a first test experiment, we will use this machine to study the IR resonance enhanced multi photon ionization and fragmentation of C_{60}; with up to a few Joules of tuneable IR light circulating inside the cavity, extremely efficient pumping of vibrational energy – up to more than 100 eV – should be possible in this system. In future experiments, we will study vibrational modes with low IR absorption cross section, like the M-C stretch of metal carbonyls, and it will become possible to investigate coherent IR multi-photon absorption processes. Last but not least, the mechanical (optical dipole) force which can be exerted on gas phase molecules inside the FEL cavity when the laser wavelength is close to an optically allowed vibrational transition will be exploited to manipulate molecules.

To be able to perform preparatory and complementary experiments to those carried out at the FELIX facility, we have set up different table-top laser systems at the FHI. These systems are either based on a Nd:YAG pumped IR optical parametric oscillator and amplifier (IR OPO/OPA), or on a tuneable dye laser in combination with non-linear frequency mixing techniques. These systems can produce light pulses of ~ 5 ns, and are currently used to cover the region between 3 and 5 µm. Although the energy per pulse of these laser systems is only limited to a few mJ, their superior bandwidth down to 0.05 cm^{-1} compensates for this in many experiments. To extend the available wavelengths further into the infrared, we are also experimenting with the production of pulsed mid-IR laser radiation via stimulated backward Raman scattering in crystalline para-hydrogen at 4 K.

To become more independent from the FELIX facility in the future, and to open up the unique possibilities offered by the far-infrared pulsed radiation for the ongoing research in the other experimental departments of the FHI as well, we are planning to set up an IR-FEL with the associated user-stations on the FHI campus. A proposal detailing the scientific case and requesting the required investment and running budget is currently under preparation.

Infrared excitation of gas-phase molecules and clusters (Gert von Helden).

The main area of research remains the IR-spectroscopic investigation of the structure and dynamics of small molecules and molecular complexes as well as of molecules of biological relevance in the gas phase. The experiments on small molecules are performed using standard molecular beam methods. Molecules with a sufficient vapour pressure are directly seeded in the expansion gas. As a prototypical system for the study of dispersive intra- and intermolecular forces, we have produced isotopically mixed $(C_6H_6)(C_6D_6)$ benzene dimers in this way. We have studied the C-H stretch region for the two distinct conformational structures of this T-shaped species, and we have identified two-body collisions between the carrier gas atoms and the benzene dimers to be responsible for an efficient conversion between the conformational structures. Low vapour pressure and temperature sensitive compounds can be brought into the molecular beam using laser desorption. One of the species that has been extensively investigated during the last two years is the amino acid phenylalanine. This work is part of the Collaborative Research Center 450 "Analysis and control of ultrafast photoinduced reactions". In preparation for future experiments in which we aim to influence and control the abundance of different conformers of amino acids, we have measured the mid- and far-IR spectra of six distinct conformers of phenylalanine. From these spectra, their conformational structure has been unambiguously determined. Knowing the potential energy landscape, the observed conformer abundances can be understood and first experiments to influence the conformational distribution in the molecular beam have been performed. Laser desorption of a tryptophan-graphite powder mixture, and entrainment of the tryptophan in a moisturized argon expansion, has been used to unravel the structure of tryptophan complexed with a distinct number of water (from zero to six) or methanol (from zero to nine) molecules. This study has shown that there is a gradual transition from the gas phase neutral structure of this amino acid to the zwitterionic solvated structure, starting when five solvent molecules are attached.

Another possibility for bringing large molecules into the gas phase is electrospray ionization (ESI). In that technique, molecules are brought directly from solution into the gas phase as charged species with an internal energy distribution around room temperature. Those ions can be mass selected and investigated using IR spectroscopic techniques. The species that we have investigated thus far range from small peptides to an entire protein, containing more than 1500 atoms.

Since earlier this year, a new experimental setup has been under construction. The core of the instrument is a commercial tandem mass spectrometer equipped with an ESI source. The instrument is being modified to allow two types of novel experiments. In the first type of experiments, isomers of molecules having the same composition but different shapes, are separated exploiting the fact that they have different collision cross sections and diffusion constants. The molecules shape-selected in that manner can be then investigated using spectroscopic techniques. Examples range from linear and cyclic isomers of small carbon clusters to differently folded peptides and proteins. In the second type of experiments, charged species will be embedded in helium nanodroplets. There, molecules are cooled to equilibrium temperatures of about 0.4 K. In addition, the helium “solvent” atoms provide an ideal matrix for spectroscopic investigations, as their interactions with the solute are weak and their evaporation can be used as a probe for light absorption. Species of interest for such investigations are clusters and biomolecules as well as reactive species.

Spectroscopy and chemistry of metal clusters and cluster complexes (André Fielicke).

Getting insight into the structure of gas-phase transition metal clusters and analyzing their surface chemistry to obtain well defined *model* and *reference* systems for heterogeneous catalysts is the main goal of our research. Until now, most of our experiments have made use of FELIX as an intense and tuneable IR source. After the cancellation of the beam time period at FELIX in 2006, we took the opportunity to move the molecular beam setup, which is normally permanently installed at the FELIX facility, to the FHI for extensive maintenance and repair. The machine has been upgraded with a high-purity gas inlet system and a temperature controlled source extension which can be used to obtain thermo-chemical information.

A few years ago, we demonstrated far-IR multiple photon dissociation spectroscopy on the rare gas complexes of transition metal clusters as a new tool to measure their vibrational spectra and to get information on their structures via comparison with theory. By now, the far-IR vibrational spectra of clusters of all transition metals of group 5 of the periodic table (V, Nb, Ta) have been recorded in the size range of about 3 to 20 atoms. For several cluster sizes, the spectra of these various metal clusters are rather similar, pointing to structural similarities, as predicted by theory. During the last year we have focused on metals more relevant for catalysis, such as cobalt and rhodium. For these metals, the spectra for a particular size are rather different from those for V, Nb, and Ta. We hope to learn more about the structures of the Co and Rh clusters from ongoing DFT based theoretical investigations (*Karsten Reuter,* theory dept., FHI).

In a collaboration with *David M. Rayner* (NRC Canada) we have studied the interaction of CO with gold clusters in different charge states, *i.e.,* as anions, neutrals, or cations. The measurement of the internal CO stretching frequency ν(CO) for CO bound to clusters of different size and charge states provides a reference system for estimating charging effects in deposited clusters. In collaboration with *Frank de Groot* and *Bert Weckhuysen* (University of Utrecht, The Netherlands) we have studied the interaction of 3d transition metal clusters with hydrogen and CO to get insight into the fundamentals of Fischer-Tropsch synthesis and related hydrogenation reactions. Together with the group of *Peter Lievens* (University of Leuven, Belgium) we have investigated the influence of transition metal doping on the structures of silicon clusters.

During the last years, we have designed and constructed a new molecular beam setup for the study of transition metal clusters and their complexes in the gas phase. In this setup, information on the vibrational structure of the clusters can be obtained via mid-IR photodissociation spectroscopy using a para-hydrogen Raman shifter. Information on the electronic structure of the clusters can be obtained via photodetachment of size-selected anionic clusters. For this, a velocity map imaging photoelectron spectrometer is coupled to the mass spectrometer. Obviously, high resolution electronic spectroscopy also provides an alternative approach to obtain vibrational information. One specific future target is the study of the size and cluster-structure dependence of the activation of molecular nitrogen on ruthenium clusters.

Vibrational spectroscopy of gas phase ions (Knut Asmis).

During the last two years we have continued our research on the structure, stability and reactivity of mass-selected cluster ions in the gas phase using IR spectroscopy. A large effort has been put into the construction of a new tandem mass spectrometer with a 10 K ring electrode ion trap, which is now fully operational and used both at the FELIX facility and as part of the commercial table-top laser system at the FHI. Within the Collaborative Research Center 546 "Structure, dynamics and reactivity of transition metal oxide aggregates" we have focused on characterizing the structure-reactivity relationship of metal oxide clusters. We have performed the first measurement of the infrared spectra of mixed metal oxide clusters, we have identified unexpected structures in aluminum oxide clusters, and we have spectroscopically characterized the activation of methane by $V_4O_{10}^+$. Our research on ion solvation and strong hydrogen bonding is part of the Research Training Group 788 "Hydrogen bonding and hydrogen transfer". In particular, the studies on the stepwise hydration of the electron, $e^-\cdot(H_2O)_{15-50}$, and the sulfate dianion, $SO_4^{2-}\cdot(H_2O)_{3-24}$, allowed for an unprecedented insight into how water molecules arrange around these chemically and biologically relevant species at a molecular level. Using the new tandem mass spectrometer, we have been able to identify the infrared signature of the shared proton in the protonated ammonia dimer, a prototypical system for strong hydrogen bonding.

Cold molecules

Getting full control over both the internal and external degrees of freedom of neutral, gas phase molecules has been an important goal in molecular physics during the last decades. We have been exploring and exploiting the possibility of slowing down and trapping neutral molecules by the use of time-varying inhomogeneous electric fields. It is well known that beams of molecules with an electric dipole moment can be deflected and focused with static inhomogeneous electric fields. This approach has been extensively and successfully used in the field of atomic and molecular beams ever since the Stern and Rabi era. However, this manipulation exclusively involved the transverse motion of the molecules. It was only in

1999, that we experimentally demonstrated that appropriately designed arrays of electric fields in a so-called “Stark decelerator” can also be used to influence and control the longitudinal (forward) velocity of the molecules in a beam, *e.g.,,* to decelerate a beam of neutral polar molecules. Since then, the ability to produce focused packets of state-selected accelerated or decelerated molecules has made a whole variety of new experiments possible.

The operation principle of the Stark decelerator is based on the notion that a molecule in a quantum state in which the dipole moment is anti-parallel to an external electric field will feel a force in the direction of the low electric field. Therefore, if an electric field with a field gradient along the molecular beam axis is applied, a molecule in such a “low-field seeking” state will be decelerated on its way from a region of low electric field into a region of high electric field. If the electric field is switched off while the molecules are still in the region of high electric field, kinetic energy is permanently removed from the molecules. In the Stark decelerator, this process can be repeated until the average velocity is reduced to an arbitrarily low value. A properly timed switching of the electric fields ensures that a bunch of molecules can be kept together in the forward direction (“phase stability”) throughout this deceleration process. Transverse stability is achieved by using an electrode geometry that produces a minimum of the electric field on the molecular beam axis, thereby continuously focusing the beam. Although the forces that can thus be exerted on neutral particles are many orders of magnitude smaller than those exerted on charged particles, the various schemes allow to perform all the operations on neutral polar molecules that are successfully used throughout on charged particles.

In order to obtain a maximum initial density of state-selected molecules at a minimum initial temperature, we make use of the process of adiabatic cooling in a pulsed gas expansion. In a pulsed supersonic expansion, high number densities per quantum-state can be reached at a temperature of around 1 K. Typical velocities in a molecular beam are in the 250-3000 m/s range, thus preventing trapping of these dense low-temperature samples in the laboratory frame. The process in our Stark decelerator can be viewed as slicing a bunch of molecules with a very narrow velocity distribution (determined by the settings of the decelerator) out of the original beam, and decelerating (or accelerating) this to any desired velocity. In this process the phase-space density, defined as the number of molecules per unit volume and per unit momentum space, remains constant and one can thus efficiently transfer the high phase-space densities from the moving frame of the molecular beam to, for instance, the laboratory frame. More generally, the molecular beam exiting the Stark decelerator has a continuously tuneable laboratory velocity and a narrow velocity distribution and can be used for a large variety of experiments.

Since the first demonstration of the Stark decelerator, we have experimentally investigated its operation characteristics in great detail. We have demonstrated the possibility to guide molecules on overtones of the frequency with which the electric fields are switched, and we have studied the coupling of the transverse motion to the longitudinal motion in the decelerator. Together, this has enabled us to reach a complete, experimentally verified description of the complex three-dimensional motion of the molecules through the decelerator. The decelerated beams of molecules have subsequently been loaded into a variety of traps. In these traps, electric fields are used to keep the molecules confined in a region of space where they can be studied in complete isolation from the (hot) environment. In our first experiments of this kind, we demonstrated trapping of ammonia molecules in a quadrupole electrostatic trap, but we have demonstrated trapping in more versatile geometries as well. Apart from ammonia, we have also demonstrated the deceleration and trapping of OH radicals. The long interaction time afforded by the trap has been exploited to measure the infrared radiative lifetime of vibrationally excited OH radicals, for instance.

For many applications, deceleration and trapping of polar molecules in “high-field seeking” states is required, if only because the lowest energy level of any molecule is high-field seeking. Manipulation of molecules in high-field seeking states is generally required if one aims to get full control over heavy diatomic molecules or over large (bio-) molecules. It might appear straightforward to apply the electric field deceleration method to molecules in high-field seeking states by simply letting the molecules fly out of, instead of into, regions of a high electric field. For the motion of the molecules in the forward direction, this is indeed true. However, since Maxwell's equations do not allow for a maximum of the electric field in free space, *e.g.,* on the molecular beam axis, transverse stability cannot be maintained easily; molecules in high-field seeking states have the tendency to crash into the electrodes, where the electric fields are the highest. The same situation is encountered in charged particle accelerators where this problem has been resolved by applying the alternate gradient (AG) focusing method. We have shown that this principle can be applied to polar molecules when using electrostatic dipole lenses, and AG deceleration of molecules in high-field seeking states has been demonstrated. To trap molecules in high-field seeking states we have developed various AC electric traps.

Deceleration and trapping of polar molecules (Bas van de Meerakker).

A few years ago, we developed a new generation Stark deceleration and trapping machine, in which we have been able to decelerate ground-state OH radicals and to confine them in an electrostatic quadrupole trap. During the last two years, we have significantly improved the overall performance of this machine and performed a number of experiments using the trapped molecules. In particular, we have implemented a more efficient scheme to load the molecules into the trap, and we have studied the trap loss resulting from optical pumping due to blackbody radiation.

The deceleration and trapping machine has been used to decelerate and trap other molecular species as well. In a proof-of-principle experiment, we have produced and decelerated a beam of metastable NH ($a^1\Delta$) radicals. This is important, as metastable NH offers good prospects for trap reloading schemes using magnetic traps. We also demonstrated the first electrostatic trapping of CO molecules in the electronically metastable $a^3\Pi$ state, and accurately determined the quantum-state specific radiative lifetimes in this state.

We are currently developing a magnetic trap for neutral molecules, which can be mounted behind the Stark decelerator. In this trap, the OH radicals can be magnetically confined both in the upper and lower Λ-doublet component of the $^2\Pi_{3/2}$, J=3/2 ground state, which offers interesting possibilities for the observation of collision processes between the trapped molecules. This magnetic trap will also be used to confine and accumulate NH ($a^1\Delta$) radicals; the production of beams of NH ($a^1\Delta$) is currently being optimized using different precursors like HN_3 and HNCO.

The beams exiting the Stark decelerator can be transversely and longitudinally focused, both in velocity and in real space, giving full six-dimensional control over the motion of the molecules. These beams thereby offer interesting advantages for collision studies. We have therefore started a new research line to exploit Stark decelerated molecular beams in crossed beam scattering studies. To test the feasibility of this approach we have performed a proof-of-principle experiment, scattering a decelerated beam of OH radicals with a beam of Xe atoms, and studying the opening up of inelastic scattering channels. At present, we are constructing a new crossed molecular beam machine consisting of two Stark decelerators, oriented orthogonally to get a 90 degrees crossing angle of the molecular beams. With this machine we will be able to study molecule-molecule collisions at a collision energy between 1 cm^{-1} and 500 cm^{-1} with an overall energy resolution of about 1 cm^{-1}. This project is part of the ESF collaborative project (EuroQUAM) on “Collisions of cold polar molecules” (2007-2010).

The molecular synchrotron (Rick Bethlem).

A few years ago, we demonstrated an electrostatic storage ring for neutral polar molecules. In its simplest form, a storage ring is a trap in which the molecules – rather than having a minimum potential energy at a single location in space – have a minimum potential energy on a circle. The advantage of a storage ring over a trap is that packets of molecules with a non-zero mean velocity can be confined. While circling the ring, these molecules can be made to interact repeatedly, at well-defined times and at distinct positions with electromagnetic fields and/or other particles. To fully exploit the possibilities offered by a ring structure, it is imperative that the molecules remain in a bunch as they revolve around the ring. This ensures a high density of stored molecules and, moreover, makes it possible to inject multiple – either co-linear or counter propagating – packets into the ring without affecting the packet(s) already stored. We have recently demonstrated such a molecular synchrotron.

As discussed above, molecule-molecule collisions can be studied in a crossed molecular beam setup. Alternatively, one may perform these studies in a ring. Whereas in the crossed beam geometry the particles encounter each other only once, in a ring they can be made to meet each other many times. A new synchrotron consisting of 40 segments, to be used as future low-energy collider, is currently being constructed.

Micro-structured devices to manipulate polar molecules (Horst Conrad).

In this project we aim to manipulate and control polar molecules using electric field gradients produced by micro-structured electrodes. The ultimate goal is to produce a variety of molecule manipulation tools, including lenses, mirrors, guides, decelerators, storage rings and traps, all integrated on a chip.

By miniaturizing electrode geometries high electric fields, and even higher electric field gradients, can be produced using modest voltages. A few years ago, we demonstrated that the electric field gradients generated above a planar array of 20 µm wide gold electrodes, spaced 20 µm apart and with a voltage difference of a few hundred Volt between adjacent electrodes, can be used to retroreflect a beam of polar molecules, *i.e.,* we demonstrated a micro-structured mirror for polar molecules.

Since then, we have worked on the realization of a micro-structured electrode array to guide and to decelerate polar molecules. Rather than working with switched fields (as in the normal decelerators), we apply sinusoidal waveforms to the electrodes such as to generate a travelling potential well above the micro-structured array. As it is difficult to produce and to sensitively detect the molecules closely above the electrode array, we follow the experimental approach of selecting a small fraction of a conventional pulsed molecular beam, and send these molecules along the electrode array. There, their velocity distribution is changed, and we subsequently detect the molecules when they come off the electrode array again. A new, very compact, molecular beam machine has been set up for these experiments. This summer, we have successfully demonstrated the guiding and deceleration of metastable CO molecules above a micro-structured electrode array in this machine. This work will become part of an EU-funded project (STREP) on “Nano-optics for molecules on chips” (2008-2011).

Diffraction of polar molecules from an electrostatic grating (Wieland Schöllkopf).

In this new project, we aim to demonstrate molecule diffraction from electrostatic gratings. This project has become possible with the transfer of a dedicated molecular beam diffraction machine from the MPI in Göttingen (Prof. J. Peter Toennies) to the FHI. In this experiment, a beam of CH_3F seeded in argon impinges on a reflection grating under grazing incidence. The reflection grating is formed by the electrostatic field above the surface of a micro-structured array of electrodes. As described above, this field acts as a mirror for polar molecules in low-field seeking states, but, due to the field corrugation, also as a diffraction grating. Reflection diffraction gratings for polar molecules have potential application as coherent beam splitters in molecular matter-wave interferometers.

Deceleration and trapping of large (bio-) molecules (Jochen Küpper).

During the last two years, we have performed extensive measurements and modeling to understand and optimize the operation characteristics of our alternate gradient (AG) decelerator molecular beam machine. With this machine, presently consisting of 27 electric field stages, one can decelerate molecules both in low-field seeking and in high-field seeking states. Moreover, the AG decelerator design allows for independent control over the transverse focusing and the deceleration properties. In all experiments we have detected the molecules at the exit of the decelerator via laser induced fluorescence, using a frequency-doubled narrow-linewidth (1 MHz) continuous wave dye-laser. For good long-term frequency-stability this laser is locked to a frequency-stabilized helium-neon laser. We have demonstrated the deceleration of ground-state OH radicals, both in low-field seeking and in high-field seeking states. In addition, we have decelerated different quantum states of benzonitrile. In the near future, we will extend the experimental setup to 54, and eventually 81, deceleration stages, to enable deceleration to low velocities. We plan to perform these experiments initially on OH and benzonitrile and to proceed to larger molecules, like tryptophan and small model peptides, thereafter.

We have performed feedback-control experiments using evolutionary strategies for the optimization of various decelerator beamlines in the department. Initially, we have optimized the deceleration and trapping of OH radicals. Since then, we have implemented the feedback-control optimization in a graphical user-interface within the data-acquisition software (KouDA) that is used in the department, and the automated optimization of experimental parameters has been used in a variety of experiments.

In a separate experiment, a one meter long alternate gradient quadrupole focuser has been set up. With this device individual conformers of (bio-) molecules can be selected and spatially separated, exploiting the fact that these conformers generally have different electric dipole moments (μ). The different transverse forces the conformers experience while moving through the quadrupole enables m/μ-selection, similar to the m/q-selection of charged particles in a quadrupole mass filter. We have demonstrated this by the spatial separation of the cis- and trans-conformers of 3-aminophenol in a molecular beam. We will continue these works towards larger (bio-) molecules, which exist in multiple distinct conformers in supersonic jets. In combination with a laser-desorption source even considerably larger (bio-) molecules will be amenable for conformer separation with this device. The conformer selected molecules exiting the guide can, for instance, be used for laser alignment or brute-force orientation experiments.

Trapping molecules in high-field seeking states (Melanie Schnell).

For many applications of cold polar molecules, trapping of molecules in high-field seeking states is required. We have experimentally demonstrated different types of AC electric traps, and we have used these to trap ground-state ammonia molecules in high-field seeking states. We have experimentally studied the stability of the AC electric trap as a function of switching frequency and applied voltages, and we have characterized the spatial distribution and the temperature of the trapped cloud of molecules. As a side project, we demonstrated that the electrode geometry used for AC trapping can be used to create a highly versatile DC electric trap for molecules in low-field seeking states as well; we generated and characterized a rather deep quadrupole, a hexapole, a double-well and a donut-shaped trap. We currently pursue this direction of our research further by developing and implementing a DC electric trap with a non-zero trap minimum, *e.g.,* the electric equivalent of the magnetic Ioffe-Pritchard trap.

In a new project, we use appropriately timed pulses of near-resonant standing microwave radiation in a Fabry-Pérot type resonator to guide, decelerate, and, eventually, trap polar molecules, both in high-field seeking and in low-field seeking states. This approach offers the advantage that the force exerted on the molecules can change sign, depending on the detuning of the microwave frequency from the molecular resonance. Furthermore, the microwave trap naturally offers a very open geometry which is beneficial for future studies with trapped molecules.

Interactions of molecules with fields (Bretislav Friedrich).

During the last two years the analytic “wave model” of the longitudinal motion of molecules in a Stark decelerator has been wrapped up, and it has been verified that this description is complete. In a new project, effects are studied that arise from the combined action of static electric and non-resonant radiative fields on symmetric top molecules. Often, a very weak static electric field can convert second-order alignment by a laser into a strong first-order orientation. This enhances the ability to manipulate molecular trajectories as well as to decongest molecular spectra.

In future studies, we plan to investigate vector correlations in slow collisions of polar molecules. In addition to the differential cross sections, many other directional or vector properties of collisions are now becoming accessible in experiments with Stark-decelerated molecular beams. These vector properties offer much information not provided by energetic or other scalar properties. In principle, a vector correlation offers a means to undo the “dart-board” averaging over the random azimuthal orientations of initial impact parameters. Thus by observing one or two “extra angles” in collision experiments, a further level of molecular resolution awaits collision dynamics. We plan to develop models that will capture the collisional behaviour of polar molecules at this new level of resolution.

Sympathetic cooling of molecules (Wieland Schöllkopf).

In this project we aim to cool a cloud of trapped polar molecules via elastic collisions with a magnetically trapped, and evaporatively cooled, cloud of Rb atoms, *i.e.,* we aim to use the ultracold atoms as a refrigerant for the cold molecules. In our approach, atoms and molecules are first cooled and trapped separately and then the cold atom cloud is moved to overlay with the molecular cloud. Over the last two years we have completed the ultracold atom apparatus. It includes a thermal Rb atomic beam source, a Zeeman slower, a magneto-optical trap, a magnetic trap, and an AC electric trap. In the magnetic trap we routinely confine about $5x10^8$ Rb atoms at temperatures in the range of 100 μK. The atoms are further cooled by forced evaporation using RF sweeps. The magnetic trap is mounted on a precision mechanical translation stage that allows moving the Rb cloud over 40 cm in a few seconds into another UHV chamber, where the AC electric trap – or any other molecule trap – is located. In first experiments, we used this set-up to demonstrate AC trapping of the Rb atoms instead; absorption imaging of the cloud of trapped atoms at different phases of the AC cycle allowed for a direct visualization of the dynamics of the confinement. The next step in this project is to set up a molecular beam machine, to first study (in-)elastic collisions between the magnetically trapped atoms with a (decelerated) beam of state-selected molecules, and, eventually, to study the interactions in overlaying trapped samples of molecules and Rb atoms. This project is part of the ESF collaborative project (EuroQUAM) on “Collisions of cold polar molecules” (2007-2010).

Buffer-gas cooling and magnetic trapping of molecules (Achim Peters).

Loading of molecules into a cryogenic He-filled cell and subsequent magnetic trapping of the thermalized molecules is another proven method to produce large samples of cold trapped molecules. In collaboration with *Achim Peters*, junior professor at the Humboldt University in Berlin, we have actively pursued this approach during the last few years. The special allure of this method (originally developed by John Doyle of Harvard University, who in 2006 spent several months with us as an Alexander von Humboldt awardee) is that the cooling process is very generally applicable. The combination with magnetic trapping should in principle also work for a wide variety of paramagnetic particles, atoms as well as molecules. However, we wanted to address in this project whether this general applicability actually holds for molecules given the constraints of current magnet technology and detrimental molecular properties, such as spin-flip (inelastic) collisions.

The experimental set-up at the FHI uses a superconducting quadrupole magnet in combination with a ^{3}He-^{4}He dilution refrigerator. Atoms and molecules are introduced into the buffer gas cell via laser ablation of a solid precursor material. We have verified the performance of the system – thus far the only one operating outside Harvard University – by trapping large samples of atomic chromium with densities exceeding 10^{12} atoms per cm^3 at a temperature of 350 mK and trap lifetimes > 20 seconds.

With our current magnet, we only get a sufficient trap depth at ^{3}He buffer gas temperatures for species with relatively large magnetic moments ($\geq 4\mu_B$). We identified CrH and MnH as the most promising molecules for trapping in our current setup; in collaboration with *Tim Steimle* (Arizona State University) we determined the relevant spectroscopic properties of these molecules in the presence of magnetic fields. We succeeded in “trapping” both molecules with 1/e lifetimes in the 100-200 ms range, limited by inelastic collisions. Current experiments aim at the precise determination of the relevant collision cross sections.

Combined with already demonstrated methods for rapid extraction of the buffer gas, the observed trapping times should allow for the preparation of thermally isolated samples with then much longer lifetimes. However, seen together with the latest results of the Doyle group achieving very similar 200 ms trapping lifetimes for NH molecules, we have come to the conclusion that the general applicability of the combination of buffer gas cooling of molecules with magnetic trapping is substantially curtailed at the moment. For most of our future applications, the Stark deceleration method is better suited. We therefore intend to conclude the buffer-gas cooling project after the current PhD student is finished.

Cold neutral molecules via photodetachment of cold anions (Andreas Osterwalder).

The goal of this project is to implement an alternative to the production of cold neutral molecules that shall allow the deceleration also of large molecules with direct chemical relevance. The project has been started two years ago, with a first phase of extensive simulations to find the optimal electrode geometry for this experiment. Following the design and assembly stages of the new apparatus we performed detailed studies of our molecular beam source and ion generation, with a special focus on the beam velocity and velocity spread, as well as on clustering processes following the ionization of our precursor molecules. As a part of these investigations we determined accurate values for the threshold to photodetachment as well as for absolute photodetachment cross sections for the atomic iodide anion, our test system for all of the following studies.

The next phase then consisted in first attempts to actually decelerate the negative ions and to identify and eliminate all possible sources of perturbing stray electric fields. Due to the high sensitivity of ions to electric fields – a fact that also represents a main advantage of this technique – very good control of potential perturbations is essential. We now are confident that within the constraints of passive electric field elimination everything possible has been done. Still existing discrepancies between trajectory simulations and real measurements can thus be attributed to properties of the ion cloud itself such as space charge effects or shielding of the weak deceleration fields by the plasma generated in the supersonic expansion. Our current focus is on the understanding and elimination of these effects that prevent us from actually producing cold neutrals. Possibilities for more selective ion sources are considered as well as filters to obtain maximum control on the composition of the ion cloud entering the deceleration region, while not reducing the quality of the beam expansion.

VUV photoionization studies (Uwe Becker)

We have continued our research programme on the study of the coherence properties and localization in inversion-symmetric homonuclear diatomic molecules. In addition, a new programme on multi-photon excitation processes in free atoms, molecules and clusters has been set up at the Free Electron Laser FLASH at DESY, Hamburg.

In the first programme, we have concentrated on two topics: (i) the oscillations in the photoelectron diffraction spectra and in the partial cross-sections of homonuclear diatomic molecules, and (ii) the breakdown of symmetric electron emission patterns as the most dramatic signature of electron localization at one of the two atomic sites. In (i), we succeeded to measure the frequency of the oscillations, which represent interference patterns in momentum space. For this purpose, we resolved the core electron emission of the *g* and *u* states in N_2 over a wide range of photon energies. As predicted by Cohen and Fano, the oscillation frequency is proportional to the bond lengths, which could also be proven for the electron emission in H_2. Together with our former results from the C_{60} and C_{70} fullerenes, we now have clear evidence for Cohen-Fano oscillations with frequencies covering an order of magnitude of bond lengths or diameters. In this sense we have verified the general validity of the Cohen-Fano interference model. In addition, we observed the localization of intra-molecular scattered electrons. Its signature is the appearance of EXAFS-like oscillations with a frequency proportional to twice the bond length for electron emission along the molecular axis. These localized self-interference patterns arise due to a momentum change upon scattering larger than the reciprocal bond length and hence localize the scattered electron on one atomic site. This dynamical localization is, however, indirectly phase-coupled via the oscillation of the non-scattered electron, giving rise to a symmetric electron angular distribution in the molecular frame. Hence, both the coherent Cohen-Fano and the localized EXAFS oscillations are phase-locked with respect to each other, and one may consider EXAFS as a beat on the Cohen-Fano oscillation at twice the frequency. In (ii), in order to project the inherent asymmetry of the localization process onto a measurable quantity, asymmetric fragmentation channels or two-electron ejection (as is the case in subsequent Auger decay) have to be employed as forward/backward projection markers. For N_2 these are the fragmentation channels with non-identical fragments: $N + N^{++}$ or $N^+ + N^{++}$. The fragmentation channels of dissociative photoionization into satellite states show asymmetries in the emission probability of the electron, which travels either along with or away from the moving N^{++} fragment. The N_2:(N(1s)) photoelectron main line does not exhibit such asymmetries because its final state is the stable molecular ion N_2^+, which dissociates only due to subsequent Auger decay. For H_2 and O_2 the dissociative ionization shows the asymmetry in the electron emission in the autoionization region much more pronounced. We have demonstrated symmetry breakdown of various strengths, reaching from a few percent in N_2 to more than 60 percent in O_2. Our results are corroborated by corresponding measurements using the COLTRIMS technique. These results are important for the understanding of coherence and localization in inversion-symmetric molecular systems, and may contribute to the ongoing discussion about the individual system *versus* ensemble concept of the quantum world.

The programme on multi-photon excitation processes has been started with first experiments at FLASH, where we have ionized several atoms and molecules by simultaneous or sequential multi-photon excitation. Sequential ionization came up with a surprise: although the intensity dependencies and angular distributions clearly proved the multi-photon character of the observed process, the strength of this process, which results in photoelectron spectra of ionic targets, is similar to the main line intensity obtained from the neutral target. Given the difficulties, photoelectron spectroscopy of ionic targets has faced so far, this opens up the new field of angle and spin-resolved photoelectron spectroscopy of ions.

Electronic structure of surfaces and interfaces (Karsten Horn)

In late 2005, the solid state physics community was surprised to learn that a material as simple and basic as single layer graphene, the building block of graphite and carbon nanotubes, possesses transport properties that set it apart from all other solids. These include an unusual quantum Hall effect, ballistic transport at room temperature, an ambipolar field effect, to name a few. These properties arise from the massless “Dirac Fermion” character of its charge carriers at the Fermi level. Indeed, it has been argued that graphene can be seen as a model system for quantum electrodynamics experiments in solid state physics, and it certainly provides the clearest example of a true 2D system. We were in the fortunate position to be able to study the electronic structure of single and multilayer films of graphene from the outset, through a collaboration with *Thomas Seyller* (University of Erlangen) and *Eli Rotenberg* (ALS, Berkeley, USA). The combination of a valid layer preparation recipe, precise control of the graphene/silicon carbide interface, and high resolution band mapping were the important ingredients in this cooperation. In a series of papers we have identified the linear dispersion of bands near E_F, and the influence of doping on band shape and the emergence of gaps in the bilayer. Moreover, we were able to follow the evolution from a purely 2D to 3D behaviour as a function of layer thickness. Because of its structural simplicity, graphene is a system in which electron correlation effects can be studied very precisely, and different contributions such as electron-phonon, electron-electron and electron-plasmon coupling can be distinguished. Other experiments (STM, LEEM) have addressed issues such as growth morphology and optimization. We can anticipate that this topic, which has caused a veritable frenzy of activities in the community, will continue to be at the centre of activities in our group.

Work on chiral structures and molecular switching in molecular systems has continued, with circular dichroism, NEXAFS and STM studies on model systems such as stilbene. Using a stilbene derivative, we find that the adsorption process induces a handedness which leads to a series of long-range ordered structures which themselves are chiral. Both racemic and enantiomerically pure structures exist, and we can explain the formation of these, and their stabilities, on the basis of a few “building block” adsorption sites and general thermodynamic principles. Conformational identification was achieved using NEXAFS, both in the gas phase and the adsorbed state. These data provided the basis for an identification of “molecular switching”, *i.e.,* a conversion between cis- and trans-stilbene in the adsorbed state, induced by UV-light.

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Asmis, K.: Infrared Photodissociation Spectroscopy of Mass-Selected Cluster Ions in the Gas Phase. Freie Universität Berlin, 2006.

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Dil, J.H.: Electron confinement in thin metal films: Structure, Morphology and Interactions. Freie Universität Berlin, 2006.

Korica, S.: Photoionization and photofragmentation of fullerenes. Technische Universität Berlin, 2006.

van de Meerakker, S.Y.T.: Deceleration and electrostatic trapping of OH radicals. Radboud Universiteit Nijmegen, The Netherlands, 2006.

van Veldhoven, J.: AC trapping and high-resolution spectroscopy of ammonia molecules. Radboud Universiteit Nijmegen, The Netherlands, 2006.

Master Theses

Blitstein, P.: Construction and characterization of a para-hydrogen crystal Raman shifter for the mid-IR use. Freie Universität Berlin, 2006.

Gubbels, K.: Dynamics of Stark acceleration/deceleration: Molecules riding waves. Radboud University Nijmegen, The Netherlands, 2006.

Lützow, P.: Eine lineare AC-Falle für polare Moleküle im Grundzustand**.** Freie Universität Berlin, 2006.

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Master Thesis

Kupser, P.: Konstruktion einer Elektrosprayquelle zur Erzeugung solvatisierter Biomoleküle - Nachweis von Sekundärstrukturen in der Gasphase. Freie Universität Berlin, 2007.

Invited Talks of members of the Department of Molecular Physics

Knut Asmis

Mar 2006 American Physical Society Meeting, Baltimore, MD, USA:
Infrared Spectroscopy of Gas Phase Transition Metal Oxide Cluster Ions and
Probing the Stepwise Solvation of the Sulfate Dianion: Gas Phase Infrared Spectroscopy of $SO_4^{2-}\cdot(H_2O)_n$ *Clusters (n = 3-14, 18, 24)*

June 2006 Ion Trap Symposium of the DFG Forschergruppe Laborastrophysik, Chemnitz, Germany:
Structure and Stability of Stored Cluster Ions

Oct 2006 Findungssymposium “Free Electron Lasers: Brilliant Light Sources for new Science” (W3 Professur in Physikalischer Chemie), DESY, MPG und Universität Hamburg, Germany:
Probing the Structure of and Dynamics in Gas Phase Clusters: Experiments with Intense Radiation Ranging from the IR to the VUV and Beyond

Jan 2007 Findungssymposium (W3 Nachfolge Brede), Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany:
Cluster in der Gasphase - Struktur, Reaktivität und Dynamik

Mar 2007 hot topic talk, Symposium on Size Selected Clusters (S3C), Brand, Austria:
Probing Stepwise Hydration by Gas Phase Vibrational Spectroscopy

Apr 2007 CERC3 Young Chemists' Workshop "Time-resolved methods for studies on chemical reactions", Göttingen, Germany:
Time- and Frequency-Resolved Gas Phase Spectroscopy of Mass-selected Clusters

June 2007 Institute Seminar, Department of Physics and Astronomy, Katholieke Universiteit Leuven, Belgium:
Transition Metal Oxide Clusters

Aug 2007 Fall Meeting of the American Chemical Society, Boston, MA, USA:
Hydration: From Clusters to Aqueous Solutions

Oct 2007 International Symposium of the DFG Collaborative Research Centers 546 and 558 “From Clusters to Catalysts - Transition Metals and Transition Metal Oxides”, Erkner, Germany:
Gas Phase Infrared Spectroscopy of Vanadium Oxide Cluster Ions

Joost Bakker

Nov 2005	Arizona State University, Department of Chemistry, Tempe, AZ, USA: *Buffer-gas loading and magnetic trapping of chromium atoms and the prospects for trapping CrH molecules*
Mar 2006	Laboratoire de Photophysique Moléculaire, Orsay, France: *Structural identification of gas-phase biomolecules using infrared spectroscopy*

Uwe Becker

Oct 2005	Workshop des Arbeitskreises Philosophie in der DPG, Universität Dortmund, Germany: *Partielle Kohärenz bei molekularen Doppelspalt-Experimenten*
Nov 2005	US-Africa Advanced Studies Institute on Photon Interactions with atoms and molecules, Durban, South Africa: *Coherence and localization in core electron photoemission from diatomic homonuclear molecules*
Nov 2005	VUV-FEL User Workshop, DESY, Hamburg, Germany: *Photoelectron and photoion spectroscopy of rare gases and fullerenes by FEL radiation: First results*
Jan 2006	Gordon Research Conference on Photoions, Photoionization and Photodetachment, Buellton, CA, USA: *Coherence and decoherence in molecular double-slit experiments*
Mar 2006	ESRF Colloquium, Grenoble, France: *Coherence and decoherence in molecular double-slit experiments using synchrotron X-rays*
Apr 2006	Ultra-fast Dynamic Imaging Workshop, Imperial College, London, UK: *Time-resolved VUV and soft X-ray photoelectron spectroscopy today and tomorrow*
June 2006	PETRA III XUV Beamline User Workshop, DESY-HASYLAB, Hamburg, Germany: *User demands – update of the science case. Gas phase studies*
June 2006	International Conference on many-particle spectroscopy of atoms, molecules, clusters and surfaces, Rome, Italy: *Coherence transfer and decoherence in photon induced molecular ionization and fragmentation*

July 2006	FEL-Gasphasen Workshop, Photon Science Facility, DESY, Hamburg, Germany: *Time-resolved VUV and soft X-ray photoelectron spectroscopy today and tomorrow*
Aug 2006	International Conference on Electronic Spectroscopy and Structure, Iguassu Falls, Brazil: *Coherence and decoherence in molecular photoelectron double-slit experiments*
Sept 2006	International Wilhelm and Else Heraeus Summerschool on few-body dynamics in atomic and molecular systems, Wittenberg, Germany: *Single photon interaction with atoms and molecules*
Sept 2006	FASM 19th Annual User Meeting: A New Beginning, Lund, Sweden: *Coherence and decoherence in molecular photoelectron double-slit experiments*
Oct 2006	Colloque de Laboratoire de Chimie Physique – Materie et Rayonnement, Paris, France: *Transfer and revival of quantum coherence in molecular photoelectron double-slit experiments*
Jan 2007	XVI National Conference on Atomic and Molecular Physics, Mumbai, India: *Quantum coherence and localization in molecular core electron double-slit experiments*
May 2007	ECAMP IX Satellite Symposium on multiphoton multiple ionisation of atoms, molecules and clusters, Heraklion, Greece: *Photoelectron and ion spectroscopy of atoms, molecules and fullerenes after multi-photon ionization by FEL radiation*
June 2007	Seminar der Experimentalphysik I, Universität Würzburg, Germany: *Mehrphotonen-Ionisation freier Atome, Moleküle und Fullerene mittels Freier-Elektronen-Laser-Strahlung von FLASH*
July 2007	Atomphysikseminar der GSI Darmstadt, Germany: *Mehrphotonen-Ionisation freier Atome, Moleküle und Fullerene mittels Freier-Elektronen-Laser-Strahlung von FLASH*
Sept 2007	QuAMP 2007, University College London, UK: *Spectroscopy and dynamics with synchrotron, FEL, THz and IR sources*

Hendrick Bethlem

Oct 2005	Chemistry Colloquium, Physical and Theoretical Chemistry Lab, Oxford, UK: *Trapping polar molecules*
Jan 2006	Bijeenkomst studiegroep Spectroscopie en Theorie, Lunteren, The Netherlands: *Toward a Molecular Fountain Clock*

Feb 2006 Training School of the EU network 'European Research and Training Netwerk on Cold Molecules (COMOL)'. Les Houches, France:
Manipulating polar molecules using inhomogeneous electric fields

June 2006 Physics Colloquium, Yale, New Haven, CT, USA:
Deceleration and trapping of heavy molecules

July 2006 Physics Colloquium, JILA, Boulder, CO, USA:
Cold molecules via Stark deceleration

July 2007 388. Wilhelm und Else Heraeus-Seminar “Atomic clocks and fundamental constants – ACFC 2007”, Bad Honnef, Germany:
Manipulating polar molecules using electric fields; A molecular fountain

Markus Braune

Apr 2006 VUV-FEL Experiments Selection Workshop, Hamburg, Germany:
Multiphoton ionization and excitation of atoms and fullerenes

Aug 2007 International Symposium on (e,2e), Double Photoionization and Related Topics, Königstein, Germany:
Photoelectron Spectroscopy of rare gas atoms following multi-photon ionization by FEL radiation

Horst Conrad

May 2007 Free University of Berlin:
Manipulation of polar molecules by means of electric fields

André Fielicke

Dec 2005 Annual conference of the Spectroscopy and Dynamics Interest Group of the RSC Faraday Division, Durham, UK:
Probing the structures of pure metal clusters and metal cluster complexes

Sept 2006 CECAM workshop on Catalysis from First Principles, Lyon, France:
Probing the structures of pure metal clusters and metal cluster complexes

Jan 2007 FEL Workshop "Horizons in Vibrational Spectroscopy with Free Electron Lasers", Schloß Ringberg am Tegernsee, Germany:
Probing the structures of pure metal clusters and metal cluster complexes

July 2007 Seminar Physikalische Chemie, Universität Stuttgart, Germany:
Structure and surface chemistry of metal clusters

Bretislav Friedrich

Nov 2005	Colloquium, Technische Universität Braunschweig, Germany: *From the new world of cold molecules*
Dec 2005	Colloquium, Heriot-Watt University, Edinburgh, UK: *From the new world of cold molecules*
Mar 2006	Molecular Physics Seminar, Fritz-Haber-Institut, Berlin, Germany: *Aspects of the behavior of molecules in strong fields*
July 2006	Colloquium, Universität Potsdam, Germany: *Why are cold molecules so hot?*
Sept 2006	Colloquium, Universität Köln, Germany: *Why are cold molecules so hot?*
Sept 2006	Seminar, Universität Stuttgart, Germany: *Thermodynamic properties of molecules in electromagnetic fields*
Mar 2007	Colloquium, Technical University, Prague, Czechia: *Why are cold molecules so hot?*
Mar 2007	Colloquium, Heyrovsky Institute, Prague, Czechia: *Orientation of molecules by electromagnetic fields and its applications*
July 2007	Conference on the History of Quantum Mechanics, Max-Planck-Institut für Wissenschaftsgeschichte, Berlin, Germany: *How a bad cigar assisted at the birth of quantum mechanics*

Gert von Helden

Dez 2005	Colloquium, Technical University Berlin, Germany: *Infrared spectroscopy of neutral and ionic gas-phase clusters and biomolecules*
Dez 2005	Colloquium, University of Marburg, Germany: *Infrared spectroscopy of gas-phase peptides and proteins*
Jan 2006	Colloquium, University of Frankfurt, Germany: *Infrared spectroscopy of gas-phase peptides and proteins*
May 2006	Workshop "Carbon in Space", Menaggio, Italy: *Laboratory IR experiments on gas-phase species*
June 2006	ESF Conference “Biomolecules”, Obergurgl, Austria: *Probing gas-phase biomolecules by IR spectroscopy*

Feb 2007 FEL Workshop "Horizons in Vibrational Spectroscopy with Free Electron Lasers", Schloß Ringberg am Tegernsee, Germany:
Infrared spectroscopy of gas-phase peptides and proteins

Feb 2007 Colloquium, University of Toulouse, France:
Sensitive infrared spectroscopy of neutral and charged gas-phase molecules

Karsten Horn

Apr 2006 Colloquium, Singapore Synchrotron Light Source, National University of Singapore:
Electronic structure of strange solids

Sept 2006 International Workshop on ‘Energy Dissipation at Surfaces’ in Wesseling, Germany:
Electronic structure of low dimensional solids - what can we learn from photoelectron spectroscopy?

Oct 2006 Interdisciplinary Nanoscience Center (iNANO), University of Aarhus, Denmark:
The electronic structure of mono- and multilayer graphene

Feb 2007 DFG-Rundgespräch, Bad Honnef, Germany:
Elektronische Struktur von Graphen: Bandstruktur und Dirac Fermions

June 2007 Lecture, Mid-Term Meeting des European Network of Excellence „Complex Metallic Alloys“, Santorini, Greece:
Electronic structure of β-Al_3Mg_2

June 2007 Van-der-Waals-Zeeman Kolloquium of the Universiteit Amsterdam, The Netherlands:
Graphene: electronic structure of an intruiging material

June 2007 Kolloquium der Fakultät für Physik und Astronomie der Julius-Maximilians-Universität Würzburg, Germany:
Graphene: electronic structure of an intruiging material

July 2007 17th International Vacuum Congress (IVC-17), Stockholm, Sweden:
Electronic structure of graphene

Thorsten Kampen

Nov 2005 Institut für Physik, Chemnitz University of Technology, Chemnitz, Germany:
Elektronische Struktur niedrig-dimensionaler metallischer und organischer Schichten

Dec 2005 Institut für Physikalische und Theoretische Chemie, Universität Tübingen:
Molekulare Funktionsschichten: Ordnung, elektronische Struktur und Chiralität

Jun 2006 SONS Conference 2006, Self-Organised Nanostructures, Pisa, Italy:
Molecular Chirality

Aug 2006 International Conference on Electronic Spectroscopy and Structure, Foz do Iguaçu, Brazil:
Isomerization and Chirality in Self-Organized Molecular Structures

Oct 2006 Department of Physics and Astronomy, University of Nebraska, Lincoln, USA:
Organic molecules - self-assembly and chirality

Feb 2007 FOKUS Kompaktseminar "Spektroskopie mit Röntgenstrahlung", Lehrstuhl für Experimentelle Physik 4, Universität Würzburg:
Photoemission an Oberflächen und Adsorbatsystemen

Sanja Korica

Sept 2005 NanoEurope Fair & Conference, St.Gallen, Switzerland:
Phase dependent differences in the partial cross section oscillations of C_{70} *fullerenes*

Jochen Küpper

Jan 2006 The 36th Winter Colloquium on the Physics of Quantum Electronics, Snowbird, UT, USA:
Deceleration and trapping of neutral molecules for spectroscopic applications.

May 2006 Hauptversammlung der Deutschen Bunsen-Gesellschaft, Erlangen, Germany:
Manipulating the motion of large molecules.

Jan 2007 Physical Chemistry seminar, University of Bielefeld, Germany:
Cold Molecules: From cool *molecular physics to* cold *chemistry.*

Mar 2007 Annual meeting of the German Physical Society, Düsseldorf, Germany:
Manipulating large, neutral molecules with strong electric fields: Selecting isomers, orienting, and slowing neutral polar molecules. (Plenary lecture)

Apr 2007 Seminar of the I. Physics Institute, University of Cologne, Germany:
Manipulating large, neutral molecules with strong electric fields: Selecting isomers, orienting, and slowing neutral polar molecules.

May 2007 Hauptversammlung der deutschen Bunsen-Gesellschaft, Graz, Austria:
Spectroscopy of free radicals and radical containing entrance-channel complexes in superfluid helium nanodroplets.

July 2007 Chemistry seminar, University of Alberta, Edmonton, Alberta, Canada:
Stark deceleration of polar molecules – from small to large.

Aug 2007 Workshop on “Coherent control of ultracold molecular systems”, Vancouver, BC, Canada:
Stark deceleration of polar molecules – from small to large.

Adela Marian

June 2007 Institute of Physics (Institut za Fiziku) in Zagreb, Croatia:
Direct frequency comb spectroscopy of two-photon transitions

Bas van de Meerakker

Oct 2005 Workshop on Cold Polar Molecules, Ringberg Castle, Germany:
Stark deceleration and trapping of polar molecules

May 2005 XXI International Symposium on Molecular Beams, Crete, Greece:
Deceleration and trapping of OH radicals

Jan 2006 ISAMOP, International Seminar on Progress and Excitement in AMO Physics, Tokyo, Japan:
Stark deceleration and electrostatic trapping of OH radicals

Feb 2006 Colloquium, ETH Zürich, Switzerland:
Deceleration and trapping of OH radicals

Mar 2006 Colloquium, FOM Institute for Plasmaphysics Rijnhuizen, Nieuwegein, The Netherlands:
Deceleration and trapping of OH radicals

May 2006 Colloquium, JILA and University of Colorado, Colorado, USA:
Stark deceleration and trapping of OH radicals

Jun 2006 Pire Ecci seminar, University of California at Santa Barbara, Santa Barbara, USA:
Stark deceleration and trapping of OH radicals

Sept 2006 MOLEC XVI, European Conference on Dynamics of Molecular Systems, Trento, Italy:
Collision experiments with Stark decelerated and trapped OH radicals

Oct 2006 Wilhelm und Else Heraeus Semínar on Cold Molecules, Bad Honnef, Germany:
Experiments with Stark decelerated and trapped OH radicals

May 2007 ECAMP IX, Crete, Greece:
Deceleration and Trapping of Neutral Polar Molecules

Jun 2007 COMET XX, Arcachon, France:
Crossed beam collision experiments with Stark decelerated molecular beams

Jul 2007 Dynamics of Molecular Collisions Meeting XXI, Santa Fe, New Mexico, USA:
Scattering experiments using Stark decelerated molecular beams

Gerard Meijer

Nov 2005 Physics Colloquium, University of Duisburg-Essen, Duisburg, Germany:
Deceleration and trapping of neutral polar molecules

Nov 2005 General Colloquium, Gesellschaft für Schwerionenforschung, Darmstadt, Germany:
Accelerator physics with neutral molecules

Nov 2005 GDCh (Gesellschaft Deutscher Chemiker) Colloquium, University of Bielefeld, Germany:
Deceleration and trapping of neutral polar molecules

Dec 2005 Physics Colloquium, University of Rostock, Germany:
Deceleration and trapping of neutral polar molecules

Dec 2005 Colloquium, DESY, Hamburg:
Accelerator physics with neutral molecules

Jan 2006 Physics Colloquium, University of Mainz, Germany:
Deceleration and trapping of neutral polar molecules

Feb 2006 Physics Colloquium, University of Stockholm, Sweden:
Deceleration and trapping of neutral polar molecules

Mar 2006 EU and ESF workshop on Achievements and Perspectives of Cold Molecules, Les Houches, France:
Cold molecules at the Fritz Haber Institute in Berlin

Mar 2006 Physics Colloquium, University of Lyon, France:
Deceleration, cooling, and trapping of neutral polar molecules

May 2006 Physics Colloquium, University of Halle, Germany:
Deceleration and trapping of neutral polar molecules with electric fields

June 2006 International workshop on "Correlated and many-body phenomena in dipolar systems", Dresden, Germany:
Deceleration and trapping of neutral polar molecules

June 2006 Guest Lecture, Chemistry Department, University of Helsinki, Helsinki, Finland:
Deceleration and trapping of neutral polar molecules

June 2006 XI*th* Roermond Conference on Catalysis, Rolduc, The Netherlands:
IR spectroscopic characterization of gas-phase clusters and cluster-adsorbate complexes

June 2006	Physical Chemistry Colloquium, University of Göttingen, Germany: *Deceleration and trapping of neutral polar molecules*
July 2006	XX*th* International Conference on Atomic Physics, Innsbruck, Austria: *Slowing and trapping of polar molecules*
Aug 2006	1*st* European Chemistry Congress, Budapest, Hungary: *Deceleration and trapping of neutral polar molecules*
Sept 2006	19*th* International Conference on High Resolution Spectroscopy, Prague, Czech Republic: *Deceleration and trapping of neutral polar molecules*
Sept 2006	Gordon Research Conference on Electronic Spectroscopy & Dynamics, Les Diablerets, Switzerland: *Deceleration and trapping of neutral polar molecules*
Oct 2006	Physical seminar, Department of Chemistry, University of Georgia, Athens, GA, USA: *Deceleration and trapping of neutral polar molecules*
Nov 2006	GRI Symposium I on Cluster Science: Breakthrough advances in cluster science, Nagoya, Japan: *Infrared spectroscopic characterization of clusters and cluster complexes*
Nov 2006	Physics Colloquium, Radboud University of Nijmegen, The Netherlands: *Deceleration and trapping of neutral polar molecules*
Nov 2006	Colloquium, Institute of Theoretical Physics, Utrecht University, The Netherlands: *Deceleration and trapping of neutral polar molecules*
Nov 2006	Seminar, Dept. of Molecular and Laser Physics, Radboud University of Nijmegen, The Netherlands: *Infrared spectroscopic characterization of gas-phase clusters and cluster-adsorbate complexes*
Dec 2006	Stuttgarter Physikalisches Kolloquium, University of Stuttgart, Germany: *Deceleration and trapping of neutral polar molecules*
Dec 2006	Workshop on Catalysis and Surface Science, UC Santa Barbara, CA, USA: *Infrared spectroscopic characterization of clusters and cluster complexes*
Mar 2007	Symposium on Size Selected Clusters 2007, Brand, Austria: *Infrared spectroscopic characterization of gas-phase clusters and cluster-adsorbate complexes*

Mar 2007	Symposium Molecular Collisions at ultracold temperatures (SYMC) at the DPG AMOP-Spring meeting 2007, Düsseldorf, Germany: *Molecular collision studies with Stark-decelerated beams*
Apr 2007	DFG Round Table Discussion on "Cold Reaction Dynamics", Physikzentrum, Bad Honnef, Germany: *Molecular collision studies with Stark-decelerated molecular beams*
Apr 2007	Reunion, Radboud University of Nijmegen, The Netherlands: *Geschiedenis, achtergronden en toekomst van de Atoom- en Molekuulfysica in Nijmegen*
May 2007	XXII International Symposium on Molecular Beams, Freiburg, Germany: *Deceleration and trapping of neutral polar molecules*
June 2007	Physical Chemistry & AMO Physics Seminar, The University of British Columbia, Vancouver, B.C., Canada: *Deceleration and trapping of polar molecules*
June 2007	DAMOP/DAMP Ψ Meeting, Calgary, Alberta, Canada: *Molecular collision studies with Stark-decelerated beams*
June 2007	Physics Seminar, Dalhousie University, Halifax, N.S., Canada: *Deceleration and trapping of neutral polar molecules*
June 2007	The Fritz Haber Double-Day Symposium 2007 on "Conduction in Molecular Systems", Yad Hashmonah, Israel: *Molecular collision studies with Stark-decelerated beams*
June 2007	Danish Physical Society, Annual Meeting 2007, Plenary lecture, Nyborg, Denmark: *Deceleration and trapping of neutral polar molecules*
Sept 2007	QuAMP IV, London, UK: *Molecular collision studies with Stark-decelerated beams*
Nov 2007	Colloquium of the Gesellschaft Deutscher Chemiker, Hannover, Germany: *Deceleration and trapping of neutral polar molecules*

Andreas Osterwalder

Mar 2006	Meeting of the Cold Molecules Network, Les Houches, France: *Production of Cold Neutral Molecules by Deceleration and Photodetachment of Anions*
May 2006	Seminar für Quantenaggregate, Universität Freiburg, Germany: *Using ions in Precision Measurements*

Nov 2006 Swansea University, UK:
Cold Neutral Molecules – Applications and Novel Production Schemes

Mar 2007 DPG Tagung, Düsseldorf , Germany:
Production of Cold Neutral Molecules via Photodetachment of Decelerated Anions

Axel Reinköster

June 2006 International Conference on many-particle spectroscopy of atoms, molecules, clusters and surfaces (e,2e), Rome, Italy:
One and two-photon ionization of C_{60} *fullerenes*

July 2007 The Second International Symposium on Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale, Darmstadt, Germany:
Photoabsorption and photoionization of fullerenes and clusters

Sophie Schlunk

Sept 2007 QuAMP IV, London, UK:
Trapping of rubidium atoms by AC electric fields

Melanie Schnell

May 2006 Chemistry Seminar, Technische Universität Berlin, Germany: *Deceleration and Trapping of Ground-State Molecules: Towards Ultracold Chemistry*

May 2006 Physical Chemistry Seminar, Universität Bielefeld, Germany:
Abbremsen und Fangen polarer Moleküle: Auf dem Wege zu ultrakalter Chemie

Sept 2006 232nd Fall Meeting of the American Chemical Society, San Francisco, CA, USA:
Development and Applications of Traps for Ground-State Molecules

Sept 2006 Physical Chemistry Seminar, Harvard University, Cambridge, MA, USA:
Deceleration and Trapping of Ground-state Molecules: Towards Ultracold Chemistry

Oct 2006 Plenarsitzung der Jungen Akademie an der Berlin-Brandenburgischen Akademie der Wissenschaften und der Deutschen Akademie der Naturforscher Leopoldina, Potsdam, Germany:
Die neue coole Welt der kalten Moleküle

May 2007 10. Steinheimer Gespräche für den Hochschullehrernachwuchs des Fonds der chemischen Industrie, Rödermark, Germany:
Kalte Moleküle - ein neues Werkzeug in der Physikalischen Chemie

Wieland Schöllkopf

June 2007	Seminar, J. Heyrovsky Institute of the Czech Academy of Sciences, Prague, Czech Republic: *A Paul trap for cold neutral atoms*

Jens Viefhaus

Sept 2005	First user experiments workshop at the DESY VUV-FEL, Hamburg, Germany: *Photoionization of atoms and fullerenes*
Oct 2005	VUV/XUV Experiments at PETRA III, Hamburg, Germany: *Advanced photoelectron spectroscopic methods for atomic and molecular inner-shell studies and the characterization of XUV radiation*

Other activities of members of the Department of Molecular Physics

Uwe Becker

Treasurer: Board of the Atomic, Molecular and Optical Division (AMOPD) of the European Physical Society, 2004-2006.
Deputy Spokesman of the Fachverband Atomphysik der Deutschen Physikalischen Gesellschaft, 2005-2008.
Co-Chair: XXV International Conference on Photonic, Electronic and Atomic Collisions, Freiburg, Germany, 25th to 31st July 2007.
Co-Chair: 15th International Conference on Vacuum Ultraviolet Radiation Physics, Berlin, Germany, 29th July to 3rd August 2007.
Representative of the Max Planck Society in the BMBF Forschungsschwerpunkt 301 FLASH.
Member: Editorial Board of J. Electron Spectrosc. Relat. Phenom. (since 1998).
Member: Editorial Board of the Springer Series on Atomic, Optical and Plasma Physics (since 2006).
Member: 4GLS International Advisory Committee (since 2001).
Member: Peer Review Committee SOLEIL, France (since 2006).
Teaching: *Photoionization of Atoms and Molecules* at the Technical University of Berlin.

Horst Conrad

Teaching: *Spectroscopic methods at surfaces* at the Free University of Berlin.

André Fielicke

Teaching: lecture course on Electrochemistry, chemistry department, Humboldt University (2006).

Jochen Küpper

Teaching: *Atomic and Molecular Physics II* at the Free University of Berlin (WS 2005/06 and 2006/07, compulsory optional course 20 302).

Gerard Meijer

Member: "Raad van Bestuur FOM" (2003-2007).
Member: Board of the Atomic, Molecular and Optical Division (AMOPD) of the European Physical Society, 2004-2008.
Member: NWO SPINOZA committee (2005-2008).
Member: Programme Advisory Committee FELIX/FELICE (FOM, The Netherlands), FELBE (Dresden), FLASH (Hamburg).
Member: PCMI Advisory Board (France; 2005-2006).
Member: Beirat Fritz-Haber Minerva Center, Jerusalem (2005-2009).
Member: Editorial advisory board of Phys.Chem.Chem.Phys. (since 2002).
Initiator of the ESF EUROCORES programme on Cold Quantum Matter (EuroQUAM), together with Jeremy Hutson, Ennio Arimondo, Rudi Grimm, and Pierre Pillet.
Organization of an international workshop on "Cold Molecules", Bad Honnef, October 2006, together with Rudi Grimm (Innsbruck) and Melanie Schnell.
Organization of an international workshop on "Horizons in vibrational spectroscopy with free electron lasers", February 2007, together with Knut R. Asmis.
Teaching: *Atomic and Molecular Physics II* at the Free University of Berlin (WS 2005/06 and 2006/07), compulsory optional course 20 302).

Melanie Schnell

Seminar organizer (with Gerard Meijer and Rudi Grimm): “379. WE-Heraeus seminar on cold molecules”, Bad Honnef, Germany, October 2006
Teaching: A main course in physical chemistry at the Freie Universität Berlin “Physikalische Chemie II: Atombau und chemische Bindung” (WiSe 2006/2007, VL 21302 a+b V/Ü)
Member of the Junge Akademie an der Berlin-Brandenburgischen Akademie der Wissenschaften und der Deutschen Akademie der Naturforscher Leopoldina

Dept. of Physical Chemistry **Director until Nov. 2004: Gerhard Ertl**
Acting Director: Gerard Meijer

Group leaders:

Markus Eiswirth		
Alexander S. Mikhailov		
Bruno Pettinger		
Harm H. Rotermund	(Habilitation)	until 31.07.06

Guest scientists, staying for at least six months, paid by the FHI:

Tae-Geun Noh
Takayuki Suzuki
Ming Chun Xu
Oliver Rudzick
Dai Zhang

Guest scientists, staying for at least six months, paid from external funds:

Sergio Alonso	EU Marie Curie Fellowship
Alaa El-Shafei	Arabic Fund for Economical & Social Development
Hiroshi Kori	AvH Fellowship
Yuichi Togashi	JSPS Fellowship

Graduate students:	11
Diploma students:	0
Technicians:	5

Recent Developments in the Department of Physical Chemistry

Director until 11/ 2004: Gerhard Ertl, Acting Director: Gerard Meijer

Since the last meeting of the Fachbeirat there has been the following changes among the staff scientists:

- Harm-Hinrich Rotermund became Professor of the Department of Physics and Atmospheric Science at the Dalhousie University in Halifax, Canada in August 2006.

As the Fachbeirat is well aware, the offer by the President of the MPG, Peter Gruss, to Richard Berndt from the University of Kiel, of a Directorship at the Fritz Haber Institute as Head of the Department of Physical Chemistry was not accepted, so that this position has not yet been filled. Gerard Meijer is continuing as Acting Director, while Bruno Pettinger takes care of current affairs.

The work of the remaining groups concentrates on theoretical and experimental studies of various aspects of nonlinear dynamics in various interfacial reactions, in part within the framework of DFG Sfb 555 “Complex nonlinear processes”, as well on the development of Raman spectroscopy of nanoscale objects. Theoretical research on problems related to nanobiology is being carried out.

1. Complex systems

Self-organization is a wide-spread phenomenon in nature and manifests itself in that an ordered state is formed that is far from the thermodynamic equilibrium and often shows complex spatio-temporal dynamics. The infinite diversity of patterns in physical, chemical and biological systems can be classified with modern concepts of nonlinear dynamics and a kind of soft-control of their spatio-temporal evolvement.

In complex systems, self-organizing structures arise as a consequence of the underlying nonlinear dynamics. In the early days, research was concentrated on low-dimensional systems. Mostly nontrivial behavior in the time domain was considered, such as oscillations and deterministic chaos. Over the past decades, research efforts were increasingly focused on pattern formation in high-dimensional, spatially extended systems. Besides the classical hydrodynamic instabilities, systems of the reaction-diffusion type and complex networks are among the most widely studied examples which can be found in physics, chemistry, biology, ecology and other fields. Our research on complex systems therefore covers a broad range of topics, ranging from the observation and control of self-organizing patterns in reaction diffusion systems and corrosion dynamics to protein folding, oscillator networks, and enzyme dynamics.

In the Surface Imaging Group, experimental and theoretical research on critical non-equilibrium phenomena during the onset of pitting corrosion on stainless steel has been continued and extended to other important systems. Newly developed in-situ methods have been applied to the corrosion of aluminum and the etching and pore formation of n-InP. An interesting feature of the latter system is, that the process can be controlled by light which allows for patterning of the material. Patterned porous semiconductor structures are of great importance for the design of photonic devices and sensors.

The research on the catalytic oxidation of carbon monoxide on Pt(110) single crystal surfaces has been continued. Since a few years attention has shifted from analyzing and understanding the spontaneously emerging spatiotemporal patterns to actively influencing and manipulating the system dynamics. The experimental setup has been extended such that patterns can be simultaneously manipulated globally as well as locally. Global system parameters can be modulated by real time control of partial pressures in the reactor while local control is achieved by means of focussed laser light. Recent results include the observation of frequency locked patterns with subharmonic entrainment at high forcing frequencies. The combination of global and local manipulation allowed for observation of so-called 2p phase kinks that exist at the boundaries of cluster patterns. These observations were possible because of crucial improvements of our experimental setups, like the development of a new reflection anisotropy microscope (RAM) and the construction of novel gas driving compressor that increased the accessible forcing frequency range drastically. (Rotermund)

Theoretical investigations on control of nonequilbrium pattern formation and spatiotemporal chaos in chemical systems, including surface reactions, were continued. In cooperation with an experimental group at Synchrotron Trieste, nonequilibrium nanoscale pattern formation in surface reactions accompanied by phase separation was studied. Further progress has been done in the theoretical understanding of corrosion mechanisms of stainless steel and on approaches to control the corrosion onset and to suppress it.

Several new research directions, related to various aspects of nanobiology, were explored. Attention was focused on the operation of single-molecule protein machines and on the collective behaviour in large populations of interacting molecular machines. Molecular synchronization waves in the arrays of interacting allosteric enzymes were predicted. In cooperation with the Department of Computational Molecular Biology of the Max Planck Institute for Molecular Genetics in Berlin, properties of complex biochemical networks were analyzed. Nonequilibrium pattern formation in active Langmuir monolayers including chiral molecules has been considered; similar phenomena in biomembranes with active molecular inclusions are being investigated.

Additional research funding has been provided by DFG in the framework of Sfb 555 “Complex Nonlinear Processes”, from the European Union through the Marie Curie Research Training Network “PATTERNS: Unifying Principles in Nonequilibrium Pattern Formation”, and from the Volkswagen Foundation within its program “Complex Networks as a Cross-Disciplinary Phenomenon”.

Prof. A. S. Mikhailov has received an invitation from the Solvay Foundation to the International Solvay Chair in Chemistry in Belgium in 2009. This invitation has been accepted. (Mikhailov)

Further experimental studies of electrochemical pattern formation have been extended by lowering the conductivity of the electrolyte substantially. In formic acid oxidation on a Pt ring, decreasing conductivity leads to a richer variety of patterns, including (besides standing waves and rotating pulses which already exist for high conductivity) cluster formation, pulse reflection and propagation failure. The pattern selection seems to depend on the type of electrochemical oscillator used (NDR or HNDR), a systematic theoretical investigation using reaction-migration equations is planned.

Application of ideas from algebraic geometry (graph theory and ideal theory) to chemical reaction dynamics not only gives theoretical insight into discrete-algebraic aspects of bifurations, but also allows analytical solutions of the stationary states of kinetic models and the stability problem. The set of roots can be obtained by an intersection of the convex flux cone and a deformed toric variety obtained from the Gröbner basis of the reaction binomials. In contrast to earlier approaches involving convex geometry only, this intersection can be mapped back into standard kinetic parameters, allowing the determination of multistability and the regions where local bifurcations occur.

Recently, a new project involving discrete mathematics has been started in cooperation with the group of P. Plath (Institut für Angewandte und Physikalische Chemie, Universität Bremen). The dynamics of foam decay is characterised and modelled using order theory (in particular classical and weak majorisation). (Eiswirth)

2. Raman spectroscopy

In science and thechnology there is a strong demand to characterize even smaller entities and structures. A recently developed approach, tip-enhanced Raman spectroscopy (TERS) is very promising in this respect, it is a variant of surface enhanced Raman spectroscopy (SERS) but avoids its limitations. Both spectroscopies are based on the optical excitation of localized surface plasmons in small metal structures. In the case of TERS, surface plasmons are excited at the tip only, or between the Au (or Ag) tip of a scanning probe microscope and any (smooth) surface, whereby a very strong local field enhancement is achieved in the gap. A Au-tip / Au-substrate configuration proved to support particularly strong field enhancements. This approach has a great potential for application in research and technology as it provides a vibrational spectroscopy with very high sensitivity and nanometer resolution.

TERS spectra from various adsorbed organic and inorganic molecules were recorded. With a sharp tip of ~20 nm tip radius and the dye malachite green isothiocyanate, single-molecule sensitivity has been achieved: less than 5 molecules underneath the tip can be ‘seen’ by this technique, nevertheless providing clear fingerprint spectra. For molecules not in optical resonance with the exciting laser, such as adenine, the detection sensitivity is currently about 130 molecules. The high spatial resolution is evident from two facts: upon retracting the tip by 10 nm from the Au(111) surface, (i) the TERS intensity drops rapidly to 5% of its initial level and (ii) a blue shift of the gap resonance mode is observed, because the short range near-field coupling between tip and metal ceases.

The TERS approach has been transferred to UHV, by developing a third-generation TERS apparatus. The necessary optics, including a high numerical aperture parabolic mirror, are completely included into the UHV chamber with the parabolic mirror integrated between the STM scanner and the sample. Optical fibers deliver the incident laser beam and the inelastically scattered light to the sample and spectrograph, respectively. First results are very promising: The sharp focus ($\lambda/2$) supports a high contrast between TERS and usual Raman scattering, leading - for example - to a 4000-fold increase of the Raman signal upon tip approach for the dye brilliant cresyl blue. The underlying enhancement of Raman scattering is about 10^6. Raman mapping is also possible, e.g. the recording of an optical image with a resolution better than 50 nm, which is much below the Abbe limit of ~ $\lambda/2$.

Parallel to the UHV TERS, a setup for electrochemical TERS (EC-TERS) has been built. It uses a parabolic mirror riding on a glass plate, a configuration that serves simultaneously as an electrochemical cell and as an optical device for focusing and collecting light. This sophisticated and challenging approach is currently in the test phase.

Thus, a powerful tool for vibrational spectroscopy is being developed that provides chemical and topographic information with spatial resolution in the nanometer regime and is applicable in UHV, gaseous and liquid phases. (Pettinger)

Publications of the Department of Physical Chemistry

2005 (late publications)

Couderc-Azouani, S., J. Sidhu, T. Thurn, R. Xu, D.M. Bloor, J. Penfold, J.F. Holzwarth, and E. Wyn-Jones: Binding of sodium dodecyl sulfate and hexaethylene glycol mono-*n*-dodecyl ether to the block copolymer L64: Electromotive force, microcalorimetry, surface tension, and small angle neutron scattering investigations of mixed micelles and polymer/micellar surfactant complexes. Langmuir **21**, 10197-10208 (2005).

Davidsen, J., A. Mikhailov and R. Kapral: Front explosion in a periodically forced surface reaction. Phys. Rev. E **72**, 046214–1-7 Part 2 (2005).

Gatermann, K., M. Eiswirth and A. Sensse: Toric ideals and graph theory to analyze Hopf bifurcations in mass action systems. J. Symbolic Comput. **40**, 1361-1382 (2005).

Hagen, A., M. Steiner, M.B. Raschke, C. Lienau, T. Hertel, H. Qian, A.J. Meixner and A. Hartschuh: Exponential decay lifetimes of excitons in individual single-walled carbon nanotubes. Phys. Rev. Lett. **95**, 197401–1-4 (2005).

Kori, H. and A.S. Mikhailov: Entrainment of complex oscillator networks. In: J.F.F. Mendes, S.N. Dorogotsev, A. Povolotsky, F.V. Abreu, and J.G. Oliveira (Eds.): Science of Complex Networks. From Biology to the Internet and WWW; CNET 2004, Aveiro, Portugal, 29 Aug. – 2 Sep. 2004. AIP Conf. Proceedings **776**. American Institute of Physics, Melville, NY, 2005, p. 157-165. ISBN: 0-7354-0262-0.

Organ, L., J.R. Scully, A.S. Mikhailov and J.L. Hudson: A spatiotemporal model of interactions among metastable pits and the transition to pitting corrosion. Electrochim. Acta **51**, 225-241 (2005).

Schillinger, R., C. Bromberger, H.J. Jänsch, H. Kleine, O. Kühlert, C. Weindel, and D. Fick: Metallic Si(111)-(7-7)-reconstruction: A surface close to a Mott-Hubbard metal-insulator transition. Phys. Rev. B **72**, 115314–1-11 (2005).

Sharon, M., D. Pradhan, R. Zacharia, V. Puri: Application of carbon nanomaterial as a microwave absorber. J. Nanosci. Nanotechnol. **5** (12), 2117-2120 (2006).

Stolbov, S. and T.S. Rahman: First principles study of some factors controlling the rate of ammonia decomposition on Ni and Pd surfaces. J. Chem. Phys. **123**, 204716–1-5 (2005).

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Dornhege, Monika: Beobachtung von Prozessen an der Phasengrenze Elektrode/Elektrolyt und deren Einordnung in den Bereich der nichtlinearen Dynamik. TU Berlin 2007. 120 p.

Invited Talks of members of the Department of Physical Chemistry

Dr. M. Eiswirth

Feb 2006	Workshop on Nonlinear Dynamics and Hierarchical Self-organization Processes, Sapporo, Japan *Nonautocatalytic oscillators in chemistry and biochemistry*
Feb 2006	Osaka University, Japan *Theory of electrochemistry*
Feb/Mar/ Oct 2006	Hokkaido University, Sapporo, Japan - *Chaos – Metric and topological characterization* - *Chaos in activator-inhibitor systems* - *Pattern formation in the CO oxidation on Pt* - *Stochastic vs. deterministic nucleation in CO oxidation on Pt* - *Thermodynamic efficiency in nonlinear systems* - *Remote triggering in electrochemical systems* - *Saltatory conduction in an electrochemical reaction* - *Application of algebraic geometry to nonlinear chemistry*
Mar 2006	KIST, Seoul, Korea *Electrochemical pattern formation in constrained geometries*
Aug 2006	SIAM Life Sciences SMB, Raleigh NC, USA *Convex and toric geometry for chemical reaction systems*
Sept 2006	AIST, Tsukuba, Japan - *Thermodynamics of periodic processes* - *Diffusion-induced instabilities in stoichiometric networks*
Sept 2006	Conference Understanding of Complex Patterns Dynamics Kobe, Japan *Deterministic and stochastic modeling of a surface reaction*
Oct 2006	Osaka University, Japan *Stochastic effects in a surface reaction*
Oct 2006	Kyoto University, Japan *Toric geometry for chemical reaction dynamics*
Nov 2006	Toyota Workshop Decision Making and Uncertainty in Nonlinear Complex Systems, Helsingoer, Denmark *Stoichiometric network analysis*
Apr 2007	UAEM, Guernavaca, Mexico - *Nonautocatalytic oscillators and olfactory response* - *Electrochemical patterns on a ring*

Apr 2007 ITC, Celaya, Mexico
- Stochastic effects in a surface reaction
- Electrochemical modeling with reaction-migration systems

Sept 2007 3rd International Conference on Physics and Control, Potsdam
Geometric constraints in electrochemical pattern formation

Prof. Dr. G. Ertl

May 2006 Bunsentagung, Erlangen:
Heterogene Katalyse: Vom Idealen zum Realen

June 2006 11th Int. Conf. on Theoretical Aspects of Catalysis (ICTAC11), Schmöckwitz
Towards understanding catalysis

June 2007 Bunsen Discussion Meeting, Heidelberg
Towards the limits of surface science

Sept 2007 Ann. Meeting of the Slovak Chemical Society, High Tatras, Slovakia
Heterogeneous catalysis: From atoms to complexity

Prof. Dr. A. S. Mikhailov

Dec 2005 Seminar in the Department of Physics, Free University of Brussels (ULB), Belgium
Are enzymes molecular machines?

Jan 2006 International Workshop on Dissipative Solitons, Max Planck Institute for Complex Physical Systems, Dresden, Germany
Nonequilibrium pattern formation in chiral Langmuir monolayers

Mar 2006 Seminar in the Institute Curie, Paris, France
Nonequilibrium pattern formation in chiral Langmuir monolayers

Apr 2006 Seminar in the Institute of Industrial Science, Tokyo University, Japan
Slow ordered relaxation in random and designed elastic networks, single-molecule oscillators and prototypes of protein machines

Apr 2006 Seminar in the Research Institute of Electronic Science, Hokkaido University, Sapporo, Japan
Slow ordered relaxation in random and designed elastic networks, single-molecule oscillators and prototypes of protein machines

Apr 2006 Seminar in the Department of Mathematics and Life Sciences, Hiroshima University, Japan
Are enzymes molecular machines?

Apr 2006	Seminar in the Department of Physics, Kyoto University, Japan *Molecular synchronization waves in enzymic arrays*
May 2006	Seminar, Department of Physics, Peking University, China *Molecular synchronization waves in enzymic arrays*
June 2006	ESF Workshop “Nonequilibrium Nanoscale Fluctuations: Single Molecules, Chemical Reactions and Microfluidics”, Castle Goldrain, Italy *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
July 2006	ESF Workshop “Noise in Life”, Barcelona, Spain *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Aug 2006	Symposium “Collaborative Research between Life Science and Mathematical Science”, Hiroshima University, Japan *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Sept 2006	Symposium “Self-Organization Phenomena in Condensed Matter”, Waseda University, Tokyo, Japan *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Oct 2006	International Workshop on Synchronization: Phenomena and Analyses 2006, Institute of Industrial Science, University of Tokyo, Japan *Molecular synchronization waves in enzymic arrays*
Oct 2006	Seminar, Department of Physics, University of Bayreuth, Germany *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Dec 2006	8th RIES-Hokudai International Symposium, Hokkaido University, Sapporo, Japan *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Feb 2007	Lise-Meitner-Kolloquim, Hahn Meitner Institute, Berlin *Onset of pitting corrosion on stainless steel as a cooperative critical phenomenon*
Mar 2007	1st Ladenburg-Discourse “From Bio-Inspired Logistics to Logistics-Inspired Bio-Nanoengineering”, Daimler-Stiftung, Ladenburg, Germany *Design of robust functional networks: A model study of biological signal transduction*

Apr 2007	German-Canadian Matheon-Mitacs Workshop “Complex Networks in Life Sciences”, Erkner, Germany *Design of robust functional networks: A model study of biological signal transduction*
July 2007	International Workshop “Nonlinear Collective Behavior: Networks, Swarming and Reaction-Diffusion Dynamics”, University of Leiden, Netherlands *Relaxation phenomena in complex elastic networks and design principles of molecular machines*
Sept 2007	3rd International IEEE Scientific Conference on Physics and Control (PhysCon 2007), Potsdam, Germany *Sudden onset of corrosion on stainless steel as a cooperative critical phenomenon*
Oct 2007	399th WE-Heraus Seminar “Synergetics: Self-Organization Principles in Animate and Inanimate Systems”, Bad Honnef, Germany *Design and statistical properties of robust functional networks*

Dr. B. Pettinger

May 2006	International Symposium on Surface Imaging/Spectroscopy at the Solid/Liquid Interface, Krakow, Poland: *Tip-enhanced Raman spectroscopy from metal surfaces and electrodes*
June 2006	NIS Colloquium: Raman Spectroscopy: a powerful technique to characterize nano-materials, Torino, Italy *Tip-enhanced Raman spectroscopy (TERS): a Sensitive spectroscopic Tool with nm Resolution*
Aug 2006	Seminar at Tokyo Institute of Technology, Yokohama, Japan *Tip-enhanced Raman spectroscopy from interfaces*
Aug 2006	Tsukuba satellite symposium on Single Molecule and Tip-enhanced Raman Scattering, Tsukuba, Japan *On the sensitivity and the local nature of tip-enhanced Raman spectroscopy*
July 2007	Vibrations at Surfaces 12, Erice, Italy *Tip-enhanced Raman Spectroscopy: Toward Single-Molecule Detection*
Sept 2007	Colloquium Spectroscopicum Internationale XXXV, Xiamen, China *TERS: Single-Molecule Sensitivity, High Spatial Resolution and Applicability to Different Environments such as UHV*
Sept 2007	Workshop of the Department Chemical Physics: “Bridging the Gap between Catalysis and Surface Science”, Ringberg Castle, Tegernsee *Application of tip-enhanced Raman spectroscopy (TERS) in UHV. First results.*

Prof. Dr. H. H. Rotermund

Sept 2005	Workshop on Nonlinear Pattern Dynamics in Complex and Reactive Fluids Kyoto, Japan *Patterns in surface reactions: the oscillatory case – experiment*
Aug 2005	Surface Science Summer School, Univ. of Nottingham, U.K. *Reaction diffusion system*
Apr 2006	2006 UK Condensed Matter and Materials Physics Conference, Exeter, U.K. *Shedding light on surface reactions*
Sept 2006	Workshop on Patterns, Portoroz, Slovenia *Real time imaging and control of pattern formation during catalysis*

Other activities

Prof. A. S. Mikhailov

DFG Collaborative Research programme (SFB 555) "Complex Nonlinear Processes": Member of the Steering Committee (Vorstand), co-organizer of bi-weekly seminars "Complex Nonlinear Processes in Chemistry and Biology" (honorary chairman: Prof. G. Ertl)

EU Marie Curie Research Training Network "PATTERNS: Universal Principles of Nonequilibrium Pattern Formation", organization of the midterm review meeting (Berlin, January 2007)

ESF Program "STOCHDYN: Stochastic Dynamics – Fundamentals and Applications", organization of the International Workshop "Nonequilibrium Nanoscale Fluctuations: Single Molecules, Chemical Reactions, and Microfluidics" (Castle Goldrain, Italy, July 2006)

Organization of the 4th International Symposium "Engineering of Chemical Complexity" (Berlin, June 2006)

Organization of Harz Seminars "Structure Formation in Chemistry and Biophysics" (Hahnenklee, Germany, February 2006 and February 2007)

Lecture course "From Cells to Societies: Models of Complex Coherent Action", Department of Physics, Kyoto University, Japan, April – June 2007.

Editor, journal *Physica D: Nonlinear Phenomena* (Elsevier publishers, Netherlands)

Theory Department

Director: Matthias Scheffler

Group leaders:

Johan Carlsson	
Klaus Hermann (50% head of the Joint Network Center, GNZ)	(Habilitation)
Joel Ireta	
Peter Kratzer (moved to a professorship position at University of Duisburg-Essen, April 2006)	(Habilitation)
Angelos Michaelides (moved to a readership position at University College London, October 2006)	
Karsten Reuter (Independent Junior Research Group)	(Habilitation)

Guest scientists staying for at least six months, paid by FHI:

Marvin A. Albao
Sami Amira
Imad Belabbas
Volker Blum
Arianna Borrelli
Nadia Elghobashi
Martin Fuchs
Ricardo I. Gómez Abal
Wei Guo
Felix Hanke
Mahbube Hortamani
Limin Liu
Evgeni Penev
Matthew Probert
Patrick Rinke
Jürgen Spitaler
Mira Todorova

Guest scientists staying for at least six months, paid from external funds:

Javier Carrasco	AvH Fellow
Matteo Cavalleri	AvH Fellow
Huiqiu Deng (jointly with the Independent Junior Research Group)	
S. Javad Hashemifar	AvH Fellow
Paula Havu	
Ville Havu	AvH Fellow
Timo Jacob (Emmy-Noether Fellow since May 2007)	Liebig Fellow
Hong Jiang	
Christine Kolczewski	
Benjamí Martorell Masip	Catal. Govt.
Horia Metiu (jointly with E.K.U. Groß)	AvH Awardee
Angelos Michaelides	EURYI Award
Mats Persson	AvH Awardee
Xinguo Ren	
Angel Rubio (jointly with E.K.U. Groß)	AvH Bessel Awardee
Ersoy Şaşioğlu	
Abhishek K. Singh	UCSB
Alexandre Tkatchenko	AvH Fellow
Sudha Venkatachalam	AvH Fellow
Enge Wang	AvH Awardee
Weitao Yang	AvH Awardee
Hongsuk Yi	

MPG Fellow Group at FU Berlin: E.K.U. (Hardy) Groß
Sangeeta Sharma

Graduate students: 21 (3 of those jointly with the Independent Junior Research Group)

Diploma students: 4

Recent Developments in the Theory Department

Director: Matthias Scheffler

I. General Remarks

The main research directions of the *Theory Department* continue to be focused on understanding fundamental aspects of the chemical and physical properties of surfaces, interfaces, clusters, and nanostructures. Much of this work is related to heterogeneous catalysis, and some work is also done in the field of biophysics and environmental chemistry. Major new insight (and the uncovering of new effects) nearly always comes as a result of the development of new experimental or new theoretical tools. Therefore, we devote significant effort to the development of new techniques, methods, and computer codes. Of course, we also strive to apply these codes to timely and important scientific problems.

The *Theory Department* realized from early on, since its foundation in 1988, the importance of "multi-scale modeling from first principles". This involves the linkage of density-functional theory (DFT) with thermodynamics, continuum descriptions (e.g. elasticity theory), and, in particular, statistical mechanics. Currently, this became a "hot" topic and multi-scale modeling is a "buzz-word", as it has become widely accepted that there is a need to develop methods that address all relevant time and length scales (from fs to s in time, from nm to mm in space). While the goals are ambitious and significant new concepts still need to be developed, the potential payoff would be tremendous, offering unprecedented simulation and modeling capabilities. Perhaps more importantly, failure implies a lack of predictive capability for virtually all of the important processes of functional surfaces, bulk materials, clusters, molecules, and other nanometer-scale systems.

Electronic-structure theory (DFT or quantum chemistry methods) is the base (the finest scale) in the hierarchical set of methodologies. In principle, if electronic-structure theory can be developed to the point of giving quantitative and reliable predictions, then this accuracy can be propagated up the chain of methods to successively increasing spatial and temporal scales. Conversely, if the accuracy is lacking at the base, there is little hope for accurate predictions at any level of modeling that follows. Starting from electronic-structure theory the suitable output must be linked to molecular dynamics (MD), kinetic Monte Carlo (kMC), and other methodology, finally enabling a proper description of the statistical mechanics, i.e., the proper time and lengths scales and ensemble averages. These various simulation methodologies must be connected by robust, error-controlled links with knowledge of uncertainty. Thus, when crossing the scales the quantum-chemistry accuracy, that is available at the lower scale, must be maintained when moving up in the hierarchy. Indeed, such "error-control" has always been a central concern of the work at the FHI.

For polyatomic systems, DFT with present-day exchange-correlation functionals has proven to be an excellent technique for calculations of structures and vibrations, but is not as good for certain types of binding interactions. Accurate treatments of strong electronic correlations, hydrogen bonding, van der Waals interactions, and MD for electronically excited states are still challenging with DFT, and therefore are major research priorities (see Section III below). Here, quantum chemistry, as well as time-dependent DFT, the *GW* approach, reduced-density-matrix-functional theory, and the quantum Monte Carlo method are being employed and improved and cross-validated with respect to accuracy and efficiency.

While considerable progress has been achieved in multi-scale modeling in recent years, we also note that substantial advances are still required in terms of the basic theory and concepts, since it is currently still not known how to cross all of the scales in both *forward and reverse* directions. Progress will require new theoretical methods in materials science, chemistry, and physics, as well as new mathematical and computational approaches to deal with scale-crossing and the inherent inclusion of uncertainty in the equations.

Currently, much progress has been made with the *ab initio* kMC method, the third level in the hierarchy (above *ab initio* MD), in which rate constants calculated from *ab initio* MD or from transition-state theory can be used as parameters (also with updates "on the fly"). Sometimes the critical "spark" that triggers a significant change of the material's properties will come from a process that only happens after micro- or milliseconds or even longer. The *ab initio* kMC approach is reaching the point where certain issues can be tackled with rigor over the relevant time scales of seconds or minutes (e.g. defect diffusion and annealing, crystal growth, corrosion, heterogeneous catalysis). Advances that include (for example) systems without a lattice, the proper treatment of excited electronic states, and dissipation of heat must be developed and require new concepts and strategies. Above the kMC level in the hierarchy (e.g. links to continuum mechanics and rate equations), however, all connections are tenuous at best. In spite of more than a decade of research in this area, there has only been limited success, so far.

The challenging developments outlined above will be needed for the modeling and understanding of materials properties and functions that are of interest to the work at the FHI. Obviously, they will also impact many other areas of material sciences, biophysics and biochemistry, as well as earth- and atmospheric sciences.

Central to all our research is the desire and responsibility to educate and train top-quality students and postdocs. The lively atmosphere paired with high-quality science of the *Theory Department* forms the basis for productive and fruitful research. The large number of applications we get from highly motivated young scientists is testimony to our success in this regard. This is, for example, reflected in the number of Alexander von Humboldt (AvH) fellows (scientists younger than 40 years) and AvH senior scientists.

In October 2004, in a joint action of the *College of Engineering* and the *College of Mathematical, Life & Physical Sciences* of the *University of California Santa Barbara*, Matthias Scheffler was appointed "Distinguished Visiting Professor for Computational Material Science and Engineering". Since 2006 he has been part of the faculty at UCSB and spends three months per year in Santa Barbara, though in periods of only 2-3 weeks length. The group leader structure of the *Theory Department* ensures that students, postdocs, and visitors are well supervised and accommodated. Indeed, the collaboration between the FHI *Theory Department* and UCSB has been fruitful, and the exchange of researchers (in both directions) most stimulating. The opportunity of research visits at the UCSB also provides a strong incentive to young, talented researchers at the FHI. Some other activities are now added in bullet form:

- The "UCSB-MPG program" supports joint activities and exchange of students and postdocs between scientists working in *Materials Science* in the whole MPG and UCSB since 2005. The coordinators are Matthias Scheffler for the MPG and Anthony Cheetham for the UCSB.
- At the *Dalian Institute of Chemical Physics (CAS)*, the premier catalysis-science institute in China, a *Max Planck Partner Group* "First-Principles Theory of High-Pressure Oxidation Catalysis" has been established in January 2006. In Dalian, the group leader is Weixue Li, and the FHI partners are Karsten Reuter and Matthias Scheffler.
- We are also part of another program involving the Dalian institute: "The Partnership for International Research and Education at the University of California: electron

chemistry and catalysis at interfaces" (PIRE-ECCI). This activity, managed by the UCSB, helps to intensify collaborations through the exchange of graduate students.

- In March 2006, Joachim Sauer has been appointed *External Scientific Member* of the FHI. This documents also the close ties that he and his group have had with the FHI over the years.
- Finally, it is a pleasure to mention the new MPG initiative to support outstanding senior university lecturers by appointing them as *Max Planck Fellows*. Since the summer of 2006, Hardy Gross has been such a *Max Planck Fellow*, and his appointment is connected with some financial support provided by the MPG for his group.

Last but not least we gratefully mention the extraordinary support the *Theory Department* has received from special programs of the *Max Planck Society* since 2006, particularly from the MPG President:

- Karsten Reuter's Junior Research Group, initially fully paid by the FHI (Theory) basic budget, is covered by an additional financial plan since January 2007.
- The initiative for a new high-level computer, prepared by 31 Max Planck directors (from astrophysics, plasmaphysics, biology, chemistry, and material sciences), and coordinated by the MPG Computer Center in Garching, was successful. Consequently, in early 2008 the present IBM Regatta (p5) will be replaced by a new IBM p6 computer (6400 processors). Obviously this will serve the whole MPG, but the FHI *Theory Department* will get a fair share.
- An initiative on "Multi-Scale Modeling of Condensed Matter" (MMM), bringing together 6 Max Planck institutes (including the FHI *Theory Department* and its *Independent Junior Research Group*) was funded by the President's *"Strategischer Innovationsfonds"*. In its first of two potential phases it runs from August 2006 to July 2009.

The following Section describes aspects concerning the personnel and related activities. Then in Sections III and IV some recent highlights of work performed in the *Theory Department* are briefly outlined: Section III summarizes conceptual, methodological, and technical developments, which enable us to study new types of problems and/or improve the accuracy of calculations. Then, in Section IV, the main fields that are studied in the *Theory Department* are listed and some recent results mentioned.

Most of the work performed in collaboration with Karsten Reuter is not discussed here, as it is covered in his Chapter on the activities of the *Independent Junior Research Group*.

II. Personnel and Related Activities

Since the last visit of the *Fachbeirat* in November 2005 several noteworthy developments have taken place with the following scientists receiving impressive awards and/or offers of prestigious positions:

- Peter Kratzer accepted a W2 professorship position (Theoretical Physics) at the *University Duisburg-Essen* and started there, in April 2006. Some collaboration with him continues, and he is still supervising two Ph.D. students at the FHI.
- Angelos Michaelides accepted an offer of a Readership from the *London Centre for Nanotechnology* and *Department of Chemistry* of *University College London.* He has been there since October 2006 but still spends about half of his time at the FHI.
- Since May 2007 Timo Jacob is leading a DFG funded *Emmy-Noether Junior Research Group*. Around spring 2008, he will move to the *Institute for Electrochemistry* at the *University of Ulm*.
- Joel Ireta, who taught us about biophysics since eight years, assumed a professorship position in the *Chemistry Department* of the *Universidad Autónoma Metropolitana* in Mexico City, and is working there since September 17, 2007. Also with him several projects will continue.

Members of the *Theory Department* were and are actively taking part in several *Collaborative Research Centers* (Sonderforschungsbereiche (SFB)) of the *German Research Foundation* (Deutsche Forschungsgemeinschaft (DFG)) which reflects the close contacts and collaboration with the Berlin universities and other research institutes. In addition, they take part in DFG *Priority Programs* (Schwerpunktprogramme (SPP)) and various *Networks of Excellence* and other European (EU and ESF) and international programs. Some of the collaborations with industry (e.g. Siemens and Osram) are supported by the BMBF. The full list of external funding (without the Humboldt foundation and the DAAD) reads:

- EU – Network of Excellence (NoE): Nanoscale Quantum Simulations for Nanostructures and Advanced Materials (NANOQUANTA), coordinator: R. Godby; M. Scheffler, A. Schindlmayr, P. Rinke
- EU – Network of Excellence (NoE): Self-Assembled Semiconductor Nanostructures for New Devices in Photonics and Electronics (SANDiE), coordinator: M. Grundmann; P. Kratzer, M. Scheffler
- EU – Network of Excellence (NoE): Integrated Design of Catalytic Nanomaterials for a Sustainable Production (IDECAT), coordinator: G. Centi; R. Schlögl, H.-J. Freund, M. Scheffler
- EU – Specific Targeted Research Project (STREP)$^{(IG)}$: Oxidation of Nanomaterials (NanO_2), coordinator: A. Stierle, until 03/2007; K. Reuter, M. Scheffler
- EU – Marie Curie Host Fellowship for Early Stage Research Training (EST)$^{(IG)}$: Molecular Networks at Phase Boundaries (MONET), coordinator: J. N. Andersen; A. Michaelides, K. Reuter, M. Scheffler
- EU – Marie Curie Actions, Human Resources and Mobility: $\Psi_{\mathbf{k}}$ Training in Computational Nanoscience, chair: P. Dederichs; M. Scheffler
- EU – Integrated Infrastructure Initiative (I3): Distributed European Infrastructure for Supercomputing Applications (DEISA), chair: V. Alessandrini; H. Lederer, M. Scheffler
- ESF – Physical and Engineering Sciences Committee (PESC): Towards Atomistic Materials Design ($\Psi_{\mathbf{k}}$), chair: P. Dederichs and V. Heine; M. Scheffler
- ESF – Physical and Engineering Sciences Committee (PESC): Molecular Simulations in Biosystems and Material Science (SimBioMa), chair: B. Smit; M. Scheffler
- SFB 296: Growth-Correlated Properties of Low-Dimensional Semiconductor Structures, project A5, spokesperson: D. Bimberg, until 12/2006; P. Kratzer, M. Scheffler
- SFB 546: Structure, Dynamics, and Reactivity of Aggregates of Transition Metal Oxides, project C6, spokesperson: J. Sauer; K. Hermann

- SFB 658$^{(IG)}$: Elementary Processes in Molecular Switches at Surfaces, project C4, spokesperson: M. Wolf; K. Reuter, M. Scheffler
- SPP 1091$^{(IG)}$: Bridging the Gap between Ideal and Real Systems in Heterogeneous Catalysis, spokesperson: R. Imbihl, until 11/2006; K. Reuter, M. Scheffler
- BMBF – Federal Ministry of Education and Research ("Verbundprojekt"): Virtual Development of Ceramic and Composite Materials with Tailored Transport Properties (VEKTRA), coordinator: S. Lampenscherf (Siemens); M. Scheffler
- DFG – Emmy Noether Program: Theoretical Modeling of Electrochemical Systems; T. Jacob
- DFG – Bilateral Cooperation (POL): First-priciples Studies of Adsorbate Structures at Metal and Oxide Surfaces, until 12/2006; M. Scheffler, A. Kiejna
- ARC – Australian Research Council, Discovery Project: *Ab initio* Theory in Complex Materials and Surfaces: Prediction and Design of Functional Structures; C. Stampfl, M. Scheffler, A. Freeman
- UCSB – University of California, Santa Barbara; College of Engineering and College of Mathematical, Life & Physical Sciences; M. Scheffler
- IFP – Institut Français du Pétrole$^{(IG)}$, Ph.D. Student Program: Kinetic Monte Carlo Simulations of Gas Solid Reactions and Applications to Hydrotreating Catalysts; K. Reuter, M. Scheffler

The superscript$^{(IG)}$ indicates a collaboration with the *Independent Junior Research Group* of Karsten Reuter.

Scientists of the *Theory Department* were also involved in various services to the surface-science and electronic-structure communities worldwide. For example, they lecture at the *Free University* and the *Technical University Berlin* as well as at the *International Max Planck Research School*. Particularly pertinent during the last two years was finding a modus for continuing the $\Psi_{\mathbf{k}}$–network. This is an umbrella organization comprising the whole electronic-structure community in Europe and beyond. It fosters the communication among researchers, and it stimulates and partially supports the preparation of European research proposals, workshops, and summer schools. The $\Psi_{\mathbf{k}}$–network also organizes the large $\Psi_{\mathbf{k}}$–conference every 5 years (one of the international key meetings in the field, attracting more than 600 participants). The next one is scheduled for September 2010 in Berlin (organized by M. Scheffler). As the present funding will end next year (after a successful 10 years of funding by the ESF) a non-profit "company limited by guarantee", Psi-k.org, is being founded that "lives" from fees paid by its members (research groups at universities and research institutes). For the coming years the chairman, Peter Dederichs, already succeeded to secure the (basic) finances in this manner.

Scientists of the *Theory Department* organized or co-organized conferences on topics in surface science and biophysics, and coordinated several international workshops and summer schools on methods for electronic-structure calculations, impacting upon the careers of numerous students of theoretical surface science. This list includes:

- 10th DICP - Dalian Institute of Chemical Physics, Symposium on "Chemical Physics of Materials", 1 - 3 June, 2006, Dalian, China; organizers: Weixue Li (Chinese Academy of Sciences, Dalian, China), K. Reuter, and M. Scheffler
- International Conference on "Theoretical Aspects of Catalysis" 11 - 14 June, 2006, Schmöckwitz, Germany; organizers: K. Hermann (FHI) and J. Sauer (Humboldt University, Berlin, Germany)
- Workshop on "Advances in Computational Materials Science", 21 - 24 June, 2006, Schloss Ringberg, Rottach-Egern, Germany; organizers: A. Michaelides and M. Scheffler
- Ψ_k and CECAM (Centre Européen de Calcul Atomique et Moléculaire), Workshop on "Catalysis from First Principles", 11 - 14 September, 2006, Lyon, France; organizers: A. Michaelides, M. Scheffler, K. Reuter, J. Nørskov (Technical University of Denmark, Lyngby), and J. Hafner (University of Vienna, Austria)
- 11th Nanoquanta Workshop on "Electronic Excitations: A Decade of Applications of the Bethe-Salpeter Equation", 19 - 22 September, 2006, Houffalize, Belgium; co-organizer: P. Rinke
- SANDiE Workshop on "SAN Simulation", 4 - 5 October, 2006, Duisburg, Germany; organizer: P. Kratzer
- Ψ_k and CECAM (Centre Européen de Calcul Atomique et Moléculaire), Workshop on "Simulations of Novel Carbon Materials", 25 - 28 October, 2006, Lyon, France;

organizers: A. Fasolino (Radboud University Nijmegen, The Netherlands) and J. Carlsson

- EURYI - European Young Investigator, Awardees Symposium on “Complexity and Diversity in Matter, Molecules, Life and Society”, 29 November - 2 December, 2006, Strasbourg, France; co-organizer: A. Michaelides
- Workshop on “Multi-Scale Approaches to Nanomechanics”, 5 - 7 February 2007, Lyon, France; organizers: R. Perez (Universidad Autónoma de Madrid, Spain) and K. Reuter
- Symposium on “Exact-Exchange Based DFT Functionals Meet Quasiparticle Energy Calculations: Exciting prospects for solids”, 6 March, 2007, at APS March Meeting / Denver, USA; organizers: P. Rinke and M. Scheffler
- Reunion conference for IPAM's “Bridging Time and Length Scales in Materials Science and Bio-Physics” Program, 10 – 15 June 2007, Lake Arrowhead, California, USA; organizers: Ch. Ratsch (Institute for Pure and Applied Mathematics (IPAM), Los Angeles, USA), R. Caflisch (UCLA, Los Angeles, USA), and M. Scheffler
- 12th Nanoquanta Workshop on “Electronic Excitations: Time-Dependent Density-Functional Theory, Advances and Prospects”, 18 - 22 September, 2007, Centre CNRS Paul Langevin, Aussois, France; co-organizer: P. Rinke
- Workshop on “Electronic Structure Theory at the Water Surface”, 6 - 11 October, 2007, Rijeka, Croatia; organizers: T. Jacob and M. Scheffler
- Workshop on “Non-Adiabatic Dynamics at Surfaces”, 22 - 25 October, 2007, Schloss Reisensburg, Germany; organizers: J. Behler (University of Bochum), P. Rinke, K. Reuter, and M. Scheffler
- MMM - Max Planck Initiative on “Multi-Scale Materials Modeling of Condensed Matter”, Graduate School, 28 October - 2 November, 2007, Sant Feliu de Guixols, Spain; co-organizers: K. Reuter and M. Scheffler
- Symposium on “Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations”, 27-28 February, 2008, at DPG Spring Meeting / TU Berlin, Germany; organizers: P. Rinke and M. Scheffler

- UCSB-MPG Workshop on "Inorganic Materials for Energy Conversion, Storage, and Conservation", 20-22 February, 2008, Lake Arrowhead, California, USA; organizers: T. Cheetham (UCSB, Santa Barbara, USA), J. Maier (MPI-FKF, Stuttgart, Germany), R. Seshadri (UCSB, Santa Barbara, USA), and M. Scheffler
- Marie-Curie $\Psi_{\mathbf{k}}$ Training Summer School on "Modern Concepts for Creating and Analyzing Surfaces and Nanoscale Materials" May 12 - 16 (2008), Sant Feliu de Guixols, Spain; organizers: K. Fichthorn (Pennsylvania State University, USA), M. Scheffler, and M. Fuchs.

III. New Concepts, Methods, and Techniques

III.1 Beyond Today's Density-Functional Theory

At present, DFT is the best method for describing the electronic, magnetic, structural, and vibrational properties of poly-atomic systems. If combined with the supercell approach, one can ensure that the treatment of the exchange-correlation (xc) functional remains the only relevant approximation. Different routes are taken to scrutinize and to correct present-day xc treatments:

Local xc correction approach

In the course of an earlier quantum Monte Carlo study [C. Filippi, S.B. Healy, P. Kratzer, E. Pehlke, and M. Scheffler, *Quantum Monte Carlo calculations of* H_2 *dissociation on Si(001)*. Phys. Rev. Lett. **89**, 166102 (2002)] it occurred to us that the *differences* between the local-density approximation and the essentially exact treatment of xc may be very short ranged. This idea is now being systematically explored. We also note that Joachim Sauer's group at the Humboldt University independently came to essentially the same conclusion when treating van der Waals interactions. Our studies on various adsorbates and bulk systems also reveal the problematic performance of Hartree-Fock, Møller-Plesset perturbation theory (MP2), and of the popular B3LYP functional for the description of metallic systems. An accurate, efficient, and practical approach to correct DFT-LDA (or GGA) slab calculations has been proposed and demonstrated. (Q.M. Hu, M. Fuchs, and K. Reuter)

Reduced-density-matrix-functional theory

In the *Max Planck Fellow Group* of Hardy Gross, reduced-density-matrix-functional theory (RDMFT) was taken to a new level of accuracy. Novel approximations for the exchange-correlation energy as functional of the natural orbitals and their occupation numbers were developed which, in all aspects, are far superior to density-functional theory: (i) For correlation energies, evaluated on the so-called G2/97 test set of 148 molecules, RDMFT outperforms all presently known GGA functionals, as well as hybrid functionals such as B3LYP. (ii) Band gaps of semiconductors and insulators, which are calculated from the discontinuity of the chemical potential, are within 4% of experimental numbers. (iii) Prototypical examples of static correlation, such as the dissociation of H_2, are well described. (iv) By construction, the most advanced RDMFT functionals reproduce the correlation energy of the uniform electron gas exactly (similar to the LDA/GGA) and, hence, provide a good description of metals. All this is achieved at a numerical cost roughly equivalent to that of Hartree-Fock calculations. (E. K. U. Gross, S. Sharma, and N. Helbig)

All-electron (LAPW-based) many-body perturbation theory

Several co-workers in the *Theory Department* are developing more rigorous approaches to evaluate the electron self-energy. Here, the *GW* approach, typically applied as a first order correction to the Kohn-Sham eigenvalues, has achieved great success in the past 20 years. However, pseudopotential and all-electron calculations sometimes give noticeably different results. Employing our recently developed APW+lo G_0W_0 formulation (starting from the WIEN2k code) resolved the disturbing discrepancies, tracing them back to two approximations underlying the pseudopotential approach (linearization of core-valence xc and pseudoization of valence orbitals) which both affect the calculated quasiparticle corrections. (R. Gómez-Abal, X. Li, and C. Ambrosch-Draxl)

Defect formation energies without the band gap problem

The Kohn-Sham band-gap typically does not agree with the experimental, optical gap. This must be so even in the exact DFT, where the difference reflects the discontinuity of $\delta E_{xc}/\delta n$ with respect to the particle number. In addition, present (semi)local exchange-correlation functionals suffer from the "self-interaction" problem, which adversely affects the description of localized states, such as defect or semi-core *d*-states. By splitting the total energies of different charge states into lattice-distortion and electronic contributions and correcting the latter by G_0W_0 calculations, an approach was designed that enables us to calculate defect related properties (e.g. formation energies, charge transition levels, defect levels) without the Kohn-Sham band gap problem. Applications concern defects at surfaces of III-V semiconductors and the self-interstitial in silicon. (P. Rinke, M. Hedström, and A. Schindlmayr)

How good is DFT for the description of hydrogen bonds?

Biological systems and water clusters are largely stabilized by hydrogen bonds. The precise understanding into how different DFT xc functionals deal with this type of interaction is, however, quite shallow. Departing from the often pursued "ostrich approach", we have used MP2 calculations at the complete basis set limit as a benchmark reference to examine the performance of 16 popular DFT xc functionals with respect to their performance in describing hydrogen bonds in small water clusters. Analysis shows shortcomings of all functionals and an increasingly poor description as the H-bond angle deviates from being linear, indicating an improper treatment of van der Waals interactions. This becomes even more relevant in larger clusters: For the low-lying isomers of the water hexamer, all xc functionals predict a different energetic ordering than MP2. To assess the effect of correlations beyond MP2, we performed diffusion quantum Monte Carlo calculations (QMC). Our QMC results confirm the energetic ordering of the isomers obtained from MP2 (and CCSD(T)). Thus in contrast to the "cyclic" structure preferred by DFT, our explicitly correlated calculations identify the "prism" as the ground state structure of the water hexamer. (B. Santra, A. Michaelides, and M. Fuchs)

III.2 The Atom-Centered Numeric Basis-Set Code "FHI-aims"

Over the last years, scientists in the *Theory Department* were involved in developments of several quite different electronic-structure codes, including Green-function codes, the FHI plane-wave pseudopotential code, and several important contributions to the FP-LAPW (WIEN2k) and the DMol^3 codes. Pseudopotentials are efficient, but some uncertainties are inherent [cf. e.g. Section III.1 "All-electron (LAPW-based)…" above]. Our new code ["FHI-*ab initio* molecular simulations (aims)"] therefore incorporates all electrons and the full potential. Thanks to the chosen basis, its efficiency is on par with or better than plane-wave pseudopotential codes, while the accuracy is equal to that of LAPW. Finite clusters and periodic systems are treated on an equal footing with a near $O(N)$ scaling for large systems. Important capabilities include: massive parallel scaling (in progress), Hartree-Fock exchange and MP2 perturbation theory, hybrid functionals, and G_0W_0 quasiparticle corrections. (V. Blum, F. Hanke, P. Havu, V. Havu, R. Gehrke, X. Ren, K. Reuter, P. Rinke, A. Sanfilippo, and A. Tkatchenko)

III.3 Linking Density-Functional Theory and Density-Matrix Theory

So far the theoretical description of carrier dynamics (e.g. optical excitations and subsequent phonon-assisted relaxation dynamics) was based on simplified assumptions and empirical material parameters. In collaboration with Andreas Knorr (TU Berlin) we developed an approach to handle such problems by combining DFT-LDA plus G_0W_0 calculations with density-matrix theory: Starting from a Hamiltonian in second quantization that includes electron-light and electron-phonon interactions, master equations for the population densities are derived. The method is demonstrated for the Si(100) 2x1 surface: Electrons are initially excited into the conduction band and then relax towards the minimum of the unoccupied surface band of Si(100). The population increase at the band bottom is found to exhibit two time scales, governed by a fast surface relaxation and a slower bulk relaxation. (N. Bücking, P. Kratzer, and A. Knorr)

III.4 Visualization Software Balsac, Version 3

The visualization and analysis software Balsac for periodic crystals and clusters has been completely rewritten using the full set of intrinsic MS Windows library functions. This offers complete compatibility with other PC products like e.g. presentation software. In addition, new number theoretical methods are applied inside Balsac, version 3, for fast construction of periodic lattices in two and three dimensions. As further improvements we mention the construction of ideal nanotubes of any set of crystal netplanes, animated views (with file output for post-processing), and greatly enhanced atom manipulation and graphical analysis features. Balsac, version 3, includes an extensive on-line help system providing the user with detailed explanation on all features. (K. Hermann)

IV. Applications – Some Highlights

IV.1 Structures and Total Energies

Solving atomic structures is a necessary prerequisite for analyzing and understanding the properties and function of surfaces, and of materials in general. Of particular interest, also in view of interactions and collaborations with the experimental departments of the FHI, are surfaces of transition metals and their oxides, as well as semiconductor surfaces and quantum dots.

New carbon nitride materials

Carbon nitrides are promising as very hard materials, and they also exhibit interesting properties as catalysts, but their actual structure is still debated. In collaboration with the *MPI of Colloids and Interfaces* and the FHI *Inorganic Chemistry Department* novel carbon nitride materials have been prepared and their properties investigated. The skilful combination of XRD, EELS, and TEM experiments on one side and DFT calculations on the other was crucial to clarify the synthesis route and to determine the material stoichiometry and structure. (J. Carlsson)

Structure of complex oxide surfaces

Further progress has been made to elucidate the geometric and electronic structure of complex vanadium and molybdenum oxide surfaces using DFT cluster techniques. Extended cluster models of differently terminated $V_2O_3(0001)$ surfaces (identified by STM together with theoretical structure optimizations on periodic systems by Kresse *et al.*) have been used to evaluate oxygen 1*s* core excitation (NEXAFS) spectra. The results support the vanadyl terminated half metal surface structure to be favored at very low oxygen pressure and yield a quite convincing interpretation of corresponding experimental NEXAFS spectra from the *Chemical Physics Department*. Cluster model calculations for oxygen core excitation near the bulk terminated $MoO_3(010)$ surface provide theoretical spectra in very good agreement with experimental polarization-resolved NEXAFS data. Analogous studies on MoO_3 thin films at Au(111), using structure models by Friend and Kaxiras, can explain the NEXAFS spectra only if one assumes additional surface defects (oxygen vacancies) in large amounts to be present. (M. Cavalleri, C. Kolczewski, and K. Hermann)

Surface oxides on Ag(111)

The surface oxide that has perhaps received the most attention is a *p*(4x4) phase that forms on Ag(111). For several years it was believed that the structure of this surface oxide had been ‘‘solved’’ by means of scanning tunneling microscopy (STM) experiments. Following a review paper of ours that addressed inconsistencies in the established structural model, an extensive series of DFT calculations along with new STM images from the group in Aarhus (J. Schnadt, F. Besenbacher*, et al.*) led to the proposal of a novel “Ag_6 model”. This structure is more stable than its predecessor, accounts for the observed coexistence of the *p*(4x4) phase with other structures, and highlights the potential dynamic complexity of the system that until now had not been appreciated. (A. Michaelides and K. Reuter)

Surface structure of $Fe_3O_4(100)$

A combination of DFT and low energy electron diffraction (LEED) analyses was used to determine the surface structure of $Fe_3O_4(100)$. Our previous [Phys. Rev. Lett. **94**, 126101 (2005)] DFT results on the $(\sqrt{2}\times\sqrt{2})R45^o$ reconstruction (induced by a Jahn-Teller-like distortion) was confirmed. For the detailed structure analysis a “chain-approach” (DFT→LEED→DFT→LEED) was, however, important for obtaining a trustful R-factor. (R. Pentcheva and W. Moritz)

The electronic structures of alkali adsorbates on alkali-halide surfaces

Density-functional theory and second order Møller-Plesset perturbation theory calculations indicate that halogen atoms bond preferentially to halide substrate atoms on a series of alkali halide surfaces, rather than to the alkali atoms as might be anticipated. An analysis of the electronic structure in each system reveals that this novel adsorption mode is stabilized by the formation of textbook two-center three-electron covalent bonds. (B. Li and A. Michaelides)

Interaction of water with salts, metals, and minerals

The structure and energetics of water at salt surfaces (including the dissolution of salt into water) and the nucleation and clustering of water into ice at transition metal as well as at kaolinite ($Al_2Si_2O_5(OH)_4$) surfaces has been analyzed in great detail using DFT and quantum chemistry methods. The latter system is interesting because of its relevance to cloud formation in the upper atmosphere. Specifically, kaolinite is one of the most common foreign materials found at the central nucleus of naturally formed snow flaks. Of several interesting results in this area we just mention the conclusion that many of the interesting properties of kaolinite with regard to ice nucleation are likely due to the amphoteric nature of its hydroxyl terminated surfaces. (A. Michaelides, B. Li, X. Hu, and J. Carrasco)

Adsorbate-induced faceting of Ir and Re surfaces

Using STM and LEED of T. E. Madey’s group (Rutgers University) found recently that strongly interacting adsorbates can induce facet formation on atomically rough metal surfaces, such as Ir(210) or Re($11\bar{2}1$). To understand the driving force behind this effect, we performed DFT calculations on the adsorption of oxygen and nitrogen at the facet-relevant surfaces of Ir and Re and constructed the corresponding (p, T)-surface phase diagrams. The results show how, by choosing appropriate adsorbates and annealing conditions, it is possible to tailor the surface morphology. (P. Kaghazchi and T. Jacob)

Metal/Solution Interface at Au(111) Electrodes

Although a wealth of information exists on the macroscopic behavior of metal/solution interfaces, the atomistic structure of the electric double layer and especially the ion and solvent distribution at the electrode is still largely unknown. Focusing on Au(111) in contact with aqueous H_2SO_4, DFT calculations were performed on the adsorption of sulfate and bisulfate together with coadsorbed water and/or hydronium molecules. The electron density distribution obtained for the most stable adlayer structure is found to be in perfect agreement with recent tunneling spectroscopy measurements by D. M. Kolb at the *University of Ulm*. (S. Venkatachalam and T. Jacob)

IV.2 Kinetics and Dynamics

The dynamics of atoms is studied using "on the fly" *ab initio* molecular dynamics (AIMD), e.g. for the interaction of water with NaCl. With such calculations we are able to simulate time spans of several picoseconds, and by employing Laio-Parrinello metadynamics low probability events are selectively boosted and probed. (A. Michaelides and L. Liu)

For some situations a picoseconds (maybe 1 ns) AIMD simulation provides useful information. However, in many cases this is far from sufficient and possibly misleading. For example, when one is concerned with *the function* of materials under realistic conditions a chemical reaction at a catalyst surface may only occur once every millisecond per surface unit cell, and corrosion typically proceeds with a speed of one atomic layer per minute. The method of choice for understanding such systems is the "first-principles kinetic Monte Carlo approach". If transition-state theory is applicable, which can be tested, the "first-principles kinetic Monte Carlo approach" is indeed a coarse-grained MD without loss of relevant information. In this way investigations of time spans of several seconds or even minutes become possible. Such studies are now an essential part of the research performed in Karsten Reuter's *Independent Junior Research Group*.

On the route to cross the scales beyond the *ab initio* kinetic Monte Carlo methodology, we studied the quality of phenomenological kinetics (rate equation/mean field theory). The analysis reveals dramatic limitations of this popular and widely used approach: Ignoring fluctuations and assuming a totally random structure causes severe inaccuracies. Both effects must be taken into account when error-controlled links and reverse mapping are requirements of a trustful multi-scale simulation. (S. Matera, H. Meskine, H. Metiu, and K. Reuter)

An example aiming at understanding surface reaction dynamics concerns the properties of nanoporous carbon. As shown previously, this material catalyzes the oxidative dehydrogenation of ethylbenzene. The mechanism of this reaction is still unclear. Thus, in a joint effort of experimental work in the FHI *Inorganic Chemistry Department* and the *Theory Department* the different reactions steps have been analyzed employing reactor experiments and DFT calculations of numerous, plausible reactions. Related to this work is also the question by which mechanism and on what time scales graphene-like materials will become oxidized. (J. Carlsson and F. Hanke)

IV.3 Spin-Electronics Materials

Motivated by the goals of future spintronics, there is a desire to identify magnetic thin films that are compatible with standard semiconductors. We therefore investigated various intermetallic compounds of Mn, Co, and Cr with silicon and with GaAs.

Heusler alloys: the role of finite temperature disorder and interface effects

Due to its robust ferromagnetism, even well above room temperature, the full Heusler alloy Co_2MnSi is a promising candidate material for spintronics. However, experimentally difficulties have been encountered, probably caused by disorder and still unclear surface and interface effects. Using DFT we built a cluster expansion Hamiltonian, and then employed the Monte Carlo approach to investigate the temperature dependence of alloy ordering for different Mn and Co concentration ratios. Several new (hitherto unknown) ground states were identified. One of them, having a gap at E_F in the minority spin channel, may be interesting for tunneling magneto-resistance devices. This work is supplemented by DFT calculations to model the Co_2MnSi/MgO(001) interface. (B. Hülsen and P. Kratzer)

Mn δ-doped layers in Si

Another route to achieve a spintronics-relevant material may be doping of Si with Mn. This had been discussed by several authors, typically concentrating on Mn at substitutional sites (Mn_{sub}) in analogy to Mn doped GaAs and Ge. Our DFT studies reveal that a narrow lateral doping profile, called δ-doping, of Mn impurities in Si is possible, and that a δ-layer of Mn at *interstitial sites* is even more stable that the previously proposed Mn_{sub} geometry. (H. Wu and P. Kratzer)

Ferromagnetism of CrAs layers

Recently, ferromagnetism has been observed for thin CrAs layers in GaAs(001). This was surprising, because bulk CrAs typically shows *anti*ferromagnetic behavior. Thus, the film was speculated to have a novel (unusual) structure. From DFT calculations, we conclude that under hetero-epitaxial strain, thin CrAs films assume a deformed NiAs configuration. This structure is consistent with the experimental results, and points to a *ferri*magnetic origin of the observed magnetization resulting from uncompensated magnetic moments at the CrAs/GaAs interface. (J. Hashemifar and P. Kratzer)

IV.4 Electronic Properties (Mainly Excitations)

Search for molecular switches: stilbene on Si(100)

One of the simplest molecules that may act as a switch is stilbene where the two phenyl groups can be arranged in two conformations, yielding cis- and trans-stilbene. The switching between the two species in the gas phase can be triggered by UV irradiation while this effect has not been observed for adsorbed stilbene on Si(100). Cluster model studies on the adsorbate system show that, first, strong adsorbate-substrate π bonding occurs via the central C=C double bond of adsorbed stilbene irrespective of its conformation (making an isomer transition difficult) and, second, the intra-molecular geometry of the adsorbate is affected substantially such that the structural difference between cis- and trans-stilbene is less obvious. Both results could explain the absence of radiation-induced switching of stilbene adsorbed on Si(100) by a simple geometric effect. (C. Kolczewski and K. Hermann)

Excitons in semiconductor quantum dots

The influence of inhomogeneous composition of InGaAs quantum dots on the electronic properties was studied using an empirical sp^3s^* tight-binding description. In contrast to effective-mass $\boldsymbol{k \cdot p}$ approaches, this enables us to take atomistic details of interfaces and compositional fluctuations into account. Selected eigenstates of the Hamiltonian are calculated using the folded-spectrum method, which makes it possible to look at system sizes of 10^6 atoms and more. The results explain the experimentally observed inversion of the dipole moment of quantum dot excitons and how this is affected by the quantum dot shape and the quality of the wetting layer. (A. Kleinsorge and P. Kratzer)

Spectroscopy of thin insulator films (thickness dependence)

Growing thin films of insulators on metals or doped semiconductors offers a route to experimentally study insulators with techniques such as STM and photoelectron spectroscopy. However, as previously shown from a ground state perspective, thin films must be (typically) considered a new material rather than as analogs to surfaces of bulk crystals. We now extended this work by including the spectroscopic perspective for clean and adsorbate-covered insulator films using DFT and G_0W_0 quasiparticle energy calculations. For CO as model adsorbate on the prototypical insulator/semiconductor system NaCl/Ge(100) we demonstrate that the substrate polarization significantly reduces the HOMO-LUMO gap of adsorbed CO compared to the gas phase. The degree of polarization and thus the CO gap can be varied by increasing the NaCl layer thickness. (Ch. Freysoldt and P. Rinke)

Bandgaps of semiconductors

Quasiparticle energy calculations in the G_0W_0 approximation have been successfully combined with density functional theory calculations in the exact-exchange optimized effective potential approach (EXX) to achieve a first-priciples description of the electronic structure that overcomes certain limitations of local or gradient corrected DFT functionals (LDA and GGA). Our approach proves to be particularly useful for materials, whose electronic band structure – a key quantity for devices – has been difficult to characterize experimentally (due to growth related problems) and theoretically (due to strong self-interaction effects and the band gap problem in LDA/GGA). For InN, an important material for solid state lighting, we were then able to identify the source for the puzzling, wide interval of experimentally observed band gaps as the Burstein-Moss effect. (P. Rinke, A. Qteish, and J. Neugebauer)

IV.5 Biophysics

The relative position of a residue with respect to its neighbors along the protein backbone is typically given in terms of the torsion angles φ and ψ. The frequency distribution of (φ, ψ) describes the conformational space accessible to a residue in protein structures. We investigated the influence of peptide H-bonds and long-range electrostatic interactions on the conformational space of a residue using infinite polypeptides and DFT. Employing cylindrical coordinates appears to be more convenient than the standard (φ, ψ) torsion angles. Comparing the theoretically predicted conformational space and experimentally observed backbone conformations in a large set of thousands of protein structures resolved by X-ray crystallography, we find excellent agreement in most of the configurational space, except for the so-called polyproline II (PPII) region. The analysis of this agreement and of the discrepancy sheds light on the importance of solvents and van der Waals interactions, which both are neglected in this theoretical work. (J. Ireta)

Conformations of β-sheets are the second most recurrent conformations observed in protein structures. The ideal β-sheet structure consists of two or more parallel or antiparallel strands (single peptide chains) that lay on the same plane and are hydrogen bonded to each other. Actual β-sheet motifs show an interstrand right-handed twist coupled to an intrastrand left-handed twist. Our DFT analysis reveals that these twists are actuated by compression originating from hydrogen bonds and repulsive interactions between strands. (J. Ireta)

An infinite neutral α-helix $(\mathrm{Ala})_\infty$ is the most stable helical conformation owing to the hydrogen bond cooperative effect, whereas α-helical $(\mathrm{Ala})_5$ is not even metastable in vacuo. In order to quantify and to explain the underlying cooperativity of hydrogen bonds we performed DFT calculations for finite-length helices: $(\mathrm{Ala})_n$, with n = 1-20). The results reveal how H-bond cooperativity and the termination (e.g. by alkali ions) act on the stability of gas phase helical peptides. Work towards deriving electronic “spectroscopic fingerprints” to connect theoretically predicted conformations to photoemission experiment is in progress. (V. Blum, J. Ireta, X. Ren, and P. Rinke)

A further study of H-bond cooperativity concerns infinitely long chains of hydrogen chloride (HCl), hydrogen fluoride (HF), hydrogen cyanide (HCN), formamide (H_3CNO) and 4-pyridone (H_5C_5NO). This set of molecules covers the range from weak to strong H-bonds. While the cooperativity predicted by DFT studies appears different in different systems, we find that the increase in H-bond strength correlates with the observed redistribution (polarization) in the calculated electron density on the molecules in the chain. A comparison of our results with estimates of the H-bond cooperativity from MP2, coupled cluster, and diffusion Monte Carlo calculations shows that DFT faithfully describes the cooperativity in these systems in which hydrogen bonds are not bent. (J. Ireta and M. Fuchs)

Publications of the Theory Department

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Freysoldt, C.: Ultrathin insulator films from first principles: A ground and excited-state perspective. FU Berlin 2007.

Invited Talks of the Members of the Theory Department

Volker Blum

Mar 2006 APS March Meeting, Baltimore, U.S.A.
Predicting Complex Ground State Structures from First Principles: Genetic Algorithm for Finding Accurate Coarse-Grained Hamiltonians

Sep 2006 Seminar at the Department of Physics and Astronomy, Brigham Young University, Provo, UT, U.S.A.
Between First Principles and Multiscale Modeling: Two Tales of Bridging Scales

Apr 2007 SimBioMa Workshop on Progress in Ab Initio Modelling of Biomolecules: Towards Computational Spectroscopy, Rome, Italy
Hydrogen Bonds, Cooperativity, and the Stability of Helical Polypeptides: Towards a Spectroscopic Fingerprint

Apr 2007 Seminar at the Department of Chemistry and Applied Biosciences, ETH Zürich, Lugano, Switzerland
"DFT and Beyond" with FHI-aims – a New All-Electron/Full-Potential Code Based on Local Orbitals

Jun 2007 Seminar at the Department of Materials, University of Oxford, U.K.
Hydrogen Bonds Determine Structure, but What Determines a H Bond's Strength? Cooperativity, Termination, and the Stability of Finite Polypeptide Helices

Johan Carlsson

Jan 2006 Seminar at the Department of Chemistry, University of Amsterdam, The Netherlands
A Microscopic View into Nanoporous Carbon Materials

Jan 2006 Seminar at the Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
Nanoporous Carbon Materials for Styrene Catalysis

Mar 2006 International Winterschool on Electronic Properties of Novel Materials (IWEPNM 2006), Kirchberg, Austria
Structural and Electronic Properties of Vacancies in Nanotubes and Nanoporous Carbon

Apr 2006 3rd EnerChem Meeting, Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany
Synthesis of Carbon Nitride in the Computer

Oct 2006 CANAPE Workshop on Carbon Nanotubes – Growth, Catalysis, Electronics, Berlin, Germany
Defects in Single Walled Carbon Nanotubes

Oct 2006 CECAM Workshop on Simulations of Novel Carbon Materials, Lyon, France
Simulations of Nanoporous Carbon for Chemical Applications

Dec 2006 5th ELCASS Meting, Palermo, Italy
Theoretical Insight into the Oxidation of Nanoporous Carbon Materials

Dec 2006 UK Carbon Group Meeting, London, U.K.
Theoretical Insight into the Role of Point Defects in Carbon Chemistry

Jan 2007 Seminar at the Department of Engineering, University of Cambridge, U.K.
Theoretical Insight into the Oxidation of Nanoporous Carbon Materials

Jul 2007 Seminar at the Department of Chemistry, University of Karlsruhe, Germany
Theoretical Insight into the Gasification of Graphene Based Carbon Materials

Aug 2007 Seminar at the Department of Chemistry, University of Dresden, Germany
Structural and Electronic Properties of Nanoporous Carbon Materials in an Oxygen Atmosphere

Aug 2007 NanoteC07 – International Conference on Carbon Nanoscience and Nanotechnology, University of Sussex, Brighton, U.K.
Theoretical Insight into the Oxidation of Graphene-Based Carbon

Sep 2007 CASTEP Workshop, York University, U.K.
Pseudopotentials

Ricardo Gómez Abal

May 2007 Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany
Implementation of an All-Electron G_0 W_0 *Code within the FP-LAPW Method: The Importance of Core-Valence Interactions*

Thomas Hammerschmidt

Oct 2005 IPAM Workshop on Density-Functional Theory Calculations for Modeling Materials and Bio-Molecular Properties and Functions – Materials Modeling Seminar Series, UCLA, Los Angeles, U.S.A.
Growth Properties of InAs/GaAs Nanostructures Studied with a DFT Derived Many-Body Potential

Jul 2006 Department of Electronic and Electrical Engineering, The University of Sheffield, U.K.
Growth Simulations of InAs/GaAs Quantum Dots

Oct 2006 SANDiE Workshop on Simulation of Self-Assembled Nanostructures, Duisburg, Germany
Inter-Atomic Potentials for Simulation of Strained Nanostructures

Klaus Hermann

Nov 2005 Riken Institute of Technology, Tokyo, Japan
Chemical Properties of Vanadium Oxide Surfaces and Reactive Adsorption of Small Molecules: Ab Initio DFT Cluster Studies

Nov 2005 Department of Applied Chemistry, Tohoku University, Sendai, Japan
Chemical Properties of Vanadium Oxide Surfaces and Reactive Adsorption of Small Molecules: Ab Initio DFT Cluster Studies

Nov 2005 International Symposium on Catalysis on Oxide Materials – Theory and Experiment – Sharing Needs and Capabilities, Cracow, Poland
Excitations and Reaction at Metal and Oxide Surfaces: Cluster Models Can Help to Interpret Experimental Data

Jan 2006 Colloquium, Karl-Franzens-Universität Graz, Austria
Excitations and Reactivity at Transition Metal Oxide Surfaces: Ab Initio Cluster Models for Vanadium Oxide

Apr 2006 Physics Department, Rutgers University, Piscataway, U.S.A.
Excitations and Reaction at Metal and Oxide Surfaces: Cluster Models Can Help to Interpret Experimental Data

Apr 2006 Chemistry and Biochemistry Department, Harvard University, Cambridge, U.S.A.
Excitations and Reaction at Metal and Oxide Surfaces: Cluster Models Can Help to Interpret Experimental Data

Apr 2006 CRISP Seminar, Faculty of Engineering, Solid State and Optics, Yale University, New Haven, U.S.A.
Excitations and Reaction at Metal and Oxide Surfaces: Cluster Models Can Help to Interpret Experimental Data

Apr 2006 deMon Developers Workshop, Kananaskis, Canada
Recent Developments of StoBe and Application to Systems of Catalytic Interest

May 2006 Festkolloquium Prof. Staemmler, Ruhr-Universität Bochum, Germany
Von Menschen und Molekülen: theoretische Untersuchungen zur Adsorption und Reaktion von Oberflächen

Jun 2006	Physikalisches Kolloquium, Christian-Albrechts-Universität Kiel, Germany *Ab-initio-Clusteruntersuchungen zur Röntgenabsorptionsspektroskopie: von Molekülen zur Oberfläche und zum Volumen*
Jun 2006	3rd Humboldt Conference on Computational Chemistry, Varna, Bulgaria *Ab Initio Cluster Studies for X-Ray Absorption Spectroscopy: From Molecules to Surfaces and Bulk*
Sep 2006	E-MRS Fall Meeting, Warsaw, Poland *Excitation and Reaction at Metal and Oxide Surfaces: Cluster Models Help to Interpret Experiments*
Feb 2007	Seminar at the Chemistry Department, UC Berkeley, U.S.A. *Ab Initio Cluster Studies for X-Ray Absorption Spectroscopy: From Molecules to Surfaces and Bulk*
Apr 2007	San Luis IV Symposium on Surfaces, Interfaces, and Catalysis, Cuernavaca, Mexiko *Reactivity at Metal and Oxide Surfaces: Theory Can Help to Interpret Experimental Data*
Apr 2007	CINVESTAV, Mexico City, Mexico *Excitation and Reaction at Metal and Oxide Surfaces: Ab Initio Cluster Simulations Can Help to Interpret Experimental Results*
Jun 2007	BASF, Bereich Katalyse, Ludwigshafen, Germany *Reaktivität an Metall- und Metalloxidoberflächen: ab-initio-Cluster-Rechnungen unterstützen das Experiment*
Sep 2007	IDECAT Summerschool on Computational Methods for Catalysis and Materials Science, Porquerolles, France *XAS Theory Applied to Metal and Oxide Surfaces of Catalytic Interest*
Oct 2007	ACTINET Workshop on What Can we Learn from Coupling Theoretical Chemistry with X-Ray Absorption Spectroscopy?, Avignon, France *X-Ray Absorption Theory for Oxide Surfaces of Catalytic Interest*

Björn Hülsen

Jan 2007	Graduiertenkolleg “Struktur und Dynamik heterogener Systeme”, Universität Duisburg-Essen, Germany *An Introduction to the Cluster Expansion with the Example of Pseudo-Binary* Co_2MnSi

Joel Ireta

Nov 2005 Workshop on Recent Developments in Interatomic Potentials for Materials Science and Biophysics, Institute of Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, U.S.A.
Cooperative Effects in Hydrogen Bonding

Jul 2006 Workshop on Progress in Ab Initio Modeling of Biomolecules: Methods and Applications, Lorentz Center, Leiden University, The Netherlands
Why Helices are Right-Handed and Beta-Sheets Left-Handed: Insight from First-Principles Calculations

Mar 2007 Physical Chemistry Seminar, Chemistry Department, Metropolitana University, Mexico
Influence of Long-Range Interactions and Hydrogen Bonding on the Protein Structure

Jun 2007 IPAM Reunion Conference I: Bridging Time and Length Scales in Materials Science and Bio-Physics, UCLA, Lake Arrowhead, U.S.A.
Assessing the Influence of Hydrogen Bonding and Long Range Interactions on the Protein Conformational Space

Timo Jacob

Jan 2006 Forschergruppen-Kolloquium, Universität Kiel, Germany
Modeling Electrocatalysis under Realistic Conditions

Feb 2006 Seminar für Oberflächenprobleme, Universität Bonn, Germany
Modeling Electrocatalysis under More Realistic Conditions – Oxygen Reduction Reaction

Mar 2006 Seminar at the Laboratory for Surface Modification, Rutgers University, Piscataway, U.S.A.
DFT-Studies on the Oxygen-Induced Surface Faceting of Ir(210)

Mar 2006 Lafayette College, Easton, U.S.A.
Modeling Electrocatalysis or Why Still No Fuel Cells?

Jun 2006 Seminar at the Hahn-Meitner-Institut, Berlin, Germany
Modeling Electrocatalysis under More Realistic Conditions – Oxygen Reduction Reaction

Sep 2006 Seminar at the Forschungszentrum Jülich (IWV-3), Germany
Nano-Faceted Ir(210): Probe for Structural and Size Effects in Surface Chemistry

Oct 2006 Workshop on Fuel Cell Catalysis: A Surface Science Approach, Lorentz Center, Leiden, The Netherlands
Extended Ab Initio Atomistic Thermodynamics for Electrochemical Systems

Dec 2006 Forschungsseminar "Reaktive Strömung", Institut für Wissenschaftliches Rechnen (IWR), Universität Heidelberg, Germany
Towards a More Realistic Modeling of Electrochemical Systems

Dec 2006 Annual Meeting, European Laboratory for Catalysis and Surface Science (ELCASS), Palermo, Sicily, Italy
Towards a More Realistic Modeling of Electrochemical Systems

Mar 2007 233rd National Meeting of the American Chemical Society (ACS), Chicago, U.S.A.
Towards a More Realistic Modeling of Electrochemical Systems

May 2007 Elektrokatalyse Symposium, Paul Scherrer Institut, Villingen, Switzerland
Understanding Electrochemical Systems from First Principles

Jun 2007 Seminar at the University of Strasbourg, France
Towards a More Realistic Modeling of Electrochemical Systems

Aug 2007 234th National Meeting of the American Chemical Society (ACS), Boston, U.S.A.
Bridging the Gap between Nanoparticles and Extended Surfaces in Electrochemistry

Aug 2007 234th National Meeting of the American Chemical Society (ACS), Boston, U.S.A.
Modeling Electrocatalysis

Aug 2007 234th National Meeting of the American Chemical Society (ACS), Boston, U.S.A.
Understanding Electrochemical Systems from First Principles

Aug 2007 Rutgers University, Piscataway, U.S.A.
Adsorbate-Induced Facet-Formation on Ir and Re Surfaces

Alexander Kleinsorge

Oct 2006 SANDiE Workshop on Simulation of Self-Assembled Nanostructures, Duisburg, Germany
Tight-Binding Calculations of Single-Particle States in Quantum Dots

Peter Kratzer

Dec 2005	Physikalisches Kolloquium, Universität Göttingen, Germany *Bauen mit Atomen - Computersimulationen der Struktur und der Eigenschaften von Halbleiter-Quantenpunkten*
Feb 2006	Kinetik-Seminar, Deutsche Gesellschaft für Kristallforschung und Kristallzüchtung, Halle, Germany *Adsorption, Diffusion und Nukleation bei der MBE von III-V-Halbleitern – Ergebnisse von ab initio-Methoden*
Apr 2006	Seminar at the Lehrstuhl Theoretische Chemie, Ruhr-Universität Bochum, Germany *Chemical Reactions and Surface Diffusion of Hydrogen on the Si(001) Surface – a Test Ground for Methodologies*
May 2006	Seminar at the Materials Modelling Lab, Materials Department, Oxford University, U.K. *Growth-Related Structural and Electronic Properties of InAs Quantum Dots on GaAs*
Jul 2006	Workshop on Computational Materials Theory, Bangalore, India *Epitaxial Growth of Transition-Metal Silicides on Silicon*
Jul 2006	28th International Conference on the Physics of Semiconductors, Vienna, Austria *Transition-Metal Silicides as Novel Materials for Magnet-Semiconductor Heterostructures*
Sep 2006	28th International Symposium on Semiconductor Nanostructures, Berlin, Germany *Thermodynamics and Kinetics of Quantum Dot Growth*
Sep 2006	Università di Modena-Reggio Emilia, Modena, Italy *Growth-Related Structural and Electronic Properties of InAs Quantum Dots on GaAs*
Sep 2006	Workshop on Epitaxial Growth and Fundamental Properties of Semiconductor Nanostructures, Bonassola, Italy *Atomistic Theory of InAs/GaAs Quantum Dot Growth*
Oct 2006	Seminar at the Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Germany *Silicon-Based Magnetic Semiconductor Heterostructures: Insights from Band Structure Theory*
May 2007	Symposium “Werkstoff-Simulation”, Ruhr-Universität Bochum, Germany *Bridging the Gap between Electronic Structure and Materials Properties: Nucleation, Growth, and Alloy Formation from First Principles*

Jun 2007	Symposium on Current Trends in Physics and Chemistry, Technical University of Denmark, Lyngby, Denmark *Electronic and Magnetic Properties of Co-Mn-Si Alloys from a First-Principles Cluster Expansion Method*
Jun 2007	2nd International Lund Workshop on Nanowire Growth Mechanisms (Wire Growth 2007), Lund, Sweden *Thermodynamic and Kinetic Aspects of Nanowire Growth*
Jun 2007	IPAM Reunion Conference I: Bridging Time and Length Scales in Materials Science and Bio-Physics, UCLA, Lake Arrowhead, U.S.A. *Multi-Scale Simulations of Magnetic Alloys Using a First-Principles Cluster Expansion Method*

Angelos Michaelides

Jan 2006	Theoretical Chemistry Colloquium, Ruhr-Universität Bochum, Germany *Simulating Ice Nucleation from First Principles*
Jan 2006	Computational Electronic Structure Conference, Robinson College, Cambridge, U.K. *Ab Initio Ice Growth at Metal Surfaces*
Mar 2006	DPG Frühjahrstagung, Dresden, Germany *Ab Initio Ice Growth at Metal Surfaces*
Apr 2006	Department of Theory, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany *Electronic Structure Simulations of Everyday Materials: Water, Ice and Salt*
Apr 2006	Joint Seminar at The Royal Institution of Great Britain and the Department of Chemistry, University College London, U.K. *Electronic Structure Simulations of Water-Solid Interfaces: Waltzing Water Molecules, Novel 2D Ice Phases, and More*
May 2006	Seminar at the Materials Modeling Laboratory (MML), University of Oxford, U.K. *Electronic Structure Simulations of Everyday Materials: Water, Ice and Salt*
Jun 2006	10th DICP Symposium on Chemical Physics of Materials and Inauguration Workshop of the MPG-CAS Partner Group, Dalian Institute of Chemical Physics, P.R. China *Density Functional and Quantum Chemical Simulations of Everyday Materials: Water, Ice and Salt*

Jun 2006	6th ICQS Workshop on Novel Quantum Phenomena in Condensed Matter Physics, Beijing and Hangzhou, P.R. China *Ice Hexamers at Hydrophobic Metal Surfaces: Hydration and Hydrogen Bonding Competition*
Jun 2006	Department of Chemistry, Fudan University, Shanghai, P.R. China *Salt, Water, and Ice: Density Functional and Quantum Chemical Simulations*
Jul 2006	Joint Seminar at the London Centre for Nanotechnology and Department of Physics, University College, London, U.K. *Towards a First Principles Description of Ice Nucleation and Salt Dissolution*
Aug 2006	XV International Materials Research Congress, Cancún, México *Density Functional and Quantum Chemical Simulations of Everyday Materials: Water, Ice and Salt*
Sep 2006	24th European Conference on Surface Science (ECOSS 24), Paris, France *Density Functional and Quantum Chemical Simulations of Everyday Materials: Salt and Water*
Nov 2006	European Science Forum, Heidelberg, Germany *Atomic-Scale Simulations of Water-Solid Interfaces*
Nov 2006	European Young Investigator Awardee Symposium (EURYIAS), Institut des Sciences et d'Ingénierie Supramoléculaires (I.S.I.S.), Strasbourg, France *Atomic-Scale Simulations of Water-Solid Interfaces*
Dec 2006	Department of Theoretical Chemistry, University of Potsdam, Germany *Density Functional and Quantum Chemical Simulations of Everyday Materials: Salt, Water and Ice*
Jan 2007	Department of Chemistry, The Queens University of Belfast, U.K. *On How Salt Dissolves and Ice Clusters Nucleate: Insight from Ab Initio Electronic Structure Theory*
Jan 2007	Department of Chemistry, The Queens University of Belfast, U.K. *An Introduction to the Theory of Metal Surfaces*
Jan 2007	Faraday Symposium on Adsorption and Reactions on Solid Surfaces, University College London, U.K. *An Atomic-Level Description of Salt Dissolution from First Principles*
Apr 2007	Surface Science Group, Department of Chemistry, University of Cambridge, U.K. *Salt and Water, Clay and Ice: Insight from DFT and Quantum Chemistry*

Patrick Rinke

May 2006	Nanoquanta 3rd Young Researcher Meeting, Rome, Italy *An Introduction to Quasiparticle Spectra in the GW Approximation*
Sep 2006	2nd International Workshop on Time Dependent Density-Functional Theory (TDDFT): Prospects and Applications, Benasque, Spain *The Band Gap of InN and ScN: A Quasiparticle Energy Study Based on Exact-Exchange Density-Functional Theory*
Jan 2007	13th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy *Exact-Exchange Based Quasiparticle Energy Calculations Applied to (Transition) Metal Nitrides: ScN and InN*
May 2007	3rd International Workshop on DFT Applied to Metals and Alloys, Oran, Algeria *Calculating Excitations in Large Systems with FHI-aims, a New, All-Electron DFT and GW Code*
Jun 2007	19th Annual Workshop on Recent Developments in Electronic Structure Methods, North Carolina State University, Raleigh, U.S.A. *Exact-Exchange Based Quasiparticle Energy Calculations Applied to (Transition) Metal Nitrides: ScN, InN and More*
Sep 2007	CCP2007 Conference on Computational Physics, Brussels, Belgium *Exact-Exchange Based Quasiparticle Energy Calculations Applied to (Transition) Metal Nitrides: ScN, InN and More*

Matthias Scheffler

Nov 2005	4th International Symposium on Surface Science and Nanotechnology (ISSS-4), Omiya, Saitama, Japan *Surface Chemistry and Catalysis from First Principles*
Nov 2005	Symposium at the University of Trieste, Italy *Statistical Mechanics from First Principles: Application to Nanometer-Scale Phenomena at Surfaces*
Dec 2005	PacifiChem 2005 Conference, Honolulu, Hawaii, U.S.A. *Catalytic Properties of Nanometer and Sub-Nanometer Thin Oxide Films at Surfaces of Late Transition Metals Studied by Ab Initio Statistical Mechanics*
Jan 2006	ICMR-ICTP Advanced Workshop on Recent Developments in Inorganic Materials, Trieste, Italy *The Function of Heterogeneous Catalysts: New Insights by First-Principles Statistical Mechanics*

Jan 2006	Materials Research Outreach Symposium (MROP), UCSB, Santa Barbara, U.S.A. *Catalysis from First Principles*
Feb 2006	Winter School “Computational Nanoscience: Do it yourself!”, Zentralinstitut für Angewandte Mathematik (ZAM), Forschungszentrum Jülich, Germany *Ab Initio Electronic Structure Calculations: Status and Challenges*
Mar 2006	Rundgespräch “Elektronische Struktur von Festkörpern: Experiment und Theorie”, Bad Honnef, Germany *Theorie der elektronischen Struktur von Oberflächen*
Apr 2006	5th Brazilian / German Workshop on Applied Surface Science, Mangaratiba, Brazil *Theory of Surfaces*
Apr 2006	DFTEM 2006 – bringing together two communities: International Conference on Density Functional Theory (DFT) and Transmission Electron Microscopy (TEM), Vienna, Austria *Towards an Exact Treatment of Exchange and Correlation*
May 2006	Institute for Interfacial Catalysis (IIC), Pacific Northwest National Laboratory (PNNL), Richland, WA, U.S.A. *Novel Insights into Heterogeneous Catalysis by First-Principles Statistical Mechanics*
May 2006	University of California (PIRE-ECCI), Santa Barbara, U.S.A. *Insights into the Physics of the Earth Core, Quantum Dots, Catalysis, and Mad Cow Disease*
May 2006	Physikalisches Kolloquium, Universität Würzburg, Germany *Festkörperphysik und Materialwissenschaften mit ab initio Statistischer Mechanik*
Jun 2006	11th International Conference on Theoretical Aspects of Catalysis (ICTAC-11), Schmöckwitz, Germany *Novel Insights into Heterogeneous Catalysis by First-Principles Statistical Mechanics*
July 2006	DOE Workshop on Basic Research Needs for Advanced Nuclear Energy Systems, Washington, D.C., U.S.A. *Ab Initio Modeling of Corrosion and Catalysis*
Aug 2006	PIRE-ECCI/ICMR Summer Conference, Santa Barbara, U.S.A. *From the Many-Particle Problem to the Kohn-Sham Functional; and How to Deal with Excited States (the GW Approach)*
Aug 2006	PIRE-ECCI/ICMR Summer Conference, Santa Barbara, U.S.A. *From Electronic Structure Theory to Material Science*

Aug 2006	Colloquium at the Korea Research Institute of Standards and Science (KRISS), Daejeon, S. Korea *Computational Science and Engineering from First Principles*
Aug 2006	Colloquium celebrating the 30th Anniversary of the Korea Research Institute of Chemical Technology (KRICT), Daejeon, S. Korea *Computational Nano-Scale Research – Novel Insights into the Function of Heterogeneous Catalysis*
Aug 2006	Conference on Computational Physics 2006 (CCP 2006), Gyeongju, S. Korea *Novel Insights into Heterogeneous Catalysis by First-Principles Statistical Mechanics*
Sep 2006	CCP5 Annual Conference 2006 on Phase Behaviour From Molecular Simulation, IPI, University of Bradford, U.K. *Surface Chemistry and Catalysis Studied by First-Principles Statistical Mechanics*
Dec 2006	QSD2006 – International Conference on Quantum Simulators and Design, Hiroshima University, Japan *Ab initio Multiscale Modeling of the Function of Materials: Success Stories and Unsolved Challenges*
Jan 2007	Colloquium at the Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden-Rossendorf e.V., Germany *Get Real! The Importance of Complexity for Understanding the Function of Materials*
Jan 2007	Department of Chemistry, University of Amsterdam, The Netherlands *Get Real! The Importance of Complexity for Understanding the Function of Materials*
Feb 2007	School of Physics, University of Sydney, Australia *Key Theoretical and Algorithmic Needs for Predictive Modeling of Surface Chemistry and Catalysis*
Mar 2007	20th Symposium on Surface Science (3S07), Les Arcs, France *Key Theoretical and Algorithmic Needs for Predictive Modeling of Surface Chemistry and Catalysis*
May 2007	Colloquium at the Institut für Physik, Technische Universität Ilmenau, Germany *Get Real! Ab initio Theorie der Eigenschaften und Funktionen moderner Materialien*
May 2007	Transdisziplinäres Kolloquium "Dynamische Erde", Department für Geo- u. Umweltwissenschaften, LMU, München, Germany *Frontiers in Earth Sciences – Materials Sciences and Engineering from First Principles*

Jun 2007	Colloquium at the Faculty of Science, Lund University, Sweden *Describing and Understanding the Properties and Functions of Materials from Only Atomic Nuclei and Electrons*
Jun 2007	IPAM Reunion Conference I: Bridging Time and Length Scales in Materials Science and Bio-Physics, UCLA, Lake Arrowhead, U.S.A. *Key Theoretical and Algorithmic Needs for Predictive Modeling of Surface Chemistry and Catalysis*
Jun 2007	Roberto Car 60th Birthday Symposium, ICTP, Trieste, Italy *Towards an Exact Treatment of Exchange and Correlation in Materials*
Aug 2007	11th ICFSI – International Conference on the Formation of Semiconductor Interfaces: From Semiconductors to Nanoscience and Applications with Biology, Manaus, Brazil *Transition-Metal Silicides as Materials for Magnet-Semiconductor Heterostructures*
Aug 2007	Seminar at the INMETRO – National Institute of Metrology, Standarization and Industrial Quality, Rio de Janeiro, Brazil *Get Real ! The Importance of Complexity for Understanding the Function of Materials*
Aug 2007	Seminar at the Instituto de Física, Universidade Federal do Rio de Janeiro (UFRJ), Brazil *Formation and Properties of Silicon-Based Magnetic Semiconductor Interfaces*

Independent Junior Research Group

Head: Karsten Reuter

Guest scientists staying for at least six months, paid by FHI:

Juan Beltrán

Vladimir Froltsov

Guest scientists staying for at least six months, paid from external funds:

Paula Abufager
Huiqiu Deng
(jointly with the Theory Department)
Joost Frenken

Hakim Meskine
Jutta Rogal
Li Sheng AvH Fellow

Graduate students: 16 (3 of those jointly with the Theory Department)

Diploma students: 1

Recent Developments in the Independent Junior Research Group

Head: Karsten Reuter

I. General Remarks

Following its originally defined mission the goal of the *Independent Junior Research Group (IG)* “First-Principles Statistical Mechanics” is to develop and apply predictive-quality general methodologies for multi-scale materials simulations, focusing, in particular, on links between first-principles electronic-structure calculations at the finest, molecular scale and equilibrium and non-equilibrium statistical mechanics simulations to address mesoscopic system properties. Critical to assigning the desired predictive quality to our simulations is the development of robust links between the various employed theories with error-control across the scales. At each scale, the simulations have approximations that introduce uncertainty, and bridging from one scale to another gives rise to additional uncertainty. One of the emerging central methodological research objectives of the group is therefore to overcome the present state-of-the-art, which is still dominated by *ad hoc* linkage concepts and gain control of how the multiple sources of uncertainty translate to the final multi-scale results. Only robust error-controlled links will allow to propagate the first-principles accuracy up the chain of methods to successively increasing spatial and temporal scales. This description encompasses then in particular a full reverse mapping capability, i.e., the power to analyze in detail how the electronic structure (bond breaking and bond making) actuates the resulting meso- and macroscopic materials properties, function, and performance.

With respect to the research themes the core activities of the group continue to be centered on surface chemistry and catalysis, comprising also detailed studies on gas-surface dynamics and ensemble properties of molecular networks. With the prospect to achieve a parameter-free, quantitative calculation of the macroscopic catalytic activity we have further developed our hierarchical approach of combining density-functional theory (DFT) with kinetic Monte Carlo (kMC) simulations and are applying it now to a range of model catalysts and reactions. Just initiated methodological activities aim to further advance this approach by integrating a refined description of the local heat dissipation and a treatment of the hydrodynamic flow of the chemicals over the catalyst surface. This requires to couple in a self-consistent manner the atomistic statistical simulations of the chemical reactions and processes at the solid surface with a continuum description of the heat and mass transport.

Further research themes focus on elucidating the structure and reactivity of small atomic clusters and on the interaction of organic molecules with solid surfaces. Highlights of our current work are summarized below in Sec. III (methodology) and IV (applications).

II. Funding, Personnel and Related Activities

In its third year of existence the group has reached its full size, fluctuating including visitors at around 15 members. Funding comes apart from the *IG* budget directly provided by the Max-Planck-Gesellschaft (MPG) predominantly from research projects within the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) or the European Union (EU), where projects preceded by the superscript$^{(ThD)}$ are in collaboration with the *Theory Department*.

Collaborative actions:

- EU – Specific Targeted Research Project (STREP)$^{(ThD)}$: Oxidation of Nanomaterials (NanO$_2$), coordinator: A. Stierle, until 03/2007; K. Reuter, M. Scheffler
- EU – COST Action P-19: Multi-Scale Modeling of Materials; K. Reuter
- EU – Marie Curie Host Fellowship for Early Stage Research Training (EST)$^{(ThD)}$: Molecular Networks at Phase Boundaries (MONET), coordinator: J. N. Andersen; A. Michaelides, K. Reuter, M. Scheffler
- SFB 658$^{(ThD)}$: Elementary Processes in Molecular Switches at Surfaces, project C4, spokesperson: M. Wolf; K. Reuter, M. Scheffler
- SPP 1091$^{(ThD)}$: Bridging the Gap between Ideal and Real Systems in Heterogeneous Catalysis, spokesperson: R. Imbihl, until 11/2006; K. Reuter, M. Scheffler
- IFP – Institut Français du Pétrole$^{(ThD)}$, Ph.D. Student Program: Kinetic Monte Carlo Simulations of Gas Solid Reactions and Applications to Hydrotreating Catalysts; K. Reuter, M. Scheffler
- Strategischer Innovationsfonds of the MPG President: Multi-Scale Materials Modeling of Condensed Matter (MMM); K. Reuter

Individual projects:

- DFG – Project: *Ab Initio* Description of Non-Adiabatic Effects in Dissociative Adsorption; K. Reuter, A. Groß
- EPSRC – Engineering and Physical Sciences Research Council, Project: Dynamic Processes in the Adsorption and Formation of Organic Molecules on Surfaces; W. Hofer, K. Reuter

Particularly the newly launched MPG Initiative Multi-Scale Materials Modeling embeds the group nicely into concurrent multi-scale modeling efforts at other MPG institutes, whereas the participation in the DFG Collaborative Research Centre SFB 658, as well as the group head's teaching activities and involvement in the preparations for the DFG excellence initiatives provided close contacts and links to the Berlin universities and research institutions. Strong links are furthermore maintained to several groups by means of shared Ph.D. students who conduct parts of their research in the group in Berlin. This includes the Institut Français du Petróle Paris (Prof. H. Toulhoat), the Institut für Kristallzüchtung Berlin (Dr. W. Miller), the Universidad Autónoma de Madrid (Dr. J. Merino) and the University of Liverpool (Prof. W. Hofer).

Over the past two years, the group has also continued to be actively involved in various services to the scientific and non-scientific community. Lectures were not only delivered at the Free University, at the International Max Planck Research School or at several international summer schools, but also at public events like the "Long Night of the Sciences" or the "Girls Day 2006". Further visibility has again come from the organization or co-organization of international workshops, including:

- 10th DICP - *Dalian Institute of Chemical Physics*, Symposium on "Chemical Physics of Materials", 1 - 3 June, 2006, Dalian, China; organizers: Weixue Li (Chinese Academy of Sciences, Dalian, China), K. Reuter, and M. Scheffler
- Ψ_k and CECAM (Centre Européen de Calcul Atomique et Moléculaire), Workshop on "Catalysis from First Principles", 11 - 14 September, 2006, Lyon, France; organizers: A. Michaelides, M. Scheffler, K. Reuter, J. Nørskov (Technical University of Denmark, Lyngby), and J. Hafner (University of Vienna, Austria)
- Workshop on "Multi-Scale Approaches to Nanomechanics", 5 - 7 February 2007,

Lyon, France; organizers: R. Perez (Universidad Autónoma de Madrid, Spain) and K. Reuter

- Workshop on "Non-Adiabatic Dynamics at Surfaces", 22 - 25 October, 2007, Schloss Reisensburg, Germany; organizers: J. Behler (University of Bochum), P. Rinke, K. Reuter, and M. Scheffler

The already achieved accomplishments, as well as increased recognition of the group as its own entity within the Fritz-Haber-Institut have furthermore led to the following incidences which we are particularly proud to report:

- With the granting of the doctorate to Dr. Jutta Rogal the first official Ph.D. thesis of the *IG* has been completed. The thesis work was not only marked with "*summa cum laude*", but was also awarded with the Otto Hahn Medal of the MPG for an outstanding Ph.D. thesis.
- With Dr. Li Sheng we are happy to welcome the first Alexander von Humboldt fellow that has explicitly chosen the *IG* as his host.
- In December 2006, the *IG* has officially joined the local International Max Planck Research School on "*Complex Surfaces in Materials Science*" as a new workgroup.
- Since October 2005 the group head is the elected spokesperson of all *IG* s within the Chemical Physical Technical Section (CPTS) of the MPG.

Initially, the local computer equipment of the group was restricted to a Linux cluster (3 IBM Blade Centers with 14 double 2.8 GHz Xeon processors each) and our beloved antique 23 Compaq ES-45 servers (4 shared-memory processors each). In August 2006, the group applied for 300.000 Euro to install a new local compute cluster at the MPG internal *Beratender Ausschuss für EDV-Anlagen* (BAR, advisory board for compute equipment). The proposal was rated as "exemplary" and fully granted. Since January 2007, the purchased five 16-way IBM p575 compute nodes with dual-core Power5+ (1.9 GHz) processors, 4 GB memory per core and a global file system with 5 TB net storage capacity are fully operational and provide the new computational backbone for the group's large scale calculations. Further computing time is available through access to the shared-memory IBM p690 (Power4) / p575 (Power5) computers at the MPG computing centre in Garching, as well as through successful proposals to the Distributed European Infrastructure for Supercomputing Applications

(DEISA) initiative and the Leibniz computing centre in Munich. Summing all of these components together, the computational facilities of the group are satisfactory, at present.

III. New Concepts, Methods and Techniques

III.1 Electronic-structure level

The group addresses the finest scale in the modeling hierarchy, namely the electronic structure level, now with both density-functional as well as *ab initio* quantum chemistry methods. For polyatomic systems, DFT with present-day exchange-correlation (xc) functionals has proven to be an excellent technique for calculations at this electronic structure base at an intense, but still affordable computational cost. However, it is not as good for certain types of binding interactions like van der Waals interactions that are playing a crucial role in an increasing number of *IG* projects. Ongoing activities at the electronic-structure level aim therefore at the formulation and implementation of approaches that provide a reliable energetics also in these cases and in a computationally most efficient way.

- Having contributed to the new in-house DFT code FHI-aims since its very inception, we are presently engaged in the implementation of second-order Møller-Plesset perturbation theory (MP2) as one of the computationally cheapest methods that can e.g. account (from first principles) for van der Waals interactions. In order to make the calculations computationally tractable the implementation relies on the efficiency of modern resolution of identity techniques, as well as the construction of most compact converged numeric atomic orbital basis sets. (A. Sanfilippo, X. Ren, P. Rinke, V. Blum, and M. Scheffler)
- When looking at appropriate energy differences, prominent deficiencies in present-day local (LDA) and semi-local (GGA) xc functionals like the spurious self-interaction or the lack of van der Waals interactions are intriguingly short ranged. We exploit this with a systematic, non-empirical scheme to locally correct the total LDA or GGA energy of extended systems by analyzing properly chosen clusters and employing higher-quality quantum chemistry methods. The approach works for bulk systems as

well as for defects in the bulk and at surfaces, as demonstrated in applications to the adsorption of CO or benzene at Cu(111), to Li impurities in MgO or to the equation of state of Cu bulk. (Q.M. Hu, E. McNellis, L. Sheng, M. Fuchs, and M. Scheffler)

III.2 Matching of electronic and mesoscopic regime

In the effort to integrate the various levels of theory into one multi-scale simulation, the methodologically most appropriate approach for the problems tackled in the *IG* is to link the disparate length and time scales by information passing. This information is transferred in form of first-principles parameters that then form the basis of the statistical simulations. A robust link with error-control across the scales necessitates therefore to characterize the uncertainty contained in these parameters and to scrutinize how it affects the final multi-scale modeling results.

- Lateral interactions are the ruling microscopic parameters behind the equilibrium and non-equilibrium ordering behavior of atomic or molecular networks at surfaces. Since the accuracy of these interactions should be of the order of $k_B T$ to properly describe thermal ensemble properties, we systematically studied the accuracy with which they can be determined from DFT calculations with local or semi-local xc functionals. Our analysis reveals a significantly larger uncertainty in the on-site energy, i.e., the binding energy of an isolated adsorbate, as compared to the pair or many-body lateral interactions between different adsorbates. This suggests a hybrid approach, in which the lateral interactions can be determined with present-day DFT calculations, whereas the on-site energy needs to be more accurately obtained e.g. using the local xc correction approach described above (Y. Zhang).
- The crucial microscopic input to kinetic Monte Carlo simulations are the rate constants for the individual elementary processes. The degree of rate control describes the variation of the catalytic activity (turnover frequencies) with these individual rate constants. While originally suggested to identify rate-limiting steps in experimental steady-state activity measurements, evaluation of the degree of rate control for each elementary process in the kMC simulations thus provides a natural basis for a sensitivity analysis of the effects of the uncertainty contained in the first-principles rate constants on the ultimately obtained turnover frequencies. As such, this analysis clearly identifies which rate constants are particularly crucial for a quantitative

determination of the catalytic activity, possibly requiring a higher-level calculation of the corresponding processes than possible with present-day DFT (H. Meskine, S. Matera, H. Metiu, and M. Scheffler).

III.3 Simulations at the mesoscopic scale

The focus on error-control is also reflected in the methodological work addressing the mesoscopic scale. On the one hand this concerns the validity of the level of coarse-graining underlying the statistical simulations, e.g. by scrutinizing the approximations behind the employed model Hamiltonians. On the other hand this concerns the reliability of the statistical algorithms themselves, particularly in view of the constraints imposed by a restricted amount of available first-principles data.

- A prevalent approach to address the microkinetics of heterogeneous catalysis are mean-field type rate equations. While appealing in view of its simplicity, this approach relies on a number of severe approximations: The role of fluctuations is neglected, correlations between the locations of the reactants on the surface are assumed to be absent, and the reacting mixture is considered to be an ideal solution. In contrast, kinetic Monte Carlo simulations do not need to rely on any of these approximations and can therefore be used to scrutinize the validity of the mean-field assumption behind rate equation theory. Even for a showcase system without appreciable lateral interactions, i.e., without a thermodynamic driving force for segregation (CO oxidation at $RuO_2(110)$), we find the rate equation description to be in serious error. This holds for the steady-state activity, as well as for temperature-programmed reaction data. Essentially, application of the mean-field picture in the analysis of experimental data yields in either case kinetic parameters that are wrong by several orders of magnitude and misrepresent the relative reactivities of the different surface species. (H. Meskine, S. Matera, M. Rieger, J. Rogal, H. Metiu, and M. Scheffler)
- Genetic Algorithms (GAs) and Basin Hopping (BH) are two predominantly used algorithms to identify (meta)stable isomers of small atomic clusters. Sampling the minima of the corresponding high-dimensional potential-energy surfaces, the efficiency of both approaches relies heavily on the way how new trial structures are generated (“moves”) and on algorithmic parameters that decide how the energetic

information of these trial structures is exploited for the continued sampling. In view of the high computational cost of calculating the potential-energy surface data from first priciples, we systematically compare the efficiency of the GA and BH approach, both with respect to the employed moves and with respect to their algorithmic parameters. (R. Gehrke and V. Froltsov)

IV. Applications

IV.1 Stabilizing a molecular switch at solid surfaces

Embedded into experimental activities within the local Collaborative Research Centre on molecular switches, we target the prototypical conformational switch azobenzene (C_6H_5-N=N-C_6H_5) and the effect of adsorption at noble metal surfaces on its cis-trans isomerization function. As a prerequisite to studies of ensemble properties of adsorbed molecular networks, current large-scale DFT calculations provide a detailed structural and electronic characterization of the stable (or metastable) molecular states at the surface. Particularly at Cu(111), these calculations reveal the formation of rather strong covalent bonds to the central azo-bridge (-N=N-) of the molecule which even reverse the gas phase energetic order of the two isomers at the level of the employed GGA xc functional. Since this level of theory does not properly treat van der Waals interaction of the phenyl-rings with the solid surface, ongoing work concentrates on assessing the size of this contribution through MP2 level calculations focusing on the adsorption of benzene within the local xc correction scheme described in Section III.1 above (E. McNellis, A. A. Dehghan Baghi, and M. Scheffler).

IV.2 Long-range Coulomb interactions in the molecular metal TTF-TCNQ

In order to address non-adiabatic effects in the gas-surface interaction we have previously formulated a locally-constrained DFT approach that allows to calculate the electronic ground state under the additional constraint of defined spin or charge in chosen subsystems given by atoms or groups of atoms. Exploiting that this approach can be ideally transferred to the calculation of realistic first-principles parameters for Hubbard models, we apply it now to the molecular metal TTF-TCNQ. Considering both intra- and intermolecular screening in the crystal, we confirm the importance of the suspected longer-range Coulomb interactions along the molecular stacks, as well as inter-stack coupling. Contrary to past belief, these terms do not lead to the formation of a Wigner lattice, but simply broaden the spectral function, thereby likely resolving the problems with the interpretation of angular-resolved photoemission experiments using a simple Hubbard model only. (J. Behler, L. Cano-Cortés, J. Merino, and E. Koch)

IV.3 Ensemble properties of molecular networks at metal surfaces

Determining the lateral interactions from DFT calculations, we employ the first-principles lattice-gas Hamiltonian approach to study the thermal ordering behavior of adsorbates at solid surfaces. Using low coverages of oxygen at Pd(100) as a simple model system we demonstrate the accuracy of this approach by the achieved quantitative agreement with the experimental phase diagram. Moving on to more complex molecular networks, we investigate the surprising chiral ordering behavior of the intrinsically achiral organic molecule succinic acid at Cu(110). We find the chirality to arise from a twisted adsorption mode of the molecule, with the dominant short-ranged pair interactions between the adsorbed succinic acid molecules determining their alignment in rows along the experimentally reported directions. The twisted adsorption mode induces a significant local stress in the Cu substrate, which prevents the formation of superstructure domains containing more than three adjacent rows of molecules (Y. Zhang, H. Lin, and W. Hofer).

IV.4 First-principles kinetic Monte Carlo simulations of heterogeneous catalysis

Based on first-principles rate constants calculated with DFT and transition-state theory, our first kinetic Monte Carlo simulations of heterogeneous catalysis had addressed the steady-state activity of $RuO_2(110)$ for the CO oxidation reaction over a wide range of temperatures and pressures, extending from ultrahigh-vacuum to ambient pressures and elevated temperatures. Successfully reproducing existing experimental data, the same framework is now also applied to simulate temperature-programmed reaction spectroscopy data. The results are in quantitative agreement with experiment and demonstrate that the atomic-scale information contained in the measured data complies fully with the established picture of the function of this model catalyst surface. Further first-principles kinetic Monte Carlo simulations address the stability of a sub-nanometer thin surface oxide film during the steady-state CO oxidation over Pd(100), again obtaining results that are in full agreement with available experimental data. Ongoing work is now directed to apply the approach to ever more complex systems, including the hydrodesulfurization over MoS_2 and the oxidative coupling of methane over Li-doped MgO catalysts. (M. Rieger, J. Rogal, N. Dinter, N. Zobel, L. Sheng, H. Toulhoat, P. Raybaud, and M. Scheffler)

Publications of the Independent Junior Research Group

Late 2005

Michaelides, A., K. Reuter, and M. Scheffler: When seeing is not believing: Oxygen on Ag(111), a simple adsorption system? J. Vac. Sci. Technol. A **23**, 1487-1497 (2005).

2006

Kiejna, A., G. Kresse, J. Rogal, A. De Sarkar, K. Reuter, and M. Scheffler: Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces (8 pages). Phys. Rev. B **73**, 035404 (2006).

Reuter, K.: Insight into a pressure and materials gap: CO oxidation at “Ruthenium” catalysts. Oil & Gas Science and Technology - Rev. IFP, **61**, 471-477 (2006).

Reuter, K.: Nanometer and sub-nanometer thin oxide films at surfaces of late transition metals. In: Nanocatalysis. (Eds.) U. Heiz, U. Landman. Springer Berlin 2006, 343-376. ISBN 978-3-540-32645-8.

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Schnadt, J., A. Michaelides, J. Knudsen, R.T. Vang, K. Reuter, E. Lægsgaard, M. Scheffler, and F. Besenbacher: Revisiting the structure of the $p(4 \times 4)$ surface oxide on Ag(111). Phys. Rev. Lett. **96**, 146101 (2006).

Zhang, Y., J. Rogal, and K. Reuter: Density-functional theory investigation of oxygen adsorption at Pd(11N) vicinal surfaces (N=3,5,7): Influence of neighboring steps (9 pages). Phys. Rev. B **74**, 125414 (2006).

Ph.D. Theses

Rogal, J.: Stability, composition and function of palladium surfaces in oxidizing environments: A first-principles statistical mechanics approach. FU Berlin 2006.

2007

Behler, J., B. Delley, K. Reuter, and M. Scheffler: Nonadiabatic potential-energy surfaces by constrained density-functional theory (10 pages). Phys. Rev. B **75**, 115409 (2007).

Behler, J., S. Lorenz, and K. Reuter: Representing molecule-surface interactions with symmetry-adapted neural networks (11 pages). J. Chem. Phys. **127**, 014705 (2007).

Behler, J., K. Reuter, and M. Scheffler: Non-adiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Phys. Rev. B, submitted.

Cano-Cortés, L., A. Dolfen, J. Merino, J. Behler, B. Delley, K. Reuter, and E. Koch: Spectral broadening due to the long-range Coulomb interactions in the molecular metal TTF-TCNQ. Eur. Phys. J. B **56**, 173-176 (2007).

Hu, Q.-M., K. Reuter, and M. Scheffler: Towards an exact treatment of exchange and correlation in materials: Application to the “CO adsorption puzzle” and other systems. Phys. Rev. Lett. **98**, 176103 (2007).

Reuter, K. and M. Scheffler: Erratum: Composition, structure, and stability of RuO_2(110) as a function of oxygen pressure [Phys. Rev. B 65, 035406 (2001)]. Phys. Rev. B **75**, 049901(E) (2007).

Rieger, M., J. Rogal, and K. Reuter: Effect of surface nanostructure on temperature programmed reaction spectroscopy: First-principles kinetic Monte Carlo simulations of CO oxidation at RuO_2(110). Phys. Rev. Lett., submitted.

Rogal, J. and K. Reuter: Ab initio atomistic thermodynamics for surfaces: A primer. In: RTO-AVT-142, VKI Lecture Series on “Experiment, modeling and simulation of gas-surface interactions for reactive flows in hypersonic flights”, Rhode-St-Genèse, Belgium, February 6-10, 2006 (2007).

Rogal, J., K. Reuter, and M. Scheffler: CO oxidation at Pd(100): A first-principles constrained thermodynamics study (11 pages). Phys. Rev. B **75**, 205433 (2007).

Rogal, J., K. Reuter, and M. Scheffler: First-principles statistical mechanics study of the stability of a subnanometer thin surface oxide in reactive environments: CO oxidation at Pd(100). Phys. Rev. Lett. **98**, 046101 (2007).

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Zhang, Y., V. Blum, and K. Reuter: Accuracy of first-principles lateral interactions:

Oxygen at Pd(100) [14 pages]. Phys. Rev. B **75**, 235406 (2007).

Diploma Theses

Rieger, M.: First-principles kinetic Monte Carlo simulations for temperature-programmed desorption spectroscopy. RWTH Aachen, 2007.

Invited Talks of the Members of the Independent Junior Research Group

Karsten Reuter

Dec 2005	International IFP Conference on Research Advances in Rational Design of Catalysts and Sorbents, Lyon, France *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Jan 2006	Chemistry Seminar, University of St. Andrews, U.K. *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Jan 2006	Colloquium at the Institut für Kristallzüchtung im Forschungsverbund Berlin e.V., Germany *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Feb 2006	RTO-AVT-VKI Lecture Series on Experiment, Modeling and Simulation of Gas-Surface Interactions for Reactive Flows in Hypersonic Flights, Rhode-St-Genèse, Belgium *Introduction to the Experimental Techniques of Surface Science*
Feb 2006	RTO-AVT-VKI Lecture Series on Experiment, Modeling and Simulation of Gas-Surface Interactions for Reactive Flows in Hypersonic Flights, Rhode-St-Genèse, Belgium *First-Principles Statistical Mechanics for Surface Properties and Functions*
Feb 2006	19th CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, U.S.A. *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Feb 2006	Research Seminar at the ExxonMobil Research Labs, Annandale, U.S.A. *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Mar 2006	APS March Meeting, Baltimore, U.S.A. *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Apr 2006	KNAW Conference on Multiscale Modeling: Electrons, Molecules and (Bio)Materials, Amsterdam, The Netherlands *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
May 2006	Kolloquium des SFB 555, Fritz-Haber-Institut, Berlin, Germany *First-Principles Statistical Mechanics Approaches for Heterogeneous Catalysis*

Jun 2006	10th Symposium on the Chemical Physics of Materials and Inauguration Workshop of the MPG-CAS Partner Group, Dalian Institute of Physics, P.R. China *First-Principles Statistical Mechanics Approaches to Heterogeneous Catalysis*
Jun 2006	6th ICQS Workshop on Novel Quantum Phenomena in Condensed Matter Physics, Beijing and Hangzhou, P.R. China *First-Principles Statistical Mechanics Approaches to Heterogeneous Catalysis*
Jun 2006	iNano School “Surface Reactivity and Nanocatalysis”, Fuglsø, Denmark *Bridging the Pressure Gap*
Jun 2006	Lorentz Center Workshop on Predicting Catalysis: Ammonia Production from First-Principles, Leiden, The Netherlands *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Jul 2006	Colloquium at the Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany *First-Principles Statistical Mechanics Approaches for Heterogeneous Catalysis*
Sep 2006	COST Workshop on Multiscale Modeling of Extended Defects and Phase Transformations at Material Interfaces, Wroclaw, Poland *First-Principles Statistical Mechanics Approaches to Heterogeneous Catalysis*
Nov 2006	Seminar at the Material Modeling Laboratory, University of Oxford, U.K. *Novel Insights into the Function of Heterogeneous Catalysts through First-Principles Statistical Mechanics*
Nov 2006	Seminar at the Departamento de Teória de la Materia Condensada, Universidad Autónoma de Madrid, Spain *Novel Insights into the Function of Heterogeneous Catalysts through First-Principles Statistical Mechanics*
Dec 2006	International Workshop on Computational Methods for Nanoscale Systems, Hong Kong *First-Principles Statistical Mechanics for Oxidation Catalysis*
Mar 2007	233rd National Meeting of the American Chemical Society, Chicago, U.S.A. *Microscopic Insight into the Function of Heterogeneous Catalysts from First-Principles Statistical Mechanics*

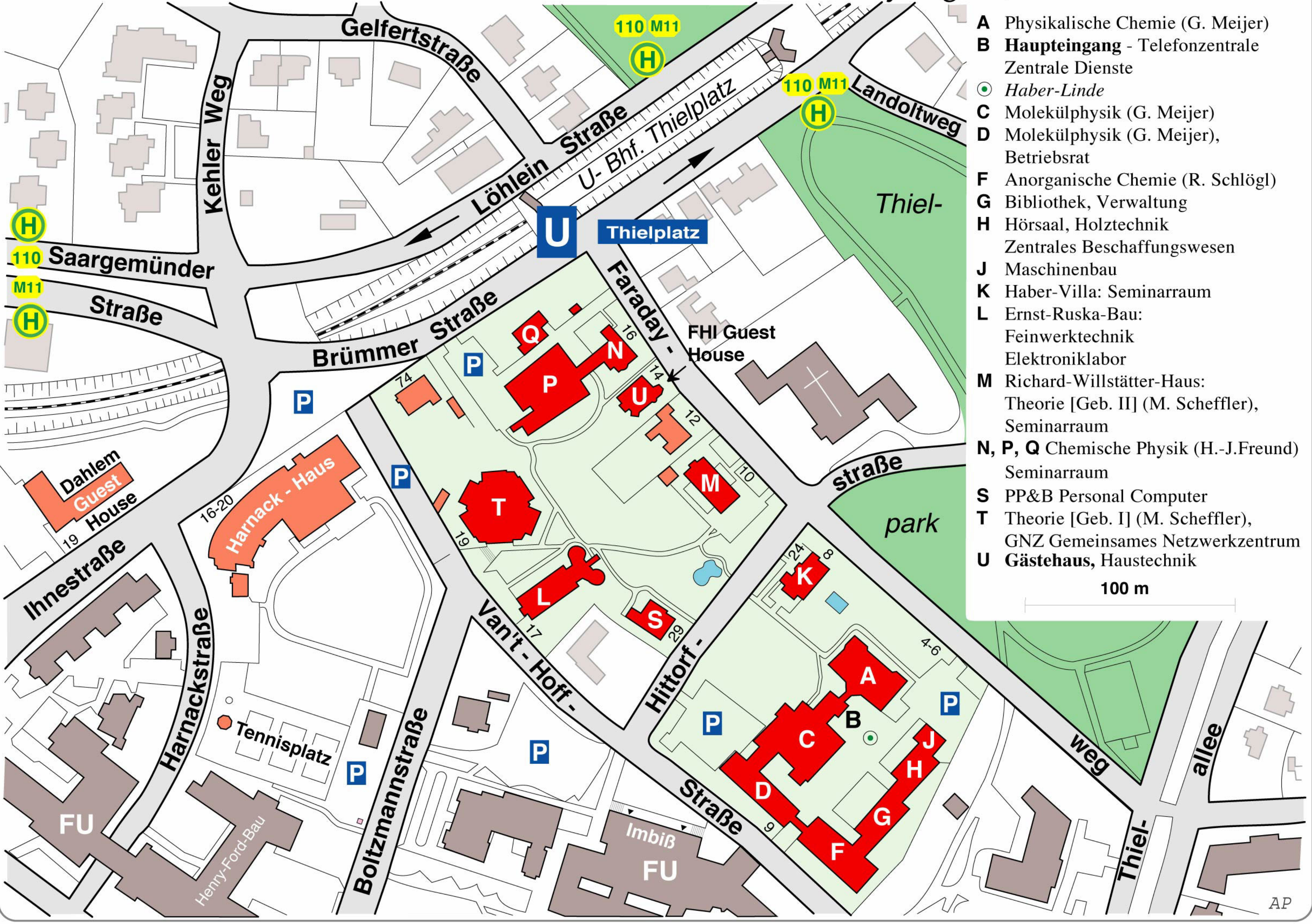
Apr 2007	Physikalisches Kolloquium, Jacobs Universität Bremen, Germany *Error-Controlled Multiscale Modeling Approaches to Surface Chemistry and Catalysis*
May 2007	Seminar at the Freie Universität Berlin, Germany *Atoms, Molecules, and Molecular Switches at Solid Surfaces: The "Cans" and "Can'ts" of Density-Functional Theory*
May 2007	Seminar "Moleküle im Rechner", Konrad-Zuse Institut, Berlin, Germany *Microscopic Insight into the Function of Heterogeneous Catalysts from First-Principles Statistical Mechanics*
Jun 2007	1st GOSPEL Workshop on Low Dimensional and Nanostructured Oxides: Bridging Surface Science and Sensor Science, Tübingen, Germany *Nanometer and Sub-Nanometer Thin Oxide Films at Surfaces of Late Transition Metals*
Jul 2007	17th International Conference on Vacuum Science and 13th International Conference on Surface Science, Stockholm, Sweden *Error-Controlled Multiscale Modeling Approaches to Surface Chemistry and Catalysis*
Jul 2007	Seminar at the Universität Tübingen, Germany *What First-Principles Statistical Mechanics Might Contribute to Sensor Science*
Aug 2007	234th National Meeting of the American Chemical Society, Boston, U.S.A. *Error-Controlled Multiscale Modeling Approaches to Surface Chemistry and Catalysis*
Aug 2007	12th Int. Conference on the Applications of Density-Functional Theory (DFT2007), Amsterdam, The Netherlands *Error-Controlled Multiscale Modeling Approaches to Surface Chemistry and Catalysis*
Sep 2007	European Congress and Exhibition on Advanced Materials and Processes (Euromat 2007), Nürnberg, Germany *Error-Controlled Multiscale Modeling Approaches to Surface Chemistry and Catalysis*

Jutta Rogal

Sep 2006	CECAM Workshop on Catalysis from First Principles, Lyon, France *A First-Principles Statistical Mechanics Investigation of the Stability of a Thin Surface Oxide in Reactive Environments*

Dec 2006	Workshop on Progress in Anisotropic Wet Chemical Etching, Levi, Finland *First-Principles Statistical Mechanics for Heterogeneous Catalysis*
Jun 2007	Workshop on Theory Meets Industry: The Impact of Density-Functional Calculations on Material Science, Vienna, Austria *Catalytic Oxidation at Surfaces: Insight from First-Principles Statistical Mechanics*

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin



A	Physikalische Chemie (G. Meijer)
B	**Haupteingang** - Telefonzentrale Zentrale Dienste
⦿	*Haber-Linde*
C	Molekülphysik (G. Meijer)
D	Molekülphysik (G. Meijer), Betriebsrat
F	Anorganische Chemie (R. Schlögl)
G	Bibliothek, Verwaltung
H	Hörsaal, Holztechnik Zentrales Beschaffungswesen
J	Maschinenbau
K	Haber-Villa: Seminarraum
L	Ernst-Ruska-Bau: Feinwerktechnik Elektroniklabor
M	Richard-Willstätter-Haus: Theorie [Geb. II] (M. Scheffler), Seminarraum
N, P, Q	Chemische Physik (H.-J.Freund) Seminarraum
S	PP&B Personal Computer
T	Theorie [Geb. I] (M. Scheffler), GNZ Gemeinsames Netzwerkzentrum
U	**Gästehaus,** Haustechnik