

INSTITUTSBERICHT **INSTITUTE REPORT** 2005-2006

MAX-PLANCK-INSTITUT FÜR CHEMIE



MAX-PLANCK-GESELLSCHAFT



BIOGEOCHEMISTRY



ATMOSPHERIC
CHEMISTRY



GEOCHEMISTRY



PARTICLE
CHEMISTRY

MAX
PLANCK
INSTITUT

INSTITUTSBERICHT

FÜR
CHEMIE

2005
2006

INSTITUTE REPORT

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VORWORT

VORWORT

Unser Institut erforscht die Erde und ihr Umfeld in unterschiedlichen Größenbereichen, vom Nanopartikel bis zum Planeten und von der Ökosystemdynamik bis zum globalen Klimawandel. Unsere wissenschaftlichen Fragestellungen entstehen oft aus der Beobachtung natürlicher Phänomene in Feldstudien. Wir untersuchen ausgewählte Komponenten des Systems Erde unter kontrollierten Bedingungen im Labor und verwenden Computermodele, um die Wechselwirkungen im System zu verstehen und die Rückkopplungs-Mechanismen aufzuklären. Wir helfen somit, Wissen und Methoden bereitzustellen, die für eine nachhaltige Nutzung der natürlichen Ressourcen und zum Schutz der Umwelt erforderlich sind. Auch sind wir durch unsere International Max Planck Research School und unser E-Learning-Programm an der wissenschaftlichen Ausbildung beteiligt.

Pensionierungen, neue wissenschaftliche Herausforderungen und Neuausrichtungen innerhalb der Max-Planck-Gesellschaft haben in den vergangenen zwei Jahren zu einer teilweisen Umstrukturierung des Instituts geführt. Nach dem Erfolg der Mars-Missionen, bei denen Spektrometer unseres Instituts an Bord der NASA-Rover verschiedene Landstellen untersucht haben, wurden die Aktivitäten im Bereich der Kosmochemie reduziert. Die Verwendung von Satellitendaten wird nun systematisch durch die Gruppe Satellitenfernerkundung, der Vorbotin der künftigen Abteilung Erdsystemchemie, betrieben. Weiterhin haben wir die Erdsystemmodellierung durch eine Kooperation mit mehreren Max-Planck-Instituten (u.a. Hamburg, Jena und Mainz) ausgebaut. Wir können auf unsere hervorragenden Mitarbeiter stolz sein, die diese nicht immer einfachen Übergänge umgesetzt haben.

PREFACE

PREFACE

The institute explores the Earth and its environment on a range of scales, from nanoparticles to planets, and from ecosystem dynamics to global climate change. Our research questions often arise from observations of natural phenomena in field studies. We investigate selected components of the Earth system under controlled conditions in the laboratory, and system interactions through computer modelling to study feedback mechanisms. We help supply the basic knowledge and methods needed for the sustainable use of natural resources and environmental protection. We are also committed to science education through our International Max Planck Research School and E-learning program.

In the past two years our institute has been partially restructured in response to retirements, new scientific challenges, and redirections within the Max Planck Society. After the success of the missions to Mars, whereby our institute's spectrometers on the NASA rovers have investigated several landing sites, the activities in Cosmochemistry have been scaled down. On the other hand, the use of satellite data has become methodical in "Satellite Remote Sensing", a forerunner group of the future department "Earth System Chemistry". We have furthermore expanded in Earth system modelling within a new cooperation between several Max Planck Institutes (Hamburg, Jena, Mainz and others). We can be proud of our excellent staff who have realised these sometimes difficult transitions.

A noteworthy event has been the delivery of the new German High Altitude – Long Range (HALO) aircraft which is currently being modified for use in atmospheric research. The institute, supported by the Max Planck

Ein weiteres bemerkenswertes Ereignis war die Auslieferung des neuen deutschen Höhenforschungsflugzeuges HALO, das nun für die Anforderungen der Atmosphärenforschung umgebaut wird. Das Institut hat sich mit Unterstützung der Max-Planck-Gesellschaft von der ersten Vorschlagsphase an sehr stark für das Zustandekommen des HALO-Projekts eingesetzt und wird dies bis nach der Instrumentierung und den ersten Tests im Jahre 2008 fortsetzen. Weiterhin haben wir uns an der Initiative „Geocycles“ der Universität Mainz beteiligt, die von der Regierung des Landes Rheinland-Pfalz in ihrem neuen „Exzellenzcluster“-Programm gefördert wird. Diese Forschungsinitiative verbindet verschiedene Aspekte des Erdsystems, von den Wissenschaften der festen Erde (einschließlich früher Erdgeschichte) über Atmosphärenchemie und -physik, Paläoklimatologie, ArchaeoScience bis hin zu Untersuchungen der Wechselwirkungen von menschlicher Kultur und Natur.

Im folgenden Bericht stellen wir unsere Institution und ihre Tätigkeitsschwerpunkte vor und geben einen kurzen Überblick unserer Forschungsergebnisse des Zeitraums 2005-2006.

Society, has been strongly committed in obtaining HALO from the early proposal phase up to its instrumentation and testing in 2008. We have also engaged in a “Geocycles” initiative by the University of Mainz, which is supported by the State government of Rheinland-Pfalz in its new “Cluster of Excellence” programme. The programme combines solid Earth science (including early Earth history), atmospheric chemistry and physics, palaeoclimate studies, ArchaeoScience, and human culture-nature interactions.

In this report we present our organisation, the central themes and a brief summary of our research results achieved in the period 2005-2006.



Prof. Dr. Jos Lelieveld
(Managing Director)

ALLGEMEINES ZUM INSTITUT

GENERAL

ALLGEMEINES ZUM INSTITUT

Geschichte und Gegenwart

Das Max-Planck-Institut für Chemie (MPI) ist das älteste unter den derzeit 80 Instituten der Max-Planck-Gesellschaft zur Förderung der Wissenschaften (MPG). Es wurde 1912 in Berlin-Dahlem als Institut der Kaiser-Wilhelm-Gesellschaft, der Vorläuferorganisation der MPG, gegründet. Nach der Zerstörung der Institutsgebäude im 2. Weltkrieg und einer provisorischen Übersiedlung nach Tailfingen/Württemberg erfolgte 1949 der Neuaufbau in Mainz auf dem Gelände der Johannes Gutenberg-Universität. Seit 1959 trägt das Institut zusätzlich den Namen "Otto-Hahn-Institut". Damit wird die große Bedeutung Otto Hahns für das Institut gewürdigt und an die Entdeckung der Kernspaltung erinnert, die er 1938 zusammen mit Lise Meitner und Fritz Straßmann an diesem Institut gemacht hat.

Wie alle anderen Einrichtungen der Max-Planck-Gesellschaft betreibt das Max-Planck-Institut für Chemie Grundlagenforschung. Um sich den verändernden wissenschaftlichen Erfordernissen anzupassen, haben sich die

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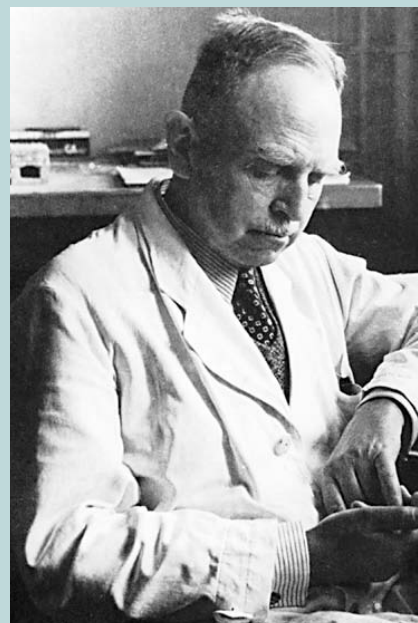
History and Present

The Max Planck Institute for Chemistry is the oldest among the currently 80 institutes of the Max Planck Society (MPG). It was founded in Berlin-Dahlem in 1912, as an institute of the Kaiser Wilhelm Society, the forerunner organisation of MPG. The institute was rebuilt in 1949 in Mainz on the campus of Johannes Gutenberg University, after it had been destroyed in World War II and temporarily relocated to Tailfingen/Württemberg. Since 1959 it has additionally been named Otto Hahn Institute to commemorate Otto Hahn's great importance for the institute and the discovery of nuclear fission, which was made in 1938 jointly by Otto Hahn, Lise Meitner and Fritz Strassmann in this institute.

Like all institutions of the MPG, the MPI for Chemistry performs basic research. To adapt to the changing scientific demands, the institute's main research has undergone multiple changes during its history. While classical chemistry was practised in the beginning, the focus has later been mainly put on radiochemistry, nuclear physics and mass spectrometry. Since the 1970's the formation and



Richard Wildstätter



Otto Hahn

ALLGEMEINES GENERAL ZUM INSTITUT

Forschungsschwerpunkte des Instituts im Laufe seiner Geschichte mehrfach gewandelt. Wurde in den Anfangsjahren die klassische Chemie betrieben, so wandte sich das Interesse später vor allem der Radiochemie, Kernphysik und Massenspektrometrie zu. Seit den siebziger Jahren des letzten Jahrhunderts sind die Entstehung, Entwicklung und Zukunft unseres Planeten und seiner Nachbarn die zentralen Forschungsthemen. Der Bogen der Forschungen spannt sich dabei von den Planeten unseres Sonnensystems über die Lufthülle unserer Erde bis zu ihrem heißen Kern. Der Schwerpunkt liegt dabei vorwiegend, aber keineswegs ausschließlich, auf chemischen und physikalisch-chemischen Untersuchungen. Insofern ist der Name MPI für Chemie auch heute noch gerechtfertigt.

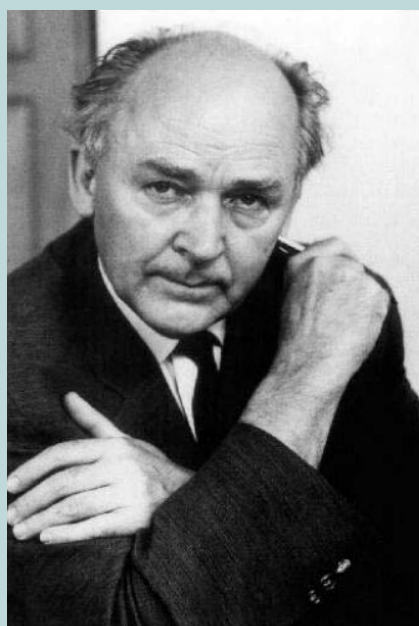
Drei Mitgliedern des Instituts wurde der Nobelpreis verliehen: Richard Wildstätter für seine Chlorophyllarbeiten (1915), Otto Hahn für die Entdeckung der Kernspaltung (1944) und Paul J. Crutzen für die Arbeiten über den Abbau des Ozons in der Stratosphäre (1995).

development of our planet and its environment have been the central issues. The research covers a wide range of topics including the planets of our solar system, the atmosphere of the Earth and its hot core. Emphasis is predominantly, though by no means exclusively, put on chemical and physical-chemical analysis. Hence, the name MPI for Chemistry continues to be relevant.

Three members of the institute have been awarded the Nobel Prize: Richard Wildstätter for his work on chlorophyll (1915), Otto Hahn for the discovery of nuclear fission (1944) and Paul J. Crutzen for his work on ozone depletion in the stratosphere (1995).



Lise Meitner



Fritz Straßmann



Paul J. Crutzen

ALLGEMEINES ZUM INSTITUT

Organisation

Heute besteht das Institut aus vier Abteilungen und zwei selbständigen Arbeitsgruppen. Jede der Abteilungen wird von einem Direktor geleitet, der als Wissenschaftliches Mitglied der MPG für seine Forschungstätigkeit eigenverantwortlich ist. Die Direktoren entscheiden gemeinsam über die Geschicke des Instituts und wählen aus ihrem Kreis im dreijährigen Turnus einen geschäftsführenden Direktor.

Die Forschungsarbeit des Instituts wird von einem internationalen Fachbeirat begutachtet. Ein Kuratorium fördert den Kontakt zur Gesellschaft und Öffentlichkeit. Neben Wissenschaftlern gehören dem Kuratorium auch Vertreter aus Politik und Wirtschaft an.

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Organisation

At present the institute consists of four departments and two independent research groups. Each of the departments is supervised by a director, who, as a scientific member of MPG has sole responsibility for the field of research. The directors decide collectively the institute's development and elect a managing director out of their circle every three years.

The institute's research is evaluated by an international Scientific Advisory Board. The Board of Trustees promotes the relation between the institute, society and the general public. Its members include representative scientific, political and industrial leaders.

ALLGEMEINES ZUM INSTITUT

GENERAL

FACHBEIRAT

SCIENTIFIC ADVISORY BOARD OF THE INSTITUTE

Prof. Dr. Halliday, Alexander N.	ETH Zürich, Schweiz
Prof. Dr. Hawkesworth, Christopher John	University of Bristol, Bristol, UK
Prof. Dr. Hoffmann, Michael R.	California Institute of Technology, Pasadena, USA
Prof. Dr. Hofmann, Thorsten	Universität Mainz
Prof. Dr. Isaksen, Ivar S.A.	University of Oslo, Oslo, Norwegen
Prof. Dr. Levin, Zev	Tel Aviv University, Ramat Aviv, Israel
Prof. Dr. Molina, Mario J.	Scripps Institution of Oceanography, University of California, San Diego, USA
Prof. Dr. Solomon, Sean C.	Carnegie Institution of Washington, Washington, DC, USA

KURATORIUM

BOARD OF TRUSTEES OF THE INSTITUTE

Dr. Baumgarten, Ludwig	Mitglied des Vorstands Deutsches Zentrum für Luft- und Raumfahrt
Beutel, Jens	Oberbürgermeister der Landeshauptstadt Mainz
Prof. Dr. Felcht, Utz-Hellmuth	Peters, Schönberger & Partner GbR, München
Junker, Reinhard	Ministerialdirektor im BMBF
Prof. Dr. Kröner, Alfred	Institut für Geowissenschaften der Universität Mainz
Dr. Leuchs, Hans-Jürgen	Geschäftsführender Gesellschafter C.H. Boehringer Sohn
Prof. Dr. Michaelis, Jörg	Präsident der Universität Mainz
Dr. Quisthoudt-Rowohl, Godelieve	Mitglied des Europäischen Parlaments
Prof. Dr. Spiess, Hans-Wolfgang	Max-Planck-Institut für Polymerforschung
Dr. Ungeheuer, Udo	Mitglied des Vorstands Schott Glas
Utner, Ferdinand	Online-Chefredakteur, Zweites Deutsches Fernsehen
Prof. Dr. Zöllner, E. Jürgen	Staatsminister für Bildung, Wissenschaft und Weiterbildung des Landes Rheinland-Pfalz

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Forschungsthemen im Überblick

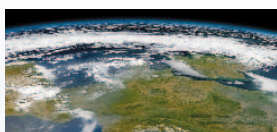
Research Topics

Die Abteilung **BIOGEOCHEMIE** (Prof. Dr. Meinrat O. Andreae) befasst sich mit Austausch und Wechselwirkungen von Spurengasen und Aerosolen zwischen Biosphäre, Hydrosphäre und Atmosphäre. Diese Prozesse werden durch Experimente im Labor, Feldmessungen und Modellrechnungen untersucht. Gegenwärtige Forschungsschwerpunkte sind: der Austausch von chemisch und physikalisch wichtigen Spurengasen zwischen dem System Boden/Vegetation und der Atmosphäre, die Bildung von Aerosolteilchen und ihr Einfluss auf das Klima, der Einfluss von Vegetationsfeuern auf die Ökologie und Luftverschmutzung sowie globale Kreisläufe von Spurenstoffen.



The **BIOGEOCHEMISTRY** Department (Prof. Dr. Meinrat O. Andreae) addresses the exchange and interactions of trace gases and aerosols between biosphere, hydrosphere and atmosphere. These processes are studied by laboratory investigations, field measurements and numerical models. The present research topics are: the exchange of chemically and physically important trace gases between the soil/vegetation system and the atmosphere, the formation of aerosol particles and their effects on climate, the impact of vegetation fires on ecology and atmospheric pollution, as well as global cycles of trace gases.

Die Abteilung **CHEMIE DER ATMOSPHERE** (Prof. Dr. Jos Lelieveld) untersucht chemische Reaktionen und globale Spurenstoffkreisläufe von Ozon und anderen reaktiven Spurengasen in der Atmosphäre. Diese Prozesse werden durch Experimente im Labor sowie Messungen in der Atmosphäre von Bodenstationen, Schiffen, Flugzeugen sowie Satelliten aus untersucht. Diese Feldmessungen werden unterstützt und analysiert mithilfe von Computermodellen zur Simulation meteorologischer und chemischer Wechselwirkungen sowie deren Einfluss auf das Klima.



The research in the **ATMOSPHERIC CHEMISTRY** Department (Prof. Dr. Jos Lelieveld) focusses on ozone and other reactive trace gases in the atmosphere, their chemical reactions and global cycles. These processes are studied by laboratory investigations and intensive ground-based, ship, aircraft and satellite measurements in the atmosphere. Numerical models that simulate meteorological and chemical interactions are used to support and analyse the field measurements and study human influences on climate.

In der Abteilung **GEOCHEMIE** (Prof. Dr. Albrecht W. Hofmann) werden die chemische Beschaffenheit und die zeitliche Entwicklung von Kruste, Mantel und Kern unserer Erde und anderer Körper des inneren Sonnensystems erforscht. Mit Hilfe sehr genauer Messungen von Isotopenhäufigkeiten der natürlichen radioaktiven Zerfallssysteme (wie z.B. Uran - Blei, Rubidium -Strontium) sowie von Spurenelementhäufigkeiten in Gesteinen und Mineralen werden neue Erkenntnisse über geologische Prozesse, wie die Bildung von Vulkaninseln oder die Entwicklung der Weltmeere, gewonnen.



The **GEOCHEMISTRY** Department (Prof. Dr. Albrecht W. Hofmann) investigates the chemical composition and chronological development of the Earth's mantle, crust and core as well as of other bodies of the inner Solar System. High-precision measurements of isotopic abundances of natural radioactive decay systems (e.g., uranium-lead, rubidium-strontium) and of trace element abundances in rocks and minerals provide new insights into a wide range of geological processes, including the formation of volcanic islands and the development of the oceans.

ALLGEMEINES GENERAL ZUM INSTITUT



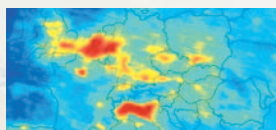
Die Abteilung **PARTIKELCHEMIE** (Prof. Dr. Stephan Borrmann), die im Jahr 2001 als jüngste Abteilung des Instituts gegründet wurde, ist eine gemeinsame Einrichtung des MPI für Chemie und des Instituts für Physik der Atmosphäre der Universität Mainz. Sie beschäftigt sich mit der chemischen Zusammensetzung und den physikalischen Eigenschaften von Aerosol- und Wolkenpartikeln in der Atmosphäre. Forschungsschwerpunkte sind zudem Untersuchungen von Größe, Anzahl, Strahlungseigenschaften und Bildungsmechanismen des Aerosols und der Wolken. Darüber hinaus werden mithilfe von Isotopenmessungen Partikel extraterrestrischen Ursprungs untersucht.

The **PARTICLE CHEMISTRY DEPARTMENT** (Prof. Dr. Stephan Borrmann), founded in 2001 as the most recent department of the institute, is a joint institution of the MPI for Chemistry and the Institute for Physics of the Atmosphere of the University of Mainz. Its research focusses on the chemical composition and physical properties of atmospheric aerosol and cloud particles. Also the sizes, number densities, shapes, radiative properties and formation mechanisms of aerosols and clouds are topics of experimental investigations. In addition, particles of extraterrestrial origin are studied by isotope measurements.



Die Arbeitsgruppe **HOCHDRUCK-MINERALPHYSIK** (Dr. Reinhard Boehler) untersucht Metall- und Mineralphasengleichgewichte, das Schmelzverhalten und thermodynamische Zustandsgrößen bei Druck- und Temperaturbedingungen des tiefen Erdmantels und Erdkerns (bis zu 2 Millionen Atmosphären und 5000 °C).

The **HIGH PRESSURE MINERAL PHYSICS** research group (Dr. Reinhard Boehler) is concerned with the determination of metal and mineral equilibria and thermodynamical properties under conditions of the deep Earth's mantle and core (up to 2 million atmospheres pressure and 5000 °C).



Die Arbeitsgruppe **SATELLITENFERNERKUNDUNG** (Dr. Thomas Wagner) ist eine Kooperation des MPI für Chemie mit dem Institut für Umweltphysik der Universität Heidelberg. Ihr Forschungsschwerpunkt ist die Entwicklung und Anwendung von Auswertelgorithmen für neuartige Satelliteninstrumente im ultravioletten, sichtbaren und nah-infraroten Spektralbereich. Solche Messungen erlauben die Untersuchung atmosphärischer Stoffkreisläufe von Schadstoffen, Treibhausgasen, Aerosolen und Wolken.

The **SATELLITE REMOTE SENSING** group (Dr. Thomas Wagner) is a co-operation between the MPI for Chemistry and the Institute of Environmental Physics, University of Heidelberg. The research focusses on the development and application of retrieval algorithms for novel UV/vis/near-IR satellite instruments. Based on these observations the atmospheric budgets of pollutants, greenhouse gases, aerosols and clouds are investigated.

ALLGEMEINES ZUM INSTITUT

Forschung und Lehre

Das Institut betreibt keine eigenständige Lehre, ist aber insbesondere durch seine Lage auf dem Universitätscampus in vielfältiger Weise in das Leben der Mainzer Johannes Gutenberg-Universität eingebunden, sowohl durch gemeinsame Forschungsprojekte als auch durch Lehrtätigkeit an der Universität.

Die **International Max Planck Research School for Atmospheric Chemistry and Physics (IMPRS)** wurde in enger Zusammenarbeit zwischen dem MPI für Chemie und den Universitäten Mainz, Frankfurt und Heidelberg im Jahre 2003 gegründet. Besonders begabten deutschen und ausländischen Studenten bietet diese Einrichtung die Möglichkeit, sich im Rahmen einer individuell strukturierten Ausbildung, die Vorlesungen, Workshops und Sommerschulen umfasst, auf die Promotion vorzubereiten.

Die IMPRS bietet einen Studienplan in Atmosphären-, Umwelt- sowie Geophysik und -chemie an. Durch die Kombination von exzellenter Forschung, modernster Geräteentwicklung, Feldmessungen und innovativen Unterrichtsmethoden wird die IMPRS zum Anziehungspunkt für talentierte und hoch motivierte junge Wissenschaftler aus der ganzen Welt. Ein Teil der Studenten arbeitet im Labor, viele beteiligen sich an Feldmesskampagnen mit Flugzeugen und Schiffen, und einige verwenden aktiv Satellitendaten und entwickeln Computermodelle.

Während ihrer Ausbildung werden die

GENERAL

Research and Education

The institute does not practice self-contained teaching. However, it is part of university life, particularly as it is located on the campus of the university of Mainz, through joint research projects and through teaching activities at the university.

The **International Max Planck Research School for Atmospheric Chemistry and Physics (IMPRS)** was established in 2003 in cooperation with the Universities of Mainz, Frankfurt and Heidelberg. The school offers talented Ph.D. students from Germany and abroad the possibility to prepare for their Ph.D. exam in an individually structured programme, which includes lectures, workshops and summer schools.

The IMPRS offers a Ph.D. curriculum in atmospheric, environmental, geophysics and -chemistry. Through the combination of high quality research, state of the art instrumentation development, field measurements and innovative education methods it attracts talented and motivated young scientists from all over the world. Part of our students work in the laboratory, many are active in field campaigns using aircraft and ships, and a number actively use satellite data and develop computer models.

During their studies our students are guided by a Ph.D. advisory committee (PAC), comprising at least 3 scientists (from both University and the Institute) with whom the student meets in regular intervals. During the PAC meetings the students present and discuss their scientific work and



ALLGEMEINES GENERAL ZUM INSTITUT

Studenten durch einen beratenden Ausschuss betreut, der aus mindestens drei Wissenschaftlern der Universität und des Instituts besteht. Mit diesen treffen die Doktoranden in regelmäßigen Abständen zusammen, stellen dabei ihre wissenschaftlichen Arbeiten vor, diskutieren die Ergebnisse und erhalten Feedback. Die Mitglieder des Ausschusses helfen den Studenten, ihre Promotion innerhalb der vorhergesehenen drei Jahre zu vollenden. Zudem berichten die Studenten am Ende des ersten und zweiten Jahres über ihre Fortschritte, die von den Ausschussmitgliedern begutachtet werden.

Die IMPRS vermittelt den Studenten nicht nur das erforderliche Fachwissen in den Geowissenschaften, ausgewählte Kurse zur Verbesserung der Präsentationsfähigkeiten ermöglichen zusätzlich eine Steigerung der Karrierechancen nicht nur in der Wissenschaft, sondern auch in der Wirtschaft oder im Ausbildungswesen. Während der jährlich im Sommer durchgeführten IMPRS-Informationstage erhalten die einzelnen Studenten Einblick in andere Labor- und Forschungseinrichtungen und tauschen untereinander Erfahrungen aus.

Seit der Gründung der IMPRS im Jahre 2003 haben insgesamt acht Studenten das IMPRS-Zertifikat erhalten, sechs davon mit der Gesamtbeurteilung „exzellent“ und zwei mit „exzellent plus“ (bis Juli 2006).

Zurzeit sind 50 Studenten in der IMPRS aufgenommen, davon 26 weibliche und 21 aus dem Ausland.

receive feedback from the senior scientists. The PAC members help the students to complete the Ph.D. work within the 3 year time frame. Besides the meetings, the students report about progress at the end of the first and second year, and the progress is assessed by the PACs.

In addition to the required knowledge in the geosciences we offer our students a selection of courses to improve their presenting and writing skills, thus enhancing career opportunities not only in science, but also in industry and education. During the annual and informal IMPRS days in summer the students gain insight in each other's laboratory and research facilities and exchange experiences.

Since the IMPRS was established in 2003, a total of 8 students have obtained the IMPRS certificate; 6 with the overall grading 'Excellent' and 2 with 'Superior' (up to July 2006).

The IMPRS currently hosts 50 Ph.D. students, of which 26 female and 21 non-native.

WWW www.atmosphere.mpg.de/school

MAX PLANCK INSTITUT

SELECTED RESEARCH REPORTS

FÜR CHEMIE

BIOGEOCHEMISTRY DEPARTMENT

ATMOSPHERIC CHEMISTRY DEPARTMENT

COSMOCHEMISTRY

GEOCHEMISTRY DEPARTMENT

PARTICLE CHEMISTRY DEPARTMENT

HIGH PRESSURE MINERAL PHYSICS GROUP

SELECTED PUBLICATIONS

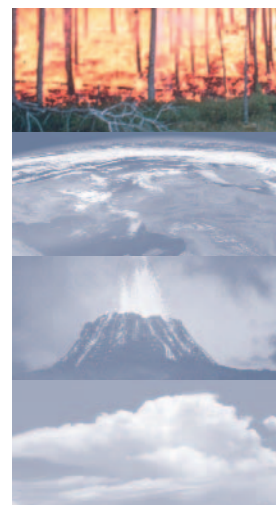
BIOGEOCHEMISTRY DEPARTMENT

Main Research Areas

Meinrat O. Andreae



Born 19 May 1949 in Augsburg. Undergraduate studies in chemistry and earth sciences, Karlsruhe and Göttingen. Ph.D. 1977 in Oceanography, Scripps Institution of Oceanography, University of California, San Diego. 1978-1982 Assist. Professor, 1982-1986 Assoc. Professor, 1986-1987 Professor of Oceanography at Florida State Univ., Tallahassee. Visiting Professor at the University of Antwerp, the University of California, Irvine, and the California Institute of Technology. Since 1987 Director and Scientific Member at the MPI for Chemistry. Member of the scientific steering committee of the "Large Scale Biosphere Atmosphere Experiment in Amazonia (LBA)" and Chair of the IGBP Core Project "Integrated Land Ecosystem Atmospheric Processes Study (ILEAPS)". Editor-in-Chief of Global Biogeochemical Cycles.



Biogeochemistry is the scientific discipline that studies the interactions of the biosphere with the Earth's chemical environment. It is an essential part of the evolving field of Earth System Science, which looks at the Earth as an integral system. Our department investigates a number of key aspects of global biogeochemistry: the role of the terrestrial biota as sources and sinks of climatically important trace gases and aerosols, the exchange of trace gases between the soil/vegetation system and the atmosphere, the effect of vegetation fires on ecology, climate, and atmospheric pollution, and the role of biogenic and other aerosols in the climate system. Our research is closely tied to the International Biosphere/Geosphere Program, and involves a high amount of international collaboration.

Current projects include the study of the exchange of volatile organic compounds by plants in tropical and Mediterranean ecosystems. One of the main objectives is to understand the role of this exchange in the carbon budget of ecosystems and the terrestrial biota as a whole.

The conversion of rainforest and savanna in the tropics into grazing and agricultural lands has a strong influence on the exchange of trace gases, and in particular on the ability of ecosystems to act as sources or sinks for a wide variety of nitrogen-containing trace gases and aerosol species. We study these effects at selected sites in the tropics and in temperate regions.

Vegetation fires are an important determinant in the ecology of many terrestrial systems. We study the role of fire in ecology, climate and atmospheric chemistry, using modelling, remote sensing, and field work in the Amazon and other regions. Gaseous and particulate emissions from vegetation fires and the products of the photochemical processing of these emissions in the atmosphere are being investigated.

Our studies show that the numbers of aerosols and cloud condensation nuclei (CCN) over pristine tropical continents are low and resemble conditions found over the oceans. Large-scale burning due to deforestation and clearing fires leads to a strong increase of aerosol and CCN concentrations, which in turn has a dramatic effect on cloud properties. This changes the mechanism of rainfall production and leads to redistribution of the transport of energy and chemical species in the tropical atmosphere. Ultimately, the effects reach far beyond the Amazon Basin and the tropics.

BIOGEOCHEMISTRY DEPARTMENT

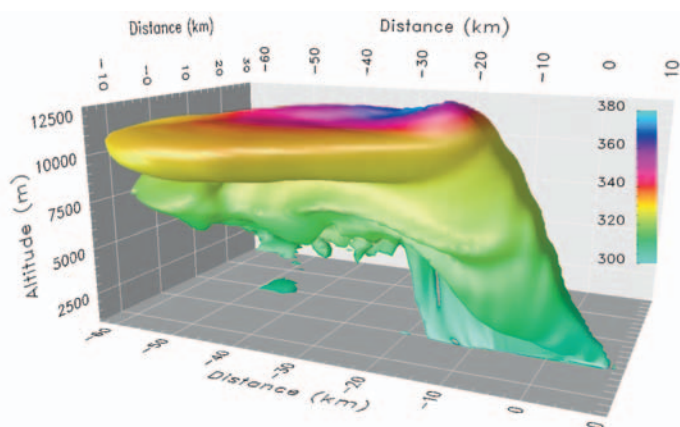
Aerosol Properties and Climate Effects

Aerosols are of central importance for atmospheric chemistry and physics, the biosphere, climate, and public health. Airborne solid and liquid particles in the nanometre to micrometre size range influence the Earth's energy balance, the hydrological cycle and atmospheric circulation, and the abundance of greenhouse and reactive trace gases. They scatter and absorb radiation; they initiate the formation of clouds and precipitation as cloud condensation nuclei (CCN) and ice nuclei (IN); and they undergo heterogeneous and multiphase chemical reactions. Airborne particles also play an important role in the spread of biological organisms, reproductive materials, and pathogens (pollen, bacteria, spores, viruses, etc.), and they can cause or enhance human, animal, and plant diseases. The physical, chemical, and biological properties of aerosols are spatially and temporally highly variable, and the quantitative understanding of particle sources, sinks, and transformation is very limited. Moreover, the description of aerosol processes and effects is hampered by a lack of universally applicable and consistent rate equations, parameters, and terminologies.

To address the scientific challenges outlined above, we develop and apply advanced measurement techniques for the physical, chemical, and biological characterisation of aerosols and air particulate matter at globally distributed sampling locations (including central Europe, Siberia, China, and Brazil), which are influenced by different types of natural and anthropogenic emissions.

Among the investigated parameters are particle concentration and size distribution, light absorption and scattering coefficients, CCN activity (dependence on particle size & water vapour supersaturation), chemical composition (black/elemental & organic carbon, organic biomolecules, inorganic ions, sulphur isotopes), and genetic signatures (amplification & sequencing of DNA). One of the recent key findings is that in spite of diverse origins and composition of aerosol particles in central Europe, their ability to grow into cloud droplets is controlled predominantly by their size.

Moreover, we develop and apply mathematical formalisms and models for the molecular elucidation of aerosol and cloud surface processes and gas-particle interactions (kinetic & thermodynamic models, detailed master mechanisms & simplified parameterisations of chemical transformation & water uptake); for the description of natural and anthropogenic particle emissions from the biosphere (wildfires & biomass burning, suspension of primary biological particles); and for the investigation of aerosol effects on the atmosphere and climate (radiation, convection, clouds & precipitation). One of the recent key findings is that strong aerosol cooling in the past may imply stronger than anticipated global warming for the future. Moreover, we found that the abundance of CCN is important for the microphysics of pyro-cumulonimbus clouds above boreal wildfires, but not so important for the associated troposphere-to-stratosphere transport of smoke, which is dominated by background meteorology and fire intensity.



Simulated aerosol isosurface of a pyro-cumulonimbus cloud with potential temperatures in color-coding (in K). The very high potential temperatures at the cloud top indicate stratospheric injection.

BIOGEOCHEMISTRY

Aerosol Emissions from Vegetation Fires

DEPARTMENT

Wide-spread natural and man-made fires are known to influence the composition of our atmosphere. These fires emit significant amounts of trace gases and particulate matter into the air, and thereby influence the budget of incoming radiation from the sun and outgoing radiation from the earth. Additionally, the emitted particles offer surfaces for heterogeneous chemical reactions, i.e., they can promote catalytic processes. So it is important to carefully characterise the surface area of emitted particles.

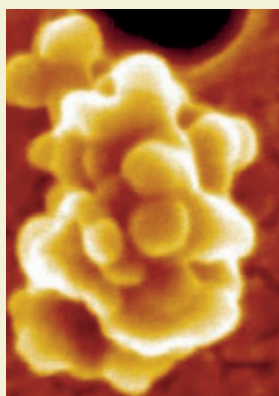
We focus here on the fractal properties of soot particles. Fractality or fractal dimension is a concept to describe complex shapes. Spheres and cubes as regular shapes have a dimension of three (they can be described by three length specifications which are perpendicular to each other). Such bodies have in common that their surface to volume ratio is constant, and therefore their surface area can be directly calculated from their volume. However, consider two spheres which are glued together – their total surface is less than the sum of the two individuals. To still be able to specify an equivalent diameter for such an aggregate of spheres, the concept of fractal dimension is used. Instead of having a dimension of two, such a combined two-sphere body will have its dimension slightly reduced. The reduction would

be enhanced if more spheres were attached to each other, because they would offer even less surface to the outside.

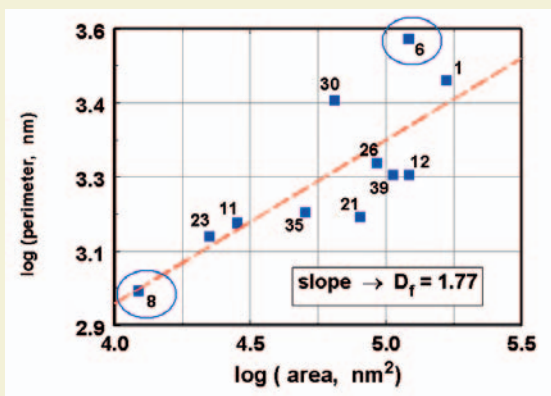
We apply this concept to soot particles, which we generated in our experimental set-up and collected on filters. The particles shown as scanning electron microscope images on this page originate from an oak fire. Soot particles typically are made of aggregates of many individual spherules.

One procedure for deriving the fractal dimension is to plot the logarithms of the projected perimeter of particles versus their projected area (their silhouette), as shown in the graph below. From the slope of the regression line, the fractal dimension can be derived – in this case it is $D_f = 1.77$. From this value, we obtain a specific surface of such particle aggregates in the range of 50 to 70 m^2 per gram soot.

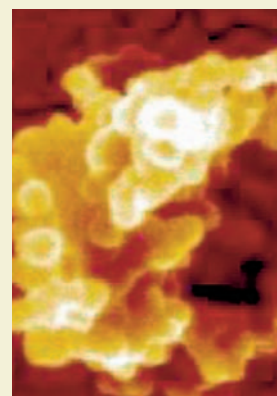
The particle 8 (left picture) shows spherules with sizes between 30 and 50 nm. Were they individual spherules of 40 nm diameter, their specific surface would have been 100 m^2 per gram soot. On the other hand, the specific surface of spheres equivalent in volume to this aerosol particle would be approximately 8 m^2 per gram. This wide variation shows that a close look at individual particles is necessary in order to understand their microphysical and chemical behaviour.



Particle 8 marked in the graph: Soot aggregate from oak fire, elongation 370 nm.



Plot to derive fractal dimension from the silhouettes of particles.



Particle 6 marked in the graph: Soot aggregate from oak fire, elongation 670 nm.

BIOGEOCHEMISTRY DEPARTMENT

Impact of Vegetation Fires on the Global Environment

Over the past decade, a growing trend of excessive fire application in land-use systems and land-use change, as well as an increasing occurrence of wildfires of extreme severities have been observed in many regions of the world. Some of the effects of wildland fires are of transboundary nature. The smoke pollution has consequences for human health and safety, loss of biodiversity, and contributes to desertification or flooding. The depletion of terrestrial carbon by fires burning under extreme conditions in some vegetation types, including peatlands, can disturb global biogeochemical cycles, notably the global carbon cycle. The Fire Ecology Research Group / Global Fire Monitoring Center (GFMC) has been involved in the development of an internationally concerted approach developing informed policies and action to reduce the negative impacts of vegetation fires on the environment and humanity. This work continues with a mandate by the United Nations to develop a strategy for international cooperation in wildland fire management based on a voluntary, legally non-binding instrument preliminarily entitled "The Fire Management Code".

Since the late 1990s the group also addresses the role of natural and anthropogenic fires in ecosystem functioning. Based on the evidence that prehistoric and historic fires have shaped ecosystem in all continents exempt Antarctica, a special emphasis is now given on the cultural history of fire application in Europe. In the history of land-use in Europe fire has always been an important element in forestry, agriculture and pastoralism. The use of fire has contributed to shape landscape patterns of high ecological and cultural diversity, e.g. heathlands, open grasslands, meadows, and swidden (shifting) agriculture sites. In the Nordic countries historic natural fires caused by lightning and burning practises have also significantly influenced the composition and structure of forest ecosystems. The rapid socio-economic changes in post-World War II Europe resulted in a change of land-use systems and landscape patterns, and the abandonment of traditional burning practises. New air quality standards and the generally prevailing

opinion in government administrations that fire would damage ecosystem stability and biodiversity, led to imposition of fire bans in most European countries.

It is now becoming evident that the abandonment of traditional cultivation and fire use methods has resulted in widespread elimination of disturbances that are crucial to maintain many valuable landscape types and ecosystems. Changing paradigms in ecology and nature conservation are currently reviving the discussion to reconsider fire-exclusion policies in certain sectors of nature conservation, forestry and landscape management. Since 1996 the group is working in the forefront of conducting research projects in the application of prescribed burning for maintaining biodiversity and landscape patterns, notably in heathland ecosystems dominated by *Calluna vulgaris* – a disturbance-dependent species that would disappear if grazing and burning would be abandoned. The question to which extent these methods affect air quality and carbon fluxes will be subject of an EU-funded integrated research programme between 2006 and 2010 with more than 31 partner institutions.



The application of prescribed fire in the maintenance of ecosystem functioning, biodiversity and cultural landscape patterns in Europe is a controversial issue addressed by integrated fire research. Photo: GFMC

BIOGEOCHEMISTRY

Nitrogen Compounds DEPARTMENT

in the Lower Atmosphere

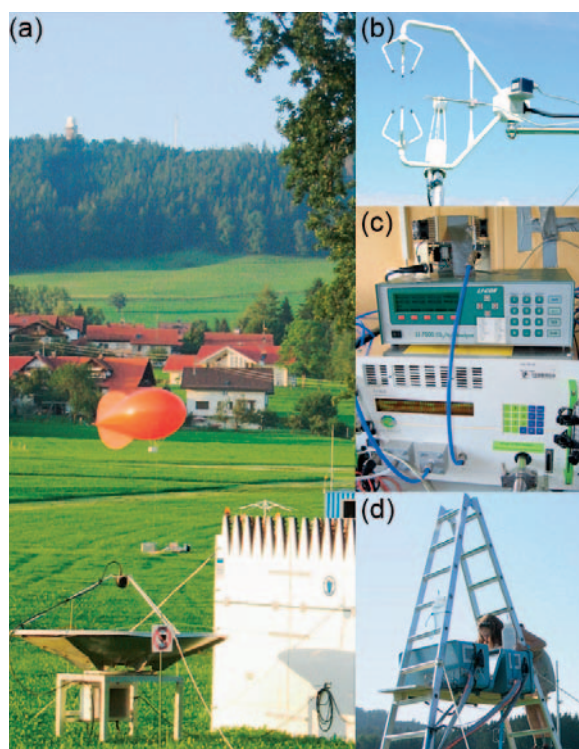
Human activities are disturbing the natural processes that control biological/chemical production and consumption of reactive nitrogen (N_r) species, especially since the 1960's. Trace gases and particles of N_r are exchanged between the biosphere and atmosphere by turbulent transport. Trace gases like nitrogen oxide (NO), nitrogen dioxide (NO_2), nitrous acid (HNO_2) and nitric acid (HNO_3) significantly influence the concentration of atmospheric hydroxyl radicals (OH), commonly called the "detergent of the atmosphere".

In summer 2005, we investigated the impact of anthropogenic emissions, chemical reactions, orographic and advection phenomena, and biological and physico-chemical properties of vegetated surfaces on the exchange, transport and chemical interconversion of gaseous and particulate N_r during a field experiment at the Meteorological Observatory of Hohenpeißenberg/Germany (Fig. a). We measured, together with the German Meteorological Service and the Universities of Cottbus and Bayreuth, the exchange of N_r between soil, plants and the near-surface atmosphere by micrometeorological techniques

(Figs. a&d). Specific and highly sensitive techniques were applied: NO and NO_2 by gas-phase chemiluminescence detection (Fig. c), NH_3 , HNO_2 and HNO_3 by a recently developed Gradient Analyser for Aerosols and Gases (GRAEGOR, Fig. d). All measurements were supported by flux and profile measurements of meteorological quantities, ozone, water vapour and carbon dioxide and by observations of the physical state of the atmospheric surface and top soil layers.

We find that even in this rural region, anthropogenic emissions strongly affect the cycling of N_r compounds. Deposition of traffic related N_r exceeded biogenic soil emissions of NO by orders of magnitude. In contrast to general wisdom, HNO_2 (generated by surface reactions during night) was not completely depleted by daytime photolysis, and HNO_2 concentrations featured unexpected diel variations. Consequently, a yet unknown daytime source of HNO_2 , stronger than its photochemical destruction, has to be postulated, which has major consequences for the atmospheric oxidant cycle.

Atmospheric dispersion of soil, plant and surface related N_r compounds is not restricted to the first few tens of metres above ground, and it continues throughout the atmospheric boundary layer (0-2 km). To quantify corresponding transport processes, we applied remote sensing techniques and direct measurements. A SODAR-RASS system ("acoustic radar") continuously measured profiles of wind speed and direction, air temperature, and turbulence up to 500 m above ground. Vertical profiles of ozone and CO_2 were measured from a tethered balloon (s. Fig. a). Our findings highlight that fluxes of biosphere-atmosphere-exchange of N_r are controlled by small scale transport processes ("turbulence"), by higher scale transport processes ("advection"), and by fast photo-chemical reactions between individual N_r compounds and ozone.



(a) SODAR-RASS and tethered balloon with Hohenpeißenberg in the background, (b) eddy covariance system, (c) fast response analysers, and (d) field deployment of the GRAEGOR system.

BIOGEOCHEMISTRY DEPARTMENT

The Vegetation as a Sink for Nitrogen Dioxide

Nitrogen dioxide (NO_2) plays a central role in tropospheric chemistry. It is involved in the formation of tropospheric ozone, acid rain and hydroxyl radicals, as well as in oxidation processes of volatile organic compounds (VOC). NO_2 exchange between plant leaves and the atmosphere takes place mainly via the leaf stomatal pores. However, in addition to such an exchange there is some discussion about additional decomposition at the leaf surface. A bidirectional exchange, i.e., deposition and emission, has been proposed, which would involve a so-called compensation point level (CP). This CP is zero when consumption and production processes balance. Forests exhibiting a high CP would serve as a source of NO_2 rather than a sink. In the literature we find a great range for NO_2 compensation points.

We are contributing to the solution of this "NO₂ conundrum", using a highly specific and sensitive technique for NO_2 analysis. Young potted trees of Beech (*Fagus sylvatica*), White birch (*Betula pendula*), Holm oak (*Quercus ilex*), and English oak (*Quercus robur*) were investigated under controlled laboratory conditions. Results were compared with data obtained during field experiments with *Quercus robur* and *Fagus sylvatica*. The NO_2 exchange was determined with two dynamic branch enclosures, one as an empty reference. All experiments were accompanied by determination of CO_2 and H_2O exchange rates. Field measurements of *Fagus sylvatica* were

conducted at the Research Centre Jülich during the ECHO (AFO 2000) campaign in 2003. For determination of the role of stomatal apertures on NO_2 uptake, a branch was cut from the tree and incubated under constant atmospheric NO_2 mixing ratios (~5 ppb) under laboratory conditions. After 4 h of acclimatisation, varying stomatal apertures were induced by infiltration of the plant hormone abscisic acid (ABA).

In the laboratory, we could exclude the existence of an NO_2 compensation point in the case of all four tree species investigated, even at very low concentrations. According to a preliminary evaluation of the field data, the oak tree in the field also did not exhibit a compensation point. Such data exclude any release of NO_2 from trees. Increasing anthropogenic nitrogen deposition into ecosystems and fertilisation might, however, change such a figure. The results further demonstrate the dominance of stomatal conductance on NO_2 exchange. A linear correlation between the ABA-controlled stomatal H_2O conductance with NO_2 uptake was observed in all experiments with all tree species. Furthermore, a reduction of the stomatal conductance under high light intensity was also closely accompanied by a decrease of NO_2 uptake in all cases. Deposition to the cuticle seemed to be of no importance. This interpretation is clearly supported by the fact that the aerodynamic resistance for NO_2 ranged around 2 orders of magnitude lower than the stomatal resistance.



Two cuvettes (stabilised Teflon film bags), one is an empty reference, the other one is enclosing a branch to investigate trace gas exchange between plants and the atmosphere.

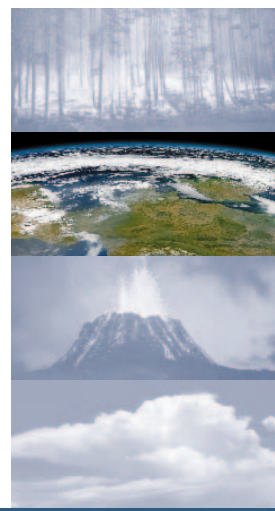
ATMOSPHERIC CHEMISTRY DEPARTMENT

Main Research Areas

Jos Lelieveld



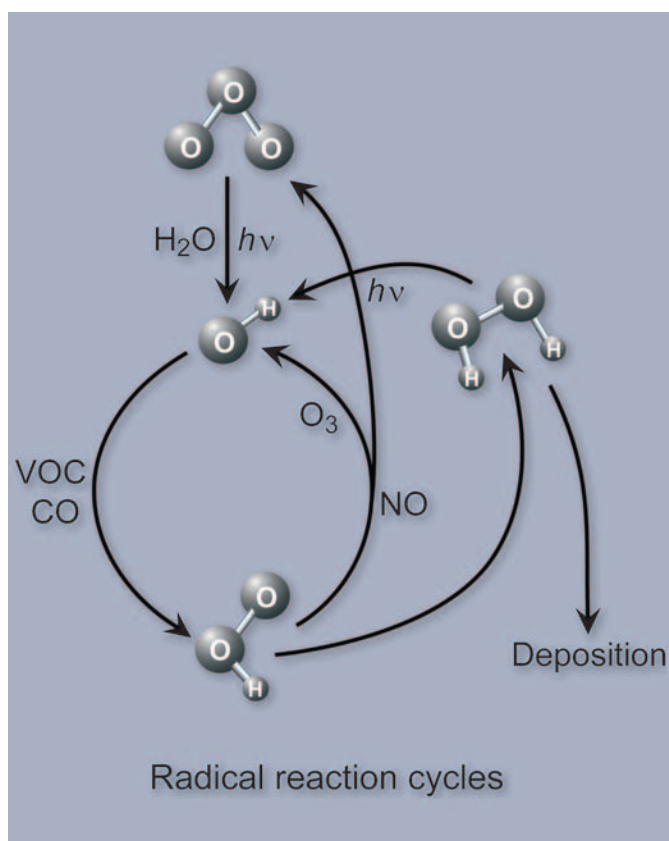
Born July 25, 1955 in The Hague, Netherlands. Undergraduate in Biology, University of Leiden. Ph.D. in Physics 1990, University of Utrecht. Research associate at Geosens B.V. in Rotterdam from 1984-1987. Atmospheric Chemistry Department of the MPI for Chemistry from 1987-1993. Extended visits at Stockholm University (1991) and the University of California, San Diego (1992). Professor in Air Quality at Wageningen University in 1993-1995. Professor in Atmospheric Physics and Chemistry at Utrecht University 1996-2000. Director of the international research school COACH (Cooperation on Oceanic, Atmospheric and Climate Change studies) 1997-2000. Director of the Atmospheric Chemistry Department since 2000. Professor in Atmospheric Physics at Mainz University, Spokesman of the International Max Planck Research School and Deputy Spokesman of the Mainz Geoscience excellence cluster.



The Earth's atmosphere contains 21% oxygen and it is uniquely oxidising. The oxidation processes transform natural and anthropogenic gases into products that can be more easily removed from the atmosphere through wet and dry deposition. This mechanism removes a multitude of gases that would otherwise accumulate and create a hothouse effect – rather than a greenhouse effect – or be toxic for life. This self-cleansing capacity of the atmosphere is regulated by radical reaction cycles that have some resemblance to those in combustion processes, in which hydrocarbons are oxidised to carbon dioxide and water vapour. On a global scale many gases, notably reactive carbon and nitrogen compounds, can have profound effects on the abundance of atmospheric oxidants. We investigate to what extent natural and anthropogenic emissions influence the self-cleansing capacity, and how they contribute to regional and global changes of our atmosphere and climate.

Our research focusses on ozone and the role of radicals in photo-oxidation mechanisms which play a central role in the self-cleansing mechanism. We develop highly sensitive instrumentation to measure trace gases, and uncover the photochemical reaction chains. We have specialised in the construction of instrumentation for application on aircraft. Laser-optical, mass spectrometric and gas chromatographic techniques, for example, are used to determine the key breakdown products of hydrocarbons and radicals. Our studies include laboratory investigations, field measurements on

aircraft and ships, and the use of satellite observations. We develop computer models to simulate the interactions of chemical and meteorological processes, and investigate the influences of atmospheric composition changes on climate.



ATMOSPHERIC CHEMISTRY DEPARTMENT

Atmospheric Chemistry Modelling

Computer models are important tools for studying the chemistry of the atmosphere. The models we use span a range of dimensions, from box models which represent the chemical processes occurring at a specific location, through cloud ensemble models which resolve the processes occurring on the scale of storms over a limited area, up to global models. These models simulate the major processes which affect the distributions of gases and aerosols in the atmosphere: emissions, photochemical reactions, gas-particle and particle-particle interactions, meteorological and transport processes, and physical loss processes such as deposition.

A major focal point is the direct interaction with the experimental research groups through the support and analysis of field measurements campaigns. We provide "chemical weather forecasts" during the campaigns in support of daily flight planning. We also help analyse the observations, particularly in light of the integrative information available from models, as well as their capacity to examine the sensitivity to uncertainties in the chemical system to place the observations into a larger perspective. This is being continually developed, for instance through the provision of web interfaces allowing field investigators to examine model output interactively, and the development of new modelling tools, such as tagged tracers and the capability to follow individual air mass motions directly using Lagrangian algorithms embedded in a Eulerian (grid-space) model.

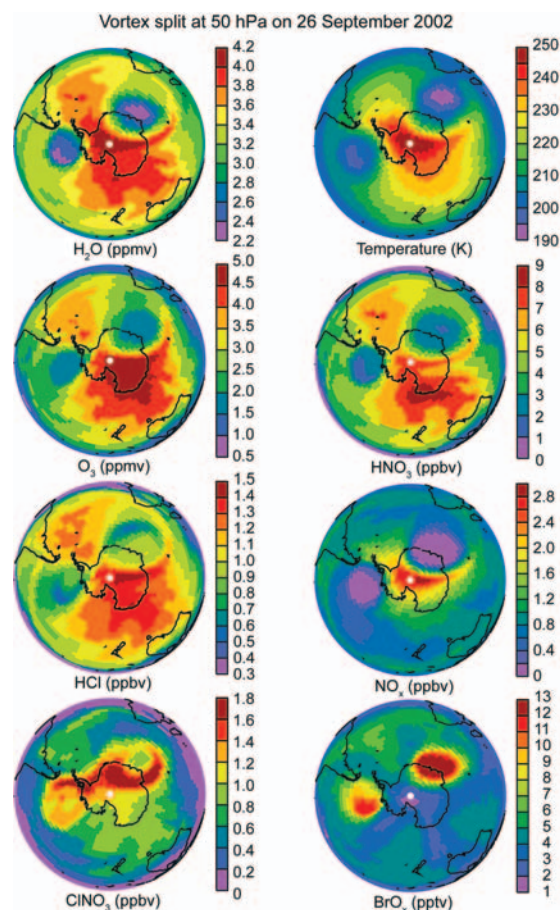
Importantly, researchers in our department contribute directly to the international evaluations of reaction kinetics compilations, which are used to specify the rates of photochemical and heterogeneous reactions in models, so that our computer codes are updated with the latest information. In turn the models are used to examine the sensitivity of the chemical system to uncertainties and new developments in laboratory assessments.

Another focus has been to establish a consistent global chemistry-climate modelling framework. This has involved the development of a standard for coupling the various processes

which are simulated in such a model, known as "MESSy", the Modular Earth Submodel System, coupled to the ECHAM5 climate model of the MPI for Meteorology. MESSy has been awarded for the advancement of scientific computation and was made available to national and international groups with the intent to provide it as open-source software.

A multi-year simulation with the chemistry-climate model of the entire lower and middle atmosphere, without artificial boundaries between the troposphere and stratosphere, has shown large advancements over earlier model versions and other similar models. Comparisons with synoptic ENVISAT data confirm the improvements both in the chemistry and the dynamics representations. The model results have provided new insights about stratosphere-troposphere exchanges, the tropospheric cleansing capacity and the water budget of the stratosphere. These results are available on request via <http://airdata.mpch-mainz.mpg.de>.

Model
 calculated
 chemistry and
 dynamics over
 Antarctica
 during a major
 stratospheric
 warming event
 in September
 2002.



ATMOSPHERIC CHEMISTRY DEPARTMENT

Atmosphere-Surface Exchanges

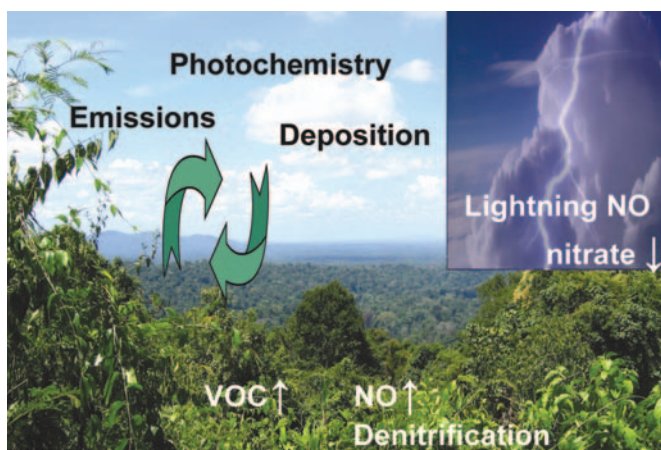
In October 2005, the field measurement project GABRIEL was carried out to investigate trace gas emissions and chemistry over the northern Amazon rainforest in Suriname and the adjacent Guyana's. Measurement flights, using a Learjet aircraft, reached up to 10 km altitude. New aspects of this campaign were the measurement of radicals and a large selection of reactive volatile organic compounds (VOCs). Additionally, several VOC instruments to assess the diel cycles were operated at the ground-based site Brownsberg in Suriname. For the first time measurements were performed over the pristine forest during the dry season, unaffected by the biomass burning which is commonplace in most of Amazonia. By comparing the output from both ground and aircraft measurements with models, an integral view on the roles of turbulence and atmospheric chemistry was gained. In addition, a smaller field campaign was completed in Finland to assess the VOC emissions of a boreal forest, used to contrast with the Amazon data.

We have engaged in an EU funded project with the aim to investigate the uptake and emission of organic trace species in seawater, by aerosol particles and in the air near the ocean surface. Our department co-ordinates this 9 partner project. A first laboratory intensive was completed, and the first of two ship-borne campaigns took place over the tropical Atlantic Ocean. Furthermore, a semi-controlled "mesocosm" experiment was conducted in Bergen,

Norway. The emission and uptake fluxes of several VOCs were quantified following a phytoplankton bloom in the Norwegian Sea using 20 m³ transparent Teflon enclosures. By adding CO₂ to the mesocosms possible future conditions were simulated and the influence of these changes on ocean biology and atmospheric chemistry can be assessed.

Collaborations between the department's experimental and modelling groups also included the analysis of peroxide exchanges between coniferous forest and the atmosphere. This analysis used peroxide profiles observed during a field campaign in Bavaria, and a chemical-meteorological model to assess the role of VOC ozonolysis in the formation of peroxides. The analysis revealed the highly efficient removal of hydrogen peroxide over coniferous forest, contrary to commonly applied model approaches, and indicated the active removal of organic peroxides by the vegetation.

The modelling of global scale atmosphere-surface exchanges has focussed on improving the representation of emissions and dry deposition of gases and aerosol particles in our chemistry-climate model. The technological, agricultural and biomass burning emission inventory has been updated and was complemented with biogenic and natural emissions, mostly calculated online in the model. This emission inventory has been used in land-use change scenario calculations, showing the importance of human-induced changes of biogenic emissions. The emission data are publicly available through <http://www.mnp.nl/edgar/>.



ATMOSPHERIC CHEMISTRY

Chemistry of Highly Reactive Species

DEPARTMENT

Most groups in the department have been active in the GABRIEL aircraft mission to study the influence of the tropical rainforest on atmospheric oxidation processes. This involved the deployment of new instruments and a specially designed aircraft inlet for highly reactive radicals, mounted on a wing pod to warrant the undisturbed sampling of ambient air. Hydroxyl (OH) radicals play a key role in the atmospheric cleansing mechanism, and their detection has been pursued by a laser-induced fluorescence technique, which also measures HO₂ radicals. For quality assurance the OH/HO₂ field instrument participated successfully in an international inter-comparison campaign.

During GABRIEL the first OH/HO₂ vertical profiles over the tropical rainforest were measured simultaneously with a host of precursor gases, photochemically active irradiance and VOC reaction intermediates with highly sensitive optical and mass spectrometric techniques, providing exciting new insights. In combination with modelling studies it has been shown that OH radicals are efficiently recycled after their initial loss by reactions with biogenic VOCs, which implies that the natural forest ecosystem contributes to the atmospheric cleansing capacity. Our measurements have also shown that thunderstorm convection over the tropical forest mixes lightning-induced NO_x with reactive VOCs of natural origin, giving rise to remarkably rapid O₃ formation.

Reactive halogen species may play an

important role in the chemistry of the marine boundary layer, both in terms of oxidation capacity and particle formation. Laboratory studies have been carried out to investigate the photochemistry and kinetics of iodine species such as IO and OIO radicals, both observed in coastal locations. Our experiments yield physical properties such as absorption cross sections, allowing accurate measurement of their photochemical lifetime and concentrations. Laser-based kinetic investigations have characterised the rate of reaction with marine traces gases and radicals and identified products.

The importance of reactive halogen chemistry on a global scale has become evident throughout the last decades, initially with a focus on chloro-fluorocarbon chemistry in the stratosphere. Nevertheless, the largest chlorine and bromine source to the atmosphere is the ocean through sea salt aerosol, and therefore reactive halogen chemistry is expected to have an influence on tropospheric chemistry, too. For the first time a global model study of halogen chemistry in the marine boundary layer was accomplished, using a prognostic calculated aerosol distribution as well as the explicit calculation of halogen release from the aerosol. The halogen chemistry mechanism including gas and aerosol phase reactions was developed as part of our chemistry-climate model. First results show pronounced maxima of reactive halogen species in the middle latitude marine boundary layer in the northern hemisphere, associated with substantial ozone loss.

GABRIEL
measurement
campaign
in Suriname.



ATMOSPHERIC CHEMISTRY

Aerosol Formation DEPARTMENT and Chemistry

Biogenic VOCs play an important role in atmospheric chemistry, e.g. in ozone formation, and their oxidation products can form aerosol particles, which affect visibility, air quality and climate. Monoterpenes and sesquiterpenes are emitted in large quantities by forests, and their reaction with ozone is considered a chief source of low-volatility compounds responsible for secondary organic aerosol (SOA) formation. Although the emissions of sesquiterpenes are expected to be substantial, they are difficult to detect due to their very short atmospheric lifetime, being of the order of minutes.

The chemical degradation and SOA formation potential of mono- and sesquiterpenes have been investigated in the laboratory, where both gas- and aerosol-phase products are determined under controlled conditions. For the structural analysis of

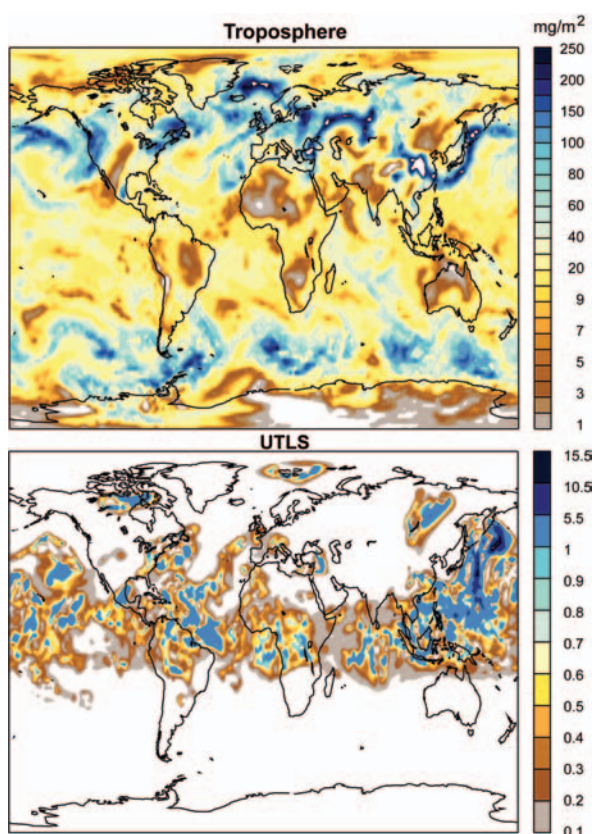
unknown VOCs, liquid chromatography/mass spectrometry employing electrospray ionisation is used, which elucidates the complex chemical structures of the oligomeric substances formed in the ozonolysis of unsaturated VOCs. We have determined the SOA yields and have shown, for example, that they increase with decreasing temperature.

Secondary aerosol particles are also formed by the gas-to-particle conversion of anthropogenic emissions and in particular their oxidation products. We have developed an aerosol-chemistry equilibrium thermodynamics model to compute the particle composition and the gas-particle partitioning of semi-volatile gases, including water. The acid-base calculations account for inorganic sulphur and nitrogen compounds, mineral cations and low-molecular weight organic acids.

We have studied the gas-aerosol partitioning, as observed during the MINOS (Mediterranean Intensive Oxidant Study) campaign in Crete, Greece. The campaign was characterised by several pronounced periods dominated by sea salt, mineral dust and biomass burning emissions. It was shown that our equilibrium model can closely reproduce the field measurements of aerosols and related gases. A key test in this respect is the gas-aerosol partitioning of ammonia and nitric acid over different aerosol types and sizes, being highly sensitive to the particle ionic composition.

By including the equilibrium model into our chemistry-climate model we have strongly improved the representations of aerosol chemistry, aerosol associated water, and the distribution of aerosol mass as a function of relative humidity. For the first time a global model can simulate hazes and thin clouds, which have a strong influence on the weather and climate. Using our chemistry-climate model, such clouds have been predicted to be abundant e.g. over the North Atlantic Ocean associated with aerosol pollution from the USA. A reanalysis of METEOSAT data, for which the retrieval normally rejects thin clouds, has shown that these new model results are realistic and accurate.

Model calculated aerosol associated water in the troposphere and tropopause region in September 2003.



ATMOSPHERIC CHEMISTRY DEPARTMENT

Transport and Chemistry at the Tropopause

Measurements of the composition of the upper troposphere and lower stratosphere (UTLS) are important for the understanding of climate change, since perturbations of trace gases (e.g. O_3 , H_2O) and aerosols in this region can substantially contribute to climate forcing. Furthermore, the UTLS is to a great extent affected by dynamical processes that determine e.g. the tropopause location. These processes range from deep convection originating near the surface to synoptic and planetary wave disturbances. The roles of transport and in-situ chemistry in the UTLS composition are highly uncertain.

Several partially oxidised VOCs (e.g. alcohols, ketones and aldehydes) are important sources of OH and HO_2 in the upper troposphere by acting as radical reservoir gases. The lifetimes and degradation products of a number of these species have been determined in laboratory investigations at a range of temperatures. New laser-based kinetic methods have been used to derive rate coefficients and photolysis quantum yields for species such as methanol and acetone. The presence of cirrus clouds in the tropopause region provides ice surfaces for trace gas interactions. Laboratory data has shown, for example, that formic acid can be temporarily removed from the gas phase by its deposition on ice particles.

The analysis of aircraft observations of a number of partially oxidised VOCs over western Europe with box-models and 3D chemistry-transport models has indicated that the most important factors determining formaldehyde (HCHO) and radical concentrations in the UTLS are the concentrations of NO, reactive VOCs (including isoprene), methylhydroperoxide, methanol, acetone as well as the level of photochemically active irradiance. Our measurements furthermore show that convective transport of hydrogen peroxide (H_2O_2) can be much more efficient than previously assumed, in spite of its high solubility in precipitation. These aircraft observations are being continued in regular mini-campaigns, and OH/ HO_2 radical measurements have been included with the aim to gain further insight into seasonal dependencies of oxidation pathways.

Civil aircraft typically cruise in the UTLS region.

Within the project CARIBIC we have modified a new Lufthansa Airbus 340-600 long-distance aircraft to regularly perform measurements near the tropopause over different parts of the globe. For the flight destinations thus far (South America, South Africa, Caribbean, South and East Asia) about half of the cruising time was spent in the UT and half in the LS. Unique and comprehensive measurements of a host of species, e.g. H_2O , O_3 , NO_x , CO, greenhouse gases, VOCs, oxidised VOCs, reactive bromine (BrO) and aerosols are being performed in the tropical upper troposphere by the A340-600 flights, carrying the 1.5 ton measurement container. The observations furthermore provide statistical information about the tropopause dynamics and the degree of mixing in the lowermost stratosphere. Interesting differences in tropopause characteristics have been observed by comparing measurements over the North Atlantic Ocean with those over continental Asia.



COSMOCHEMISTRY

Weathering and Aeolian Processes on Earth and Mars



Atmospheric dust, i.e. aeolian insoluble mineral particulate matter of terrigenous origin, is one of the most significant variables in global climate change. Ice-core records, in particular, have shown that atmospheric dust concentration exhibits extreme variability over recent glacial-interglacial cycles, with much higher levels during cold periods than during warmer periods such as the present Holocene. By comparing the Sr and Nd isotopic composition of the mineral dust extracted from ice cores with that of potential source areas, it has been shown that southern South America (Patagonia and the Pampas) was the main source for the East Antarctic plateau (Vostok and Dome C) dust during several high-dust cold intervals of the last Glacial periods. Since the dust concentration was much lower during warm periods, it is highly challenging to obtain sufficient material for isotopic analyses, which also explains the scarcity of data. Our analyses of Sr and Nd in snow from Berkner Island on the Ronne Ice Shelf, Antarctica, indicate a seasonal variability with distinct dust-sources in summer and winter.

Dust-covered in situ fragmented rock photographed by the Mars rover Spirit.

Salt-induced fragmentations of rocks on Mars were compared with mechanical weathering processes in terrestrial semi-arid environments. This reveals that salt fragmentation together with aeolian processes sculpture the Martian landscape. Data from the Mars Exploration Rovers, carrying the Alpha Particle X-Ray Spectrometer, the Mössbauer Spectrometer, the Microscopic Imager and the Rock Abrasion Tool, were used to study the chemistry of soils, undisturbed and brushed surfaces and the interior of rocks on Mars. At all landing sites the soil is basaltic with a significant amount of S (~ 2.5 wt. %) and Cl (0.8 wt. %). The Martian regolith is composed of olivine-rich basaltic fines and global windblown dust. The presence of olivine suggests that physical weathering has been more important than chemical weathering. However, substantial enhancements of Br over Cl in rocks, in sulfate-rich evaporates and in fracture filling secondary salts in veins of the Martian meteorite Nakhla, indicate alteration processes in an aqueous environment. This has probably happened later than 1.3 Ga ago since the crystallisation age of Nakhla is 1.297 Ga.

A comparable salt-induced fragmented rock (Gran Salar, Argentina).

GEOCHEMISTRY DEPARTMENT

Main Research Areas

Albrecht W. Hofmann



Born March 11, 1939 in Zeitz. Undergraduate studies in Geology at Duke University, Durham, N.C., USA and University of Freiburg i.Br. Ph.D. in Geochemistry at Brown University, Providence R.I. (1969). Scientific Assistant at Labor für Geochronologie, University of Heidelberg (1968-70), Postdoc and Scientific Staff Member at Carnegie Institution of Washington (1970-1980). Director of Geochemistry Department since 1980. Awards (Selection): Fellow American Geophysical Union (1994), V.M. Goldschmidt Medal of the Geochemical Society (1996), Foreign Associate of U.S. National Academy of Sciences (1999), Harry H. Hess Medal of the American Geophysical Union (2001).



Geochemistry is concerned with quantitative analysis of major and trace elements, and their isotopic abundances, in rocks, minerals, melts and fluids. We use these data to understand the origin and evolution of our planet and the processes that continue to shape it. The slow decay of radioactive isotopes such as uranium, thorium, potassium, rubidium, samarium and rhenium changes the isotopic abundances of the radiogenic daughter elements. From this, we can measure not only the ages of rocks, but the isotopic abundances of the daughter elements are powerful tracers of many geological processes ranging in scale from microscopic to global.

Much of our research focuses on large-scale terrestrial processes. Solid-state convection continuously turns over the Earth's interior. It is driven by heat generated from natural radioactive decay. It creates continents, ocean basins and mountains, and it causes mantle rocks to melt. These melts migrate toward the surface to create volcanoes and new continental crust. The geochemical "fingerprints" consisting of chemical and isotopic data from these melts reveal the nature and history of global cycling and recycling processes. In these cycles, oceanic crust and some continental material is returned to the deep mantle and is ultimately recycled in new volcanic eruptions.

One group led by Wolfgang Paul Award winner Alexander Sobolev is studying microscopic melt inclusions trapped in magmatic crystals. This offers a new window on melting, because these

melts preserve their primary chemistry formed in the mantle. Another group studies mantle rocks that remain behind after melting and must be dredged from the ocean floor. These studies employ a microanalytical arsenal involving an electron microprobe, an ion microprobe, and laser ablation plasma mass spectrometry.

Other studies trace the origin of ancient parts of the continental crust by measuring the ages of minerals such as zircon and garnet separated from the rocks. The radioactive elements and their daughter products, e.g. uranium and lead, are present in microgram or nanogram quantities. Their chemical separation before mass spectrometric analysis requires state-of-the-art cleanroom facilities.

We also study how global ocean circulation has changed in the geological past. This circulation resembles a global conveyor belt which transports heat from the tropics to the northern ocean. We trace ancient ocean currents by analysing lead isotopes in dated sediments. These lead isotopes are precipitated from the water column above, and this makes it possible to trace the movement of specific water masses through geological time.

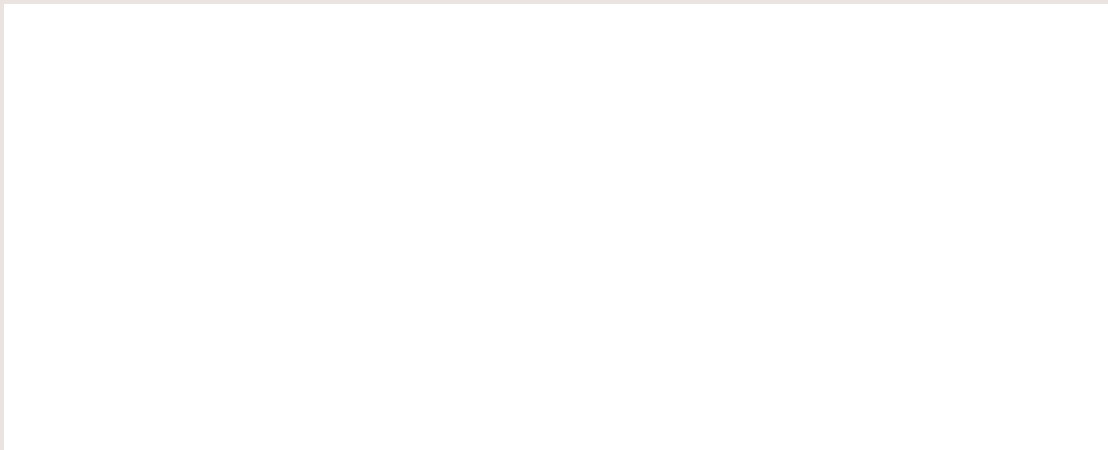
GEOCHEMISTRY DEPARTMENT

Secrets of Olivine Chemistry

The mineral olivine, also known by the name peridot, its precious-stone variety, makes up nearly half of the Earth's upper mantle. This simple, and rather pure iron-magnesium silicate has in the past held little interest to geochemists, precisely because it is so pure. Most of the trace elements used by geochemists to study important mantle processes reside in other minerals. In our laboratory, we have used olivine crystals extensively in the past, but only as "vessels" for microscopic inclusions of chilled melts (see our 2003-2004 report). But even nominally "pure" minerals contain trace elements – they are just present at very low levels. Recently we have improved our techniques for chemical microanalysis to such an extent, that we can quantitatively determine trace elements in olivine to high levels of precision. This has opened a new world. Precise data for nickel, manganese and zinc in olivines precipitated from volcanic melts tell a new story about processes taking place in the earth's mantle.

This story spells out what happens when recycled ocean crust returns from the deep

mantle toward the surface and begins to melt. The first melt reacts with olivine bearing "peridotite" and forms a new solid rock (called pyroxenite). This reaction zone can be observed in natural rock samples, so-called "xenoliths" (see photograph), plucked from the mantle by ascending melts, but it can also be reproduced in high-temperature, high-pressure experiments. Eventually, these pyroxenites melt together with ordinary mantle rocks (peridotite). When this hybrid melt ascends to the surface, it precipitates abundant olivine crystals. By measuring the nickel, manganese and zinc contents in these olivines we can determine the proportions of eclogite and peridotite deep in the mantle where the melting takes place. In this way we can quantitatively evaluate the proportions of recycled crust in many mantle-derived magmas. We find that most basalts erupting on the ocean floor contain only small amounts of recycled crust, but in some mantle plumes the proportion of recycled crust constitutes as much as half of the source rock.



Recycled former ocean crust is converted to (red garnet-bearing) eclogite by high pressure in the mantle. When eclogite melts, it reacts with normal mantle peridotite and forms a new rock consisting of the single mineral, dark green pyroxene.

GEOCHEMISTRY DEPARTMENT

Exchange at the Hydrosphere – Lithosphere Interface

Platinum group elements (Ir, Os, Ru, Rh, Pd, Pt) are unique tracers of processes involving sulphide and metal phases. These metals monitor processes deep in the Earth's interior (core-mantle differentiation; mantle melting), within the Earth's crust (evolution of magmas; formation of transition metal-rich sulphide ores) and on the Earth's surface (evolution of oceans; interaction of water/fluid with host rocks; anthropogenic addition to soil, water and atmosphere). Our group focusses on the geochemistry of these elements and the radiogenic Os isotope system, for example, to describe the metal exchange between hydrosphere and lithosphere on the ocean floor.

Near spreading centres in the midst of the oceans hot magma reaches the surface. Seawater can penetrate along fissures deep into the seafloor building convection currents which deliver up to 400 °C hot hydrothermal fluids to the ocean. The associated black smokers, chimneys that spew a flood of black mineral particles, metal deposits of Cu, Zn and Au, and the diverse biota of clams, tubeworms and shrimps have become the familiar hallmarks of hydrothermal systems. This fluid flux has strong impact on the global composition of seawater and controls many chemical and biological processes in the host rocks.

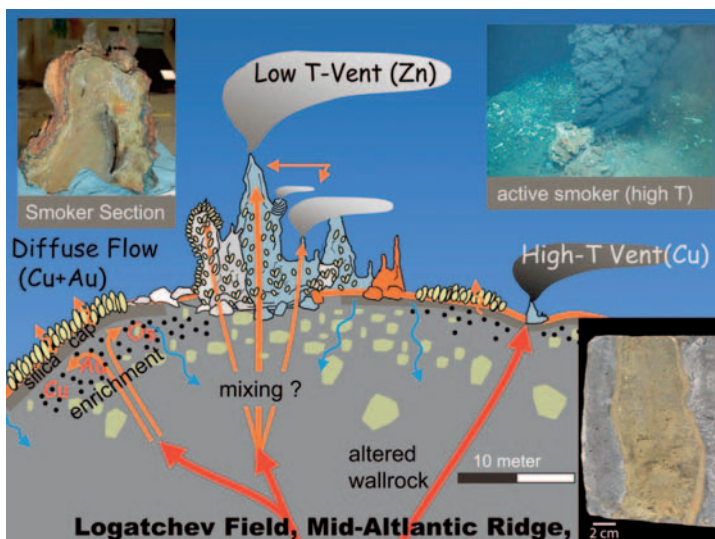
The isotopic composition of the platinum group element osmium in the oceans is governed by inputs from the continents (rivers, groundwater, aerosols), extraterrestrial matter (cosmic

dust) and from the oceanic crust (hydrothermal fluids). High-temperature hydrothermal fluids have significantly higher concentrations of platinum group elements than seawater while there is a nearly complete Os isotopic exchange between the interacting seawater and ocean lithosphere. The present-day deep oceans derive about 20 % of Os in seawater from the mantle.

The 3-dimensional distribution of these metals in host rocks and sulphides provides detailed information on their mobilisation potential. Cooling of the rising fluid, mainly caused by the mixing with cold seawater, triggers the precipitation of sulphides above and below the seafloor. Sulphur- and Os-isotope compositions in sulphides indicate that they form at variable fluid/seawater ratios, being low deep in the hydrothermal system and high directly in the smoking chimneys. Sulphide mineralogy, the metal distribution in "hot" and "cold" sulphide assemblages suggest that older, subseafloor sulphides were altered by younger, high-temperature hydrothermal fluids, a clear indication for zone refining.

Hydrothermal activity within hydrothermal systems is a multi-stage process and may take place in time intervals of thousands of years. We are developing new microanalytical techniques measuring metal concentrations and stable isotope fractionations in single mineral grains using our multi-collector inductively coupled plasma mass spectrometer which is connected to a laser ablation

system. The objective is to study the exchange of metals between host rock and fluid in order to constrain the temporal and spatial metal fluxes from mantle to ocean.



Schematic section through the Irina 2 Complex of the Logatchev hydrothermal field on the Mid Atlantic Ridge. Inserted photos show an active high-temperature black smoker, a cross section through a chimney and a sulphide vein representing a fluid flow channel. Image courtesy of T. Kuhn, IFM-GEOMAR.

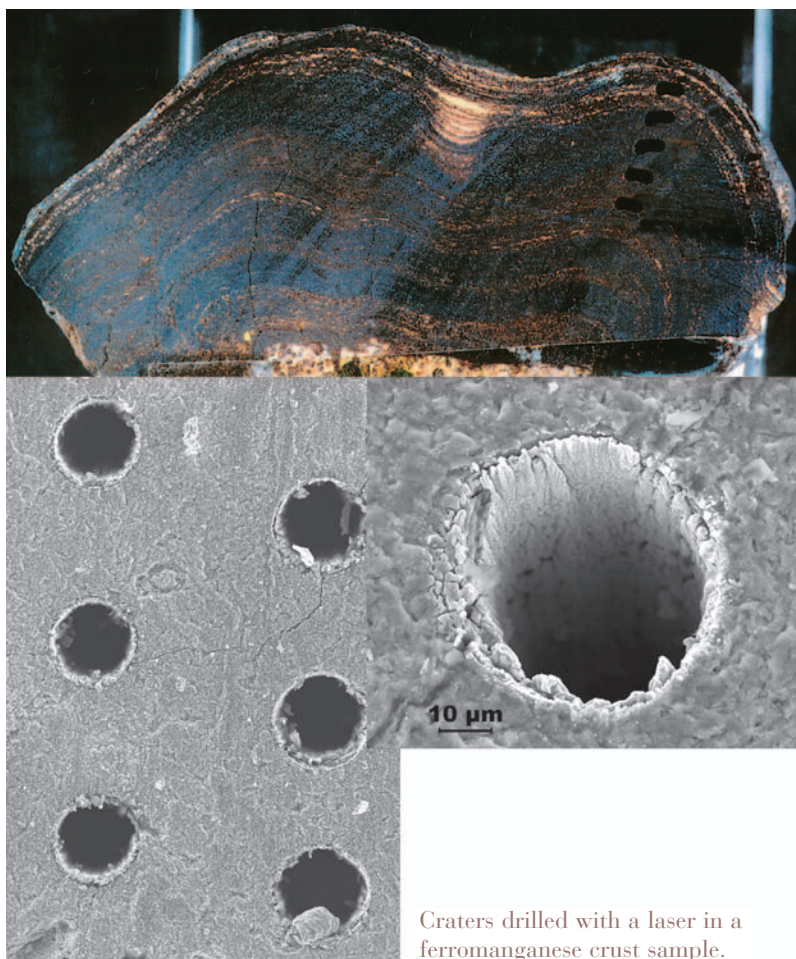
A new Tool for high Resolution Records of Seawater Composition

The most extensive deposition of manganese, the 10th most abundant element in the Earth's crust, occurs in the oceans as Fe-Mn nodules and crusts. Manganese nodules and crusts grow slowly (a few mm per million years) by direct precipitation of Mn and Fe hydroxides from ambient seawater and thus can provide a record of changes in seawater composition through time induced by modifications in the input sources to the oceans. Changes in the erosional inputs are driven by climate changes and tectonics, which ultimately modified ocean and atmosphere circulation patterns.

Of special interest for isotope geochemists is the U-Th-Pb system. Uranium and thorium have the naturally occurring and radioactive isotopes ²³⁸U, ²³⁵U and ²³²Th, which decay to ²⁰⁶Pb, ²⁰⁷Pb and ²⁰⁸Pb isotopes, respectively. The isotopic composition of Pb in manganese nodules and crusts is influenced by continental weathering (continents are uranium-rich), hydrothermal and volcanic activity at mid-ocean spreading centres (mantle is uranium-poor). Thus lead isotopes as well as trace elements can be used to fingerprint the sources and origin of material delivered to the oceans.

High-resolution records of temporal variations in seawater elemental and isotopic compositions can now be obtained with the advent of a new microanalytical technique, namely laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS). Extremely small spot sizes, between 2 and 20 μm, corresponding to a time resolution of only a few thousand years provide high quality Pb isotope and trace element data, allowing to

reconstruct seawater variations at glacial-interglacial time scales. These results could only be obtained using our highly sensitive ICP mass spectrometer Element2 and the New Wave solid-state Nd:YAG lasers UP193 and UP213, which have small wavelengths of 193 nm and 213 nm, respectively, and short pulse widths. Our first data on a Pacific manganese crust show a secular variation in ²⁰⁸Pb/²⁰⁶Pb isotope ratios which are correlated with trace element ratios. The combined trace element and Pb isotope measurements indicate that there have been pulses of hydrothermal activity during the growth of this Mn-crust reflected in distinct signatures compared with those of the hydrogenous phases of growth.



Craters drilled with a laser in a ferromanganese crust sample.

GEOCHEMISTRY DEPARTMENT

GEOROC – Geochemistry on the World Wide Web

GGEOROC is an online database compiled in the Geochemistry Department of our institute. It includes the published geochemical analyses of volcanic rocks, minerals and inclusions from worldwide occurrences (see Fig.). The GEOROC web interface allows the selection of data by bibliographic, tectonic, geographic, chemical and petrographical criteria. Currently, the database contains about 230000 geochemical analyses from 5700 publications.

Since its introduction at the end of 1999, the number of geoscientists using the database increased steadily up to around 8000 users per month. Applications of the database are, for example, compilations of the geochemical composition of volcanic ocean islands or island arcs, allowing conclusions on differences in the source material of the respective lavas.

Distribution of samples for which data are available in GEOROC (yellow dots). Blue and red dots show the samples contained in the “sister” databases PetDB and NAVDAT respectively.

Planetary Gases: Compositions, Origins, Processes

The atmospheres of the “terrestrial planets” (Venus, Earth, Mars) share common features. Main constituents are the elements carbon, nitrogen, and oxygen, either in elemental form, or in chemical compounds (such as CO₂). Additional “atmosphile elements” include the noble gases (helium, neon, argon, krypton, and xenon). Common to all these elements is that a significant fraction of the planetary inventory occurs in the atmospheres and that these elements are significantly depleted compared to their cosmic (solar) abundances. An important question is the origin and later modification of the existing inventory.

To this end we investigate materials that may have served as vehicles delivering the gaseous elements to the planets. We concentrate on the investigation of abundances and isotopic compositions of the noble gases, because in their case drawing conclusions regarding the original inventory, from what is observed today, is most straightforward. In addition, we recently installed analytical capabilities for the analysis of small (nanogram) amounts of nitrogen.

The most accessible relevant materials that may resemble the building blocks, from which the planets formed, are primitive (volatile-rich) meteorites. In these, carbon and nitrogen occur mostly in the form of a macromolecular material;

the noble gases are concentrated in a sub-fraction. Fullerenes which – because of their cage structure – have been suggested as carrier materials, seem unlikely host phases, as we have shown that C₆₀ incorporates helium efficiently, but less so the other noble gases with their larger atomic radii.

A significant portion of primitive meteoritic gases is trapped within nano-diamonds of about 2.5 nanometre size, while a small fraction occurs trapped in micrometre-sized grains of silicon carbide and graphite. These three minerals represent “stardust”. Investigations on these allow drawing conclusions concerning their history and the nuclear processes by which heavy elements are synthesised in stars. Complementing our mass spectrometric analyses, abundances and chemical state of trace elements in SiC are studied by photoelectron spectroscopy in a joint project with Johannes Gutenberg University, Mainz. Contacts to the local university are also strengthened by a seminar jointly organised with the Institute of Nuclear Chemistry.

In addition to the study of primitive materials, a significant part of our work is directed towards analysis of meteorites from Mars. Here we have shifted our attention towards characterising noble gases found in rocks affected by weathering processes on Mars vs. Earth. A project to be begun

in the near future is the noble gas study of micrometeorites (size range 0.04 to 2 mm). Because of analytical limitations, analyses so far were mostly restricted to helium only. We aim – using a high-sensitivity mass spectrometer equipped with a new type of multi-collection ion counting detector system (see Fig.) – to extend these studies to the full suite of noble gases.

New noble gas mass spectrometer during test phase of multi-collector detector for simultaneous measurement of all Xe isotopes.



GEOCHEMISTRY DEPARTMENT

Two Years on Mars: APXS Measurements

In January 2004, two NASA probes landed on the martian surface: the Mars Exploration Rovers Spirit and Opportunity. On each rover's instrument arm a small cylindrical instrument, the Alpha Particle X-Ray Spectrometer (APXS), is mounted that was designed and built under the leadership of Rudolf Rieder at the Department of Cosmochemistry. While a lifetime of several months was expected, both instruments survived the harsh martian environment for more than two years and no signs of aging are observed to date. To determine the chemical composition of a sample, the APXS sensor head is docked at the sample surface and x-ray spectra are recorded.

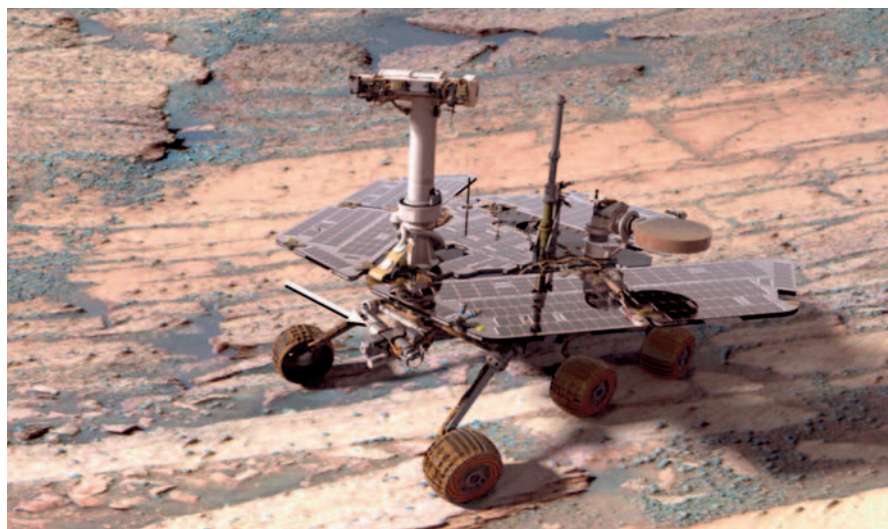
For the first 150 martian days (or sols) of its mission, rover Spirit traversed rather flat terrain at the floor of Gusev crater. At these plains, angular rocks are littered on typical martian soil. Plains rocks were identified as primitive basalts, whose comparatively fresh nature revealed that there has been little aqueous activity in Gusev crater since these basalts were emplaced. The chemical compositions of soils along the rover's traverse were very similar and comparable to those of other landing sites.

Circumstances changed when Spirit reached the Columbia Hills. These Hills are composed of ancient materials that are surrounded by the younger Gusev plains basalts. Spirit has encountered a remarkably diverse set of rocks. Based on their chemical compositions, as obtained by the APXS, several rock classes could be

identified. The rocks of the Columbia Hills preserve a rich record of geologic processes and environmental conditions, such as aqueous activities, early in martian history (several billions of years ago).

After landing in Eagle crater at Meridiani Planum, rover Opportunity spent the first 60 sols exploring rock outcrops exposed in the crater wall, as well as soils on the crater floor. The chemical composition of these rocks turned out to be very different from previously known compositions on Mars. Stunning high sulphur contents (up to 11 weight percent) were found in outcrops all along the rover's traverse, which extends to more than 7 kilometres to date. The outcrops probably result from chemical weathering of basalt in dilute aqueous solutions of sulphuric acid, followed by evaporation to produce sulphate salts that accumulated with fine grained silicates.

Most conspicuous features at Meridiani are small spherules that are found on top of soil surfaces and inside of outcrops. These spherules, which are most likely eroded from the outcrops, are very rich in iron and hematite, an iron-bearing mineral, as determined by the Mössbauer Spectrometer on board the rover. The spectral signature of hematite, as observed from orbit, motivated landing on Meridiani. The formation of hematite-rich spherules inside the outcrops also relates to ancient aqueous activities in Meridiani billions of years ago.



Special effect:
A computer generated
image of rover
Opportunity combined
with a real landscape
image of Meridiani. The
stowed instrument arm,
which carries the APXS,
is indicated by a white
arrow.

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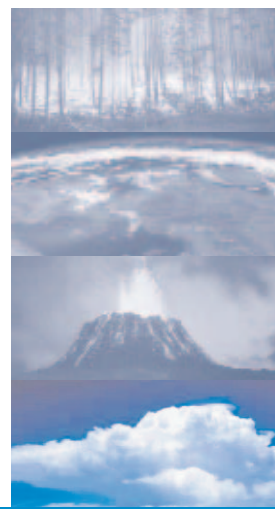
PARTICLE CHEMISTRY DEPARTMENT

Main Research Areas

Stephan Borrmann



Born 18. Januar 1959 in Mainz, Germany. "Diplom"/M.S. degree in Physics in Mainz. "Adjunct Research Instructor" at the Naval Postgraduate School in Monterey, CA, USA for two years. Ph. D student in Mainz. Postdoc for two years at the NCAR in Boulder, Colorado. Habilitation in Meteorology in Mainz and head of the Aerosol Research Group at the Forschungszentrum Jülich GmbH. Since 2000 professor for Meteorology at the Mainz University. Since 2001 Director (in part-time assignment) and Scientific Member of the Max Planck Institute for Chemistry. **Memberships in Associations:** Member of the European Geophysical Society, the German Meteorological Society, the German Physical Society. 2004 and 2005 elected member of the German Science Foundation Review Panel ("DFG Fachkollegium").



The Department of Particle Chemistry of the Max Planck Institute is structurally and conceptually linked to the Institute for Physics of the Atmosphere at the Johannes Gutenberg University in Mainz. This joint assignment of Stephan Borrmann as university professor and MPI director constitutes a close link between both institutions and is a novelty for the location of Mainz.

The research of the group is focussed on chemical composition and physical properties of aerosol and cloud particles. Sizes, number densities, shapes, radiative properties and formation mechanisms of aerosols and clouds are topics of experimental investigations. Knowledge concerning clouds and airborne, suspended aerosol particles is of importance for our understanding of climate, climate change, atmospheric chemical processes, as well as anthropogenic influences on the atmosphere. For these reasons emphasis in the department is placed upon: (1) Investigations of aerosols in the troposphere and lower stratosphere, (2) processes and properties of Polar Stratospheric Clouds, which contribute to the ozone holes, (3) the effects of commercial air traffic exhaust emissions on the atmosphere, and (4) the influence of upper tropospheric ice clouds (cirrus) on the chemical composition of the air. In addition there are (5) studies on the capabilities of cloud droplets, snow crystals, graupel and hail particles to remove ("scavenge") pollutant gases and aerosols from the atmosphere.

The methods employed cover mass spectrometric instruments for the measurement of aerosol and cloud particle chemical composition, optical and thermodynamical instruments, and a worldwide unique vertical wind tunnel. By means of this facility droplets and hydrometeors are suspended in a vertical air flow for extended periods to become amenable for detailed experiments. *In situ* atmospheric measurements are performed on board of the converted Russian espionage aircraft M-55 "Geophysika" (reaching altitudes up to 22 km), as well as other research aircraft, ships and ground stations. The efforts are aimed at enhancing our understanding of cloud related processes in order to improve weather and precipitation forecast, and also contributing to climate modelling. The methods developed in the department are applied also to environmental industrial research outside of fundamental atmospheric science. At this way our graduate students become qualified for a large variety of working fields within industry and research.

PARTICLE CHEMISTRY DEPARTMENT

Cloud and Aerosol Experiment in the Swiss Alps

Aerosol particles are solid or liquid particles from natural or anthropogenic sources that are suspended in the air. Typical number concentrations are in the order of a few hundreds to several thousands of particles per cubic centimetre of air. Only a small subset of these aerosol particles act as cloud condensation nuclei (CCN), and an even smaller subset act as ice nuclei (IN), and these subsets are not identical. The identification of ice nuclei is crucial for the understanding of heterogeneous ice nucleation in supercooled clouds, which is the main initiation process of precipitation in middle latitudes. Until today it is not well understood which chemical components (e.g. sulphuric acid, ammonium, nitrate, various organic substances, mineral dust, sea salt, soot, or other materials) contained inside or on the surface of aerosol particles enable a particle to act as an ice nucleus. While water soluble compounds are expected to favour the formation of liquid cloud droplets, insoluble materials like mineral components may favour the formation of ice particles.

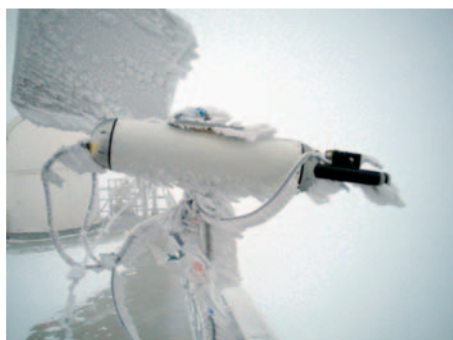
The High Alpine Research Station Jungfraujoch offers excellent opportunity to study cloud physics and chemistry, since it is located at 3500 metres altitude, and is situated in clouds about 37 percent of the time. A series of experiments was performed in the recent years at the Jungfraujoch station under the name of CLACE (Cloud and Aerosol Characterisation Experiment), in winter 2004, 2005 and 2006 under the participation of the Particle Chemistry Department of the Max Planck Institute

for Chemistry and the University of Mainz.

The CLACE projects are international co-operations, bringing together scientists from Germany, Switzerland, Denmark, United Kingdom, and Finland. A large set of instruments was employed in order to investigate the microphysical, optical, and chemical properties of the aerosol particles, the CCN, and the IN.

In order to separate the IN from the rest of the aerosol particles, a special counterflow inlet (ICE-CVI, designed by the Institute for Tropospheric Research, Leipzig) was operated during the experiments. It was designed for the sampling of small ice particles which have grown only by water vapour diffusion. The ice fraction is subsequently evaporated to make the residual particles, which are expected to be the original ice nuclei, available for analysis with various types of aerosol mass spectrometers and other devices.

The results indicate that the Wegener-Bergeron-Findeisen mechanism whereby ice crystals grow at the expense of liquid water drops, releasing formerly activated aerosols back into the interstitial phase, plays an important role in ice cloud formation. This has important implications for our understanding of weather and climate, since the presence of a few ice crystals affects the cloud microphysical and radiative properties. Furthermore, it was found that mineral dust and soot particles were enriched in the ice phase residual samples, indicating that these particles are potential ice nuclei.



PARTICLE CHEMISTRY

The Feldberg DEPARTMENT

Aerosol Experiments

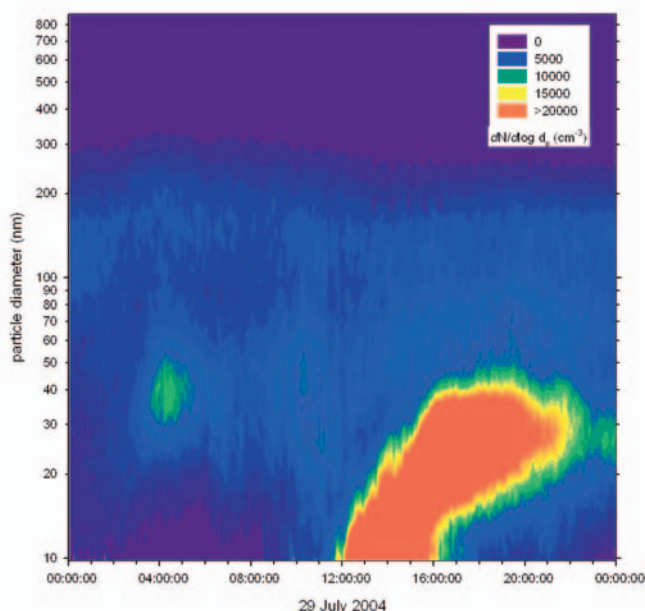
Particulate matter ("aerosol particles") suspended in the atmosphere is known to cause significant climatic effects, for example by scattering and absorbing sunlight, to determine cloud properties and to cause adverse health effects to humans. Therefore the detailed study of aerosol particles in the atmosphere is of high importance.

In the summers of 2004 and 2005 two measurement campaigns were conducted at the Taunus Observatory at Mt. Kleiner Feldberg, located in a mostly coniferous forest about 25 km northwest of Frankfurt. The aim of these campaigns was a comprehensive characterisation of the aerosol particles present at this location. The characterisation comprised the measurement of the particle number and sizes as well as the detailed mass spectrometric determination of the chemical composition of the aerosol particles. Further characterisations, for example, the determination of the ability of the aerosol particles to act as cloud condensation nuclei were measured by the Biogeochemistry Department of the institute.

Our measurements showed that the air at Mt. Kleiner Feldberg typically contained a few thousand particles per cubic centimetre. Most

particles had sizes between 50 and 200 nm in diameter and the particles were mostly composed of organic compounds (usually 50 to 75% of the aerosol mass), and contained smaller amounts of sulphates, nitrates, ammonia as well as soot inclusions. Measured total particle mass concentrations ranged between 5 and 40 $\mu\text{g}/\text{m}^3$.

During these summer measurements we encountered numerous so-called nucleation events, when the formation of new particles in the atmosphere, formed from condensable gas-phase precursors, was observed. An example of such a nucleation event is shown in the figure. The size resolved number concentration of particles is displayed by colour coding as a function of time (x-axis) and particle size (y-axis). During a nucleation event a banana-shaped contour of the particle concentrations is observed. More than 35 000 cm^{-3} newly formed particles appear around noon time at the smallest observable sizes and grow subsequently by uptake of further condensable substances during the afternoon to sizes around 30 nanometres. Our mass spectrometric measurements indicate that these particles likely grew from the condensation of organic substances, probably terpene oxidation products. Plants, especially coniferous trees, emit different gaseous terpenes like pinene or limonene. These substances are oxidised in the atmosphere by gas phase reactions with ozone, the OH radical or the nitrate radical NO_3 . Some of the oxidation products have low volatility and condense rapidly. Nucleation events were observed at Kleiner Feldberg on 25 out of 34 measurement days between mid July and mid August in 2004. It is likely that the observed particles are mostly composed of organics from natural sources but anthropogenic emissions may play a role in these processes as well, for example, by enhancing ozone concentrations ("summer smog") which accelerates the oxidation of the terpenes.



Aerosol nucleation event ("nucleation banana") observed at Kleiner Feldberg, Taunus, during the FACE measurement campaign on 29 July 2004.

PARTICLE CHEMISTRY

Ultrafine Particles DEPARTMENT

from Steelmaking

While the individual processes in the chain of steel production are well optimised with regard to economic aspects like energy and resource fluxes or automation there is still some potential to reduce the impact of these processes on air quality. Fugitive emissions from coke making, iron ore sintering or iron reduction – some of the steps from the raw materials to the finished steel – are well known as major contributors of gases and particulate matter from this sector of industry.

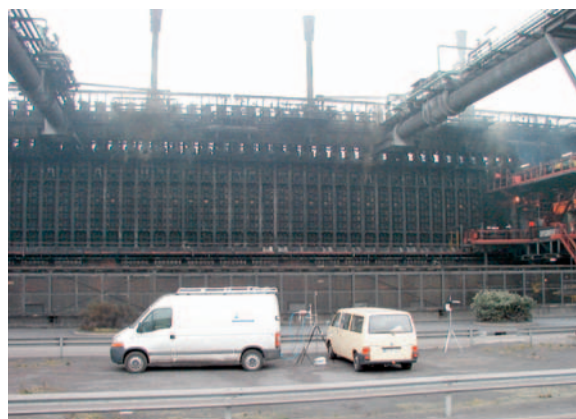
These emissions do not only contain gases relevant for the climate of the earth, but also particles that could severely impact human health. Especially the fine and ultrafine fraction of these particles, i.e. the particles with diameters $<1\ \mu\text{m}$ and $<0.1\ \mu\text{m}$ are not well studied. These small particles will consist to a significant fraction of inorganic and organic species that were emitted as vapours and condense upon cooling of the exhaust plume. Especially the polycyclic aromatic hydrocarbons (PAHs) included in these particles are known to cause adverse health effect.

Within the framework of the EU-project ULTRAFINE these particulate emissions from several steelmaking processes were investigated with a focus on ultrafine particles, i.e. particles in the size range below $0.1\ \mu\text{m}$ in diameter. The major objective of this project is to identify the processes that have the largest impact on air quality and thus on human health in affected areas. In order to measure physical and chemical particle properties with sufficient time resolution to achieve this aim, high-end aerosol

measurement technology is developed and deployed. This includes on-line measurement of particle size distributions, mass or number concentrations as well as on-line measurement of particle composition using mass spectrometry and optical methods.

Our group uses a state-of-the-art aerosol mass spectrometer to obtain size-resolved information about the chemical composition of the aerosol from steelworks processes with time resolution in the order of a minute. In a first step this instrument was characterised and data processing strategies were developed to extract the relevant information from the vast amount of measured data. Together with partners from UK, France and Germany the instrument is deployed in several steelworks facilities and the environment nearby.

In a field experiment at a coke oven battery in Dunkirk fugitive emissions from the coke-making processes were analysed. In coke ovens raw coal is converted into coke by pyrolysis – heating in the absence of oxygen. This process releases large amounts of organic and inorganic vapours that can affect human health. By nucleation or condensation onto existing particles these vapours can form or grow aerosol particles. The high time resolution of our measurements enables us to separate and identify the contribution of individual sub-processes of the coke-making to the total particulate emissions. Thus a first step in the long way towards a reduction of the steelmaking impact on ambient air quality is possible.



PARTICLE CHEMISTRY DEPARTMENT

Tropical Thunderstorms: Chasing “Hector”

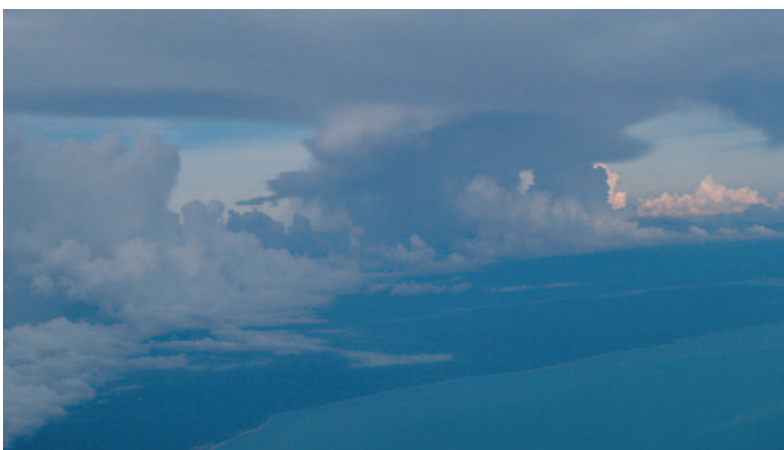
With engines roaring the M-55 “Geophysica” high altitude research aircraft is taking off climbing to 21 km on its way towards a huge thunderstorm called “Hector”. “Hector” is the isolated deep convective system shown in the photograph which forms and dissipates almost daily above the Tiwi Islands located north of Darwin, Australia. In 2005 we took part in two tropical campaigns performing experiments on atmospheric physics and chemistry of tropical thunderstorms: TROCCINOX-2 at Aracatuba in the south of Brazil and SCOUT-O3 at Darwin, Australia. Our group operates five *in-situ* instruments aboard the Russian aircraft “Geophysica” for probing aerosols and clouds. The measurements cover the large range of atmospheric aerosol particles extending from the nanometre sized condensation nuclei over cloud particles with sizes of tens to hundreds of micrometres to still larger precipitation particles and hydrometeors.

This time also the sources of stratospheric aerosol, as well as transport of water and trace gases into the stratosphere are foci of the campaigns. Within the global circulation pattern the Hadley cell is characterised by large scale updrafts in the tropical region. Inside the InnerTropical Convergence Zone (ITCZ) convective thunderstorm clouds like “Hector” form both in the northern and the southern hemispheric equatorial regions, the converging flow thus efficiently transporting air to high altitudes. Those air masses reaching the stratosphere this way are spread out there through intricate dynamical processes to mid-latitude regions, ultimately subsiding in the polar regions.

Normally during the updraft of air towards the

stratosphere water vapour freezes out forming cirrus clouds at altitudes between 16 and 18 km. By this process much of the aerosol, trace gases, and water are left behind closely below the tropopause, mostly being prevented from entering the stratosphere above. Consequently in the tropics thin ice clouds can be observed often, albeit as “sub-visual” cirrus, because these cloud layers are so tenuous that a human observer on the ground can not see them with unaided eyes. How these clouds are formed, which microphysical mechanisms maintain them, what influence they have on the chemical composition of the air in the tropopause region, and which role such ice clouds really play for freeze-drying air entering the stratosphere was among the research objectives of the “Geophysica” measurements.

Regular aircraft can not climb to the altitudes above 15 km, where these processes occur, and for this reason the single piloted, converted Russian high altitude aircraft “Geophysica” is loaded with more than 20 fully automated instruments from fifteen groups of seven EU countries, Canada, Russia, and Switzerland. Other research objectives were centred around open questions concerning the natural sources of atmospheric nitrogen oxides. One dominant source are lightnings especially in the tropics, where large numbers of thunderstorms occur every day. “Hector” – the most famous deep convective cloud – forms so regularly that the American WW II pilots used it for navigation as “Landmark Hector” when returning to Darwin from their missions and it is this reliability because of which the cloud is so well suited for atmospheric measurements.



PARTICLE CHEMISTRY DEPARTMENT

Stardust in the Laboratory

Most of the chemical elements are the products of nuclear reactions in the interior of stars. In the late stages of stellar evolution the newly formed nuclides are being dredged-up to the star's envelope and finally ejected into the interstellar medium. A significant fraction of the ejected matter condenses into nanometre- to micrometre-sized dust grains. In this way nucleosynthetic memories on the parent stars are preserved. Once ejected these stardust grains spend a long time in the interstellar medium. Finally, they eventually become part of dense interstellar gas and dust clouds, the birth places of new stars.

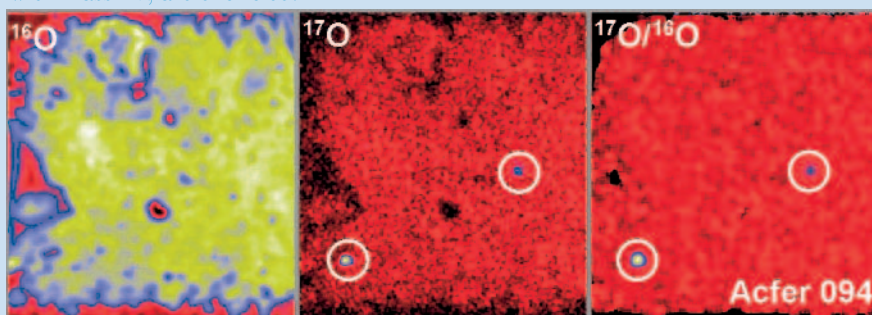
Only a small fraction of stardust grains survived the events that led to the formation of our solar system some 4.57 billion years ago. These presolar grains are characterised by large isotopic anomalies and they are found in small quantities in primitive meteorites and interplanetary dust particles (IDPs). The discovery of presolar grains has opened a new window to astrophysics as they represent a sample of stardust that can be analysed with high precision in the laboratory. Their isotopic compositions, mineralogy, and physical properties provide information on stellar nucleosynthesis and evolution, grain growth in stellar environments and on the inventory of stars that contributed matter to our solar system.

One important aspect of our studies of presolar grains was the search and isotopic characterisation of presolar silicates in Acfer 094, one of the most primitive meteorites known. For a long

time presolar silicates, the major dust component around evolved stars, could not be detected because appropriate measurement techniques were not available. Only invention of the NanoSIMS ion microprobe with its superior spatial resolution made it possible to locate the sub-micrometre-sized presolar silicate grains in thin sections of meteorites and IDPs. Our NanoSIMS studies of Acfer 094 revealed a large number of presolar silicate grains, making presolar silicates the most abundant stardust mineral in meteorites. The presolar silicates were found by oxygen isotope mapping of large areas in a thin section of Acfer 094. They exhibit O-isotopic signatures which are clearly distinct from those of the surrounding matter which is of solar system origin. From a comparison between the grain data and model predictions it can be concluded that most of the presolar silicate grains formed in the winds of red giant stars.

Comets are assumed to be at least as primitive as the most primitive meteorites and IDPs. Cometary matter may thus represent a valuable reservoir of relict stardust minerals. An important part of our future work will be the study of matter from comet Wild-2, collected and returned to Earth in January 2006 by NASA's Stardust mission. First samples have arrived in our laboratory and it is hoped that the study of this unique material will open new opportunities in the field of presolar grain research.

Oxygen isotope map of a $9 \times 9 \mu\text{m}^2$ -sized region in the Acfer 094 meteorite. Two presolar silicate grains, which have large overabundances of the oxygen isotope with mass 17, are encircled.





Melting, Structure and Viscosity of Iron at Earth's Core Conditions

The melting temperature of iron plays a key role in determining the core dynamics and understanding the thermal history of the planet. We have developed techniques to simultaneously use diamond anvils to generate the high pressures and high power infrared lasers to generate the high temperatures equivalent to the Earth's core conditions (above 1.3 Million atmospheres and above 4000 K).

The geophysically most relevant properties of iron are its structure, melting temperature, and viscosity. Iron, subjected to high pressures and high temperatures undergoes several phase transitions. The structure of solid iron at inner core conditions has been intensely debated due to the observed seismic anisotropy in the inner core. The new measurements, combining our laser-heated diamond cell and intense synchrotron radiation showed that the face-centred cubic phase was not stable above 70 GPa (about 70 000 atmospheres) and 3000 K and that the inner core is most likely made of a hexagonally close-packed phase.

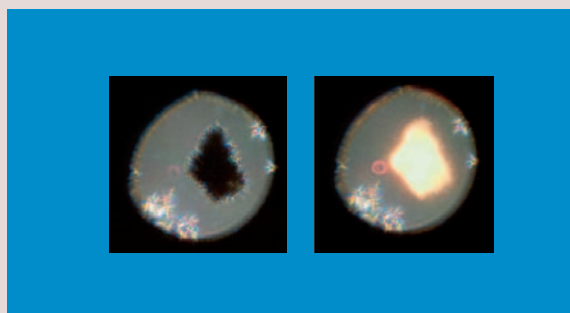
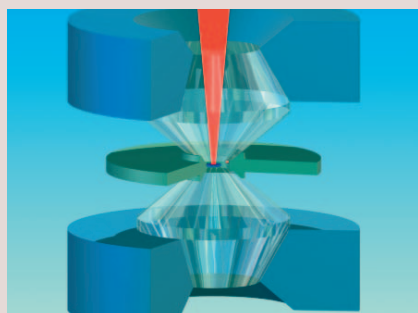
Our previous measurements of melting temperatures, which are in serious disagreement with recent theoretical *ab initio* calculations have now been confirmed using two additional independent techniques: melt detection by synchrotron X-ray diffraction and the

measurement of the latent heat of melting using time-resolved spectroscopy, an entirely new method in diamond cell application. We copied our laser-heating set up to be used at the beamline ID 27 at the European Synchrotron Radiation Facility (ESRF) in Grenoble and we are now capable of obtaining high quality X-ray patterns at thus far unreachd P-T conditions within a few seconds. Loss of long range order in iron at 90 GPa and 3000 K indicated melting.

Simultaneously we developed a new spectroscopic method that allows the study of the temperature-time function using laser pulses. At melting a significant energy loss is observed which is due to the latent heat of melting. These new measurements and a new study on the melt depression of iron caused by the light element sulphur yield rather low core temperatures of significantly below 5000 K, much lower than many other previous estimates.

The viscosity of liquid iron in the outer core is highly uncertain but theory predicts viscosities similar to that of water. We observe, however, a significant increase as a function of pressure of several orders of magnitude as evident from the vigor of motion which can be made visible in the diamond cell with a laser interference method. The outer core may thus be highly viscous.

Schematic view of a diamond anvil press. The sample in the centre is contained by a metallic gasket and an inert gas pressure medium. The sample is heated with a high power IR laser (red) and the pressure is measured using the shift of the fluorescence line of a ruby chip which is excited with a blue argon-ion laser. Also shown is a heated and unheated sample.



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MAX PLANCK INSTITUT FÜR CHEMIE

ÖFFENTLICHKEITSARBEIT
PUBLIC RELATIONS

SCHÜLERPROGRAMM
STUDENTS PROGRAM

EVENTS
EVENTS

ZENTRALE EINRICHTUNGEN
SERVICE UNITS

PERSONAL UND BUDGET
STAFF AND BUDGET

ABKÜRZUNGEN
ABBREVIATIONS

KONTAKT
CONTACT

DER WEG ZUM INSTITUT
HOW TO REACH THE INSTITUTE

ÖFFENTLICH-KEITSARBEIT

PUBLIC RELATIONS

Die primäre Aufgabe der Öffentlichkeitsarbeit ist es, die Schnittstelle zwischen den Wissenschaftlern am Institut, den Medien und dem zentralen Pressereferat der MPG zu bilden sowie die interessierten oder zu interessierenden Gruppen der Gesellschaft (z.B. Schüler, Lehrer, Studenten, Medienvertreter, Politiker, Unternehmer) über die wissenschaftlichen Arbeiten am Institut zu informieren. In den Jahren 2005 und 2006 wurden rund 20 Pressemitteilungen über herausragende Ergebnisse, über neue Techniken oder anlässlich der internationalen Expeditionen herausgegeben. Oft resultierten daraus ausführliche Berichte im Wissenschaftsmagazin „MaxPlanckForschung“, in der lokalen und überregionalen Presse sowie in Rundfunk und Fernsehen.

Das PR-Team erstellt Informationsmaterial wie z.B. Broschüren und Faltblätter über das Institut. Es bereitet die Institutsbeiträge für verschiedene Periodika und die Internetseiten der Max-Planck-Gesellschaft vor. Das Team ist zuständig für die Erstellung und Aktualisierung der allgemeinen, abteilungsübergreifenden Webseiten des Instituts. Zu den wiederkehrenden Aktivitäten gehören außerdem: Organisation und Durchführung von Gruppenführungen (Schulklassen, Studenten- und andere Gruppen), Beantwortung der Anfragen von Journalisten und Vermittlung von Gesprächspartnern sowie Kontaktpflege zu lokalen Medienvertretern und überregionalen Wissenschaftsjournalisten.

The primary merit of the public relations work is to establish an interface between scientists, media and the central press department of MPG, and to inform interested societal groups (e.g., school/university students, teachers, journalists, politicians, companies) about the scientific work at the institute. In 2005 and 2006 about 20 press releases on remarkable results, new techniques or on the occasion of international expeditions have been published. Detailed reports in the science magazine “MaxPlanckForschung”, in local and national press or broadcasting and television are often based on these releases.

The PR team produces promotional materials about the institute such as brochures and flyers. It prepares the institute's contributions to various periodicals and the website of the Max Planck Society. The team is responsible for updating the general pages of the institute's website. Other regular activities comprise, for example, organising and realising guided tours (e.g., school classes and other groups), arranging contacts between journalists and scientists, and replying to inquiries from journalists, students and other parties.

Pressekonferenz mit Bundesumweltminister Jürgen Trittin anlässlich des Starts des europäischen Klimaforschungsprojekts CARIBIC.

Press conference with Jürgen Trittin, Federal Minister for the Environment, on the occasion of the start of the European climate research project CARIBIC.



SCHÜLER-PROGRAMM

Das Max-Planck-Institut für Chemie beteiligt sich an verschiedenen Projekten für Schülerinnen und Schüler mit dem Ziel, den naturwissenschaftlichen Unterricht in den Schulen zu fördern und Schüler für naturwissenschaftlich-technische Studiengänge zu motivieren. Für einzelne Schüler bietet das Institut sowohl in den wissenschaftlichen Abteilungen als auch in der mechanischen Lehrwerkstatt Betriebspraktika an.

ESPERE und ACCENT

Seit Anfang 2003 koordiniert das Institut den Aufbau einer der größten zusammenhängenden Internet-Informationsquellen zum Klimasystem. Die achtsprachige ESPERE-Klimaenzyklopädie ist seit Mitte 2005 in ihrer deutschen Version vollständig verfügbar und wird Schulen sowie einer breiten Öffentlichkeit sowohl im Internet online und auch als Offline-Version zum kostenlosen Herunterladen angeboten. An der Gestaltung beteiligten sich Wissenschaftler aus zahlreichen Forschungsinstituten in Europa ebenso wie Didaktiker. Ein umfassender Überblick über die Zusammenhänge im Klimasystem und den menschlichen Einfluss hierauf wird auf etwa 140 Webseiten präsentiert; für die Anwendung im Schulunterricht stehen zudem zahlreiche Arbeitsblätter zur Verfügung.

Im Rahmen des ACCENT-Projekts, eines europäischen Netzwerks im Bereich der Atmosphärenforschung, erstellt das Institut das monatliche Global Change Magazin für Schulen, in dem aktuelle Berichte aus der Wissenschaft mit klassischen Inhalten der Lehrpläne in den Fächern Physik, Chemie, Biologie und Geographie verknüpft werden.

www.espere.net

www.nat-schuelerlabor.de

www.uni-mainz.de/Organisationen/ALP

STUDENTS PROGRAM

The institute participates in various projects for school students, aiming at the promotion of natural sciences at schools and the encouragement of students to take scientific-technical courses. For specific school students the institute offers courses both in the scientific departments and in training workshops.

ESPERE and ACCENT

Since the beginning of 2003 the institute has coordinated one of the biggest interrelated internet sources concerning the climate system. The complete German version of Climate Encyclopaedia ESPERE, which is released in eight languages, has been available from mid 2005 on and is offered to schools and a broad public online in the internet as well as offline as a free download version. Scientists from various research institutes across Europe and didacts contributed to its formation. About 140 websites give a comprehensive review of the coherences of the climate system and the human impact on it. In addition, numerous handouts for the use in school instruction are provided.

Within the ACCENT project, a European network concerned with atmospheric research, the institute compiles the monthly Global Change Magazine for schools. This periodical establishes a



SCHÜLER-PROGRAMM

STUDENTS PROGRAM

Ada-Lovelace-Projekt und Schülerlabor der Universität Mainz

Das Ada-Lovelace-Projekt, ein Mentorinnen-Netzwerk für Frauen in Technik und Naturwissenschaften, steht unter dem Motto „Was ich will, das kann ich“ und wendet sich insbesondere an interessierte Schülerinnen. Hier können Gruppen von Schülerinnen und Schülern Experimente selbst durchführen, wie z.B. die Messung von Methankonzentrationen mit einem Gaschromatographen oder die Dichtentrennung von Mineralen mit Schwereflüssigkeiten. Diese Versuche finden in Institutslaboratorien unter der Anleitung von jungen Wissenschaftlerinnen statt.

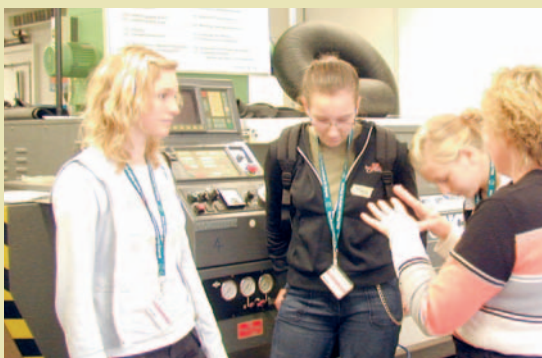
link between topical scientific reports and the classical curricula in the subjects physics, chemistry, biology, and geography.

Ada-Lovelace-Project and Student Lab of the Mainz University

The Ada-Lovelace-Projekt, a mentor-network for women in science and technology, has "What I Want, I Can Do" as its motto and is mainly directed at schoolgirls. Groups of students are given the opportunity to undertake experiments, as e.g. the measurement of methane concentrations with a gas chromatograph, or the density separation of minerals with heavy liquids. These experiments take place in the institute's laboratories, guided by young scientists.

Girls' Day 2006: Praktische Erfahrungen durch kleine Experimente und persönliche Gespräche mit Wissenschaftlerinnen fördern die Motivation, sich für einen technisch-wissenschaftlichen Beruf zu entscheiden.

Girls' Day 2006: Practical experience gathered in simple experiments and one-on-one chats with scientists encourage the decision to choose a technical-scientific career.



Schülerinnen der Martin-Luther-Schule Marburg bei der Spurengasanalyse am Gaschromatographen.

Schoolgirls perform a trace gas analysis by gas chromatography.

EVENTS

EVENTS

IdeenPark 2006

IdeasPark 2006



EVENTS

ThysenKrupp AG und das Land Niedersachsen präsentierten auf dem EXPO-Gelände in Hannover den „IdeenPark 2006“. Unter dem Motto „Technik entdecken - Zukunft gestalten“ zeigten Präsentationen von mehr als 50 Partnern aus Forschung und Wirtschaft, wie Innovationen im Zusammenspiel von Ausbildung, Forschung, Industrie und Anwendern entstehen. Das MPI für Chemie war mit dem Thema „Atmosphärenchemie und Gesundheit“ präsent. Das im Institut entworfene und gebaute Exponat „Sommersmog“ erwies sich als ein wahrer Anziehungspunkt.

Im September 2006 nahm das Institut erneut an dem von der Johannes Gutenberg-Universität organisierten "Wissenschaftsmarkt" im Mainzer Stadtzentrum teil. Spannende Präsentationen und Experimente zum Mitmachen machten die Grundlagenforschung in der Abteilung Geochemie greifbar.

EVENTS

ThysenKrupp AG and the State of Lower Saxony presented the "IdeasPark 2006" on the EXPO site in Hanover. Following the motto "Discovering Technology - Designing Future", 50 research and economy partners presented how innovation arises from the interaction of education, research, industry, and users. The MPI for chemistry contributed with the subject "Atmospheric chemistry and health". The exhibit "summer smog", designed and constructed in the institute, proved to be a main attraction.

In September 2006 the institute contributed to the "Science Market" in the city centre of Mainz, organized by Johannes Gutenberg University. Exciting presentations and experiments allowed the visitors to grasp basic research performed by the Geochemistry Department.

Mainzer Marsforscher feiern: nach zwei „irdischen“ Jahren funktionieren die beiden APXS auf dem Mars immer noch wie am ersten Tag.

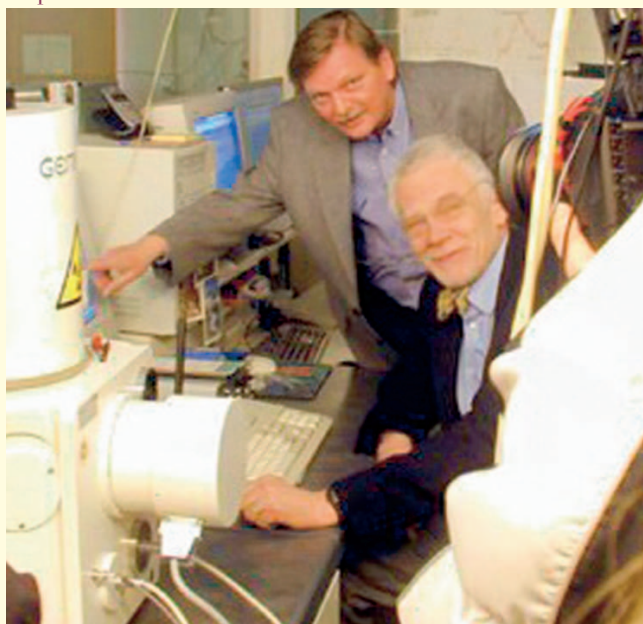
Mars researchers from Mainz celebrate: after two "terrestrial" years the two APXS on Mars still function perfectly.



© Jörg Henkel

Forschungsminister Zöllner besucht das Institut, um sich über die einzigartige Sternenstaubforschung in der Abteilung Partikelchemie zu informieren.

Minister for Science Zöllner visits the institute to catch up on the unique stardust science in the Particle Chemistry Department.



ZENTRALE EINRICHTUNGEN

SERVICE UNITS

Die Mitarbeiter der Verwaltung, der Bibliothek, der EDV-Gruppe, der Werkstätten und der Hausverwaltung bilden das infrastrukturelle Rückgrat des Instituts. Sie unterstützen die Wissenschaftler bei der Erfüllung ihrer Aufgaben und tragen wesentlich zur technischen und organisatorischen Weiterentwicklung des Instituts bei.

The staffs of the administration, the library, the computer group, the workshops and the in-house maintenance staff are the infrastructural backbone of the institute. They continuously support the researchers and contribute to the technical and organisational development of the institute.

BIBLIOTHEK

Die Bibliothek stellt die benötigte Literatur und sonstige wissenschaftliche Informationen in jedweder Form bereit. Während klassische Printmedien (Bücher, Zeitschriften) nach wie vor eine wertvolle Informationsquelle darstellen, wächst die Bedeutung elektronischer Medien, insbesondere Online-Zeitschriften, in den letzten Jahren ständig an. Literatur-Datenbanken (Georef, Web of Science etc.) wie auch Dokumentlieferdienste stellen weitere wichtige Bestandteile des Informationsangebotes dar.

Der Bibliotheksbestand umfasst wissenschaftliche Literatur aus einem weiten Bereich an Fachgebieten: Physik, Chemie, Biologie, Mathematik, Meteorologie, Geowissenschaften, Astronomie, Ökologie und Kernphysik. Im Einzelnen sind rund 28.000 Bände (Zeitschriftenbände, Monographien, Forschungsberichte, Dissertationen) sowie zahlreiche Mikrofiche-Ausgaben, CD-ROMs und Videos vorhanden.

EDV-GRUPPE

Die Bereitstellung einer modernen, problemorientierten EDV-Infrastruktur gehört zu den Hauptaufgaben der EDV-Gruppe. Dazu gehört die Serverlandschaft mit zentralen Diensten (E-Mail, Internetzugang, Datenspeicherung, PC-Services und Druckdienste) genauso wie die Sicherstellung des lokalen Netzbetriebs (LAN). Hier sind sowohl Betriebszuverlässigkeit als auch Datensicherheit gefragt. Insbesondere wird der Schutz von Ressourcen und sensiblen Daten immer komplexer und bekommt einen immer höher werdenden Stellenwert. Zu den Aufgaben gehört deshalb auch die Sensibilisierung der Nutzer gegenüber den Herausforderungen, die mit der modernen Kommunikation verbunden sind.

Auf Grund der Heterogenität der eingesetzten Endgeräte (Windows, Mac OS, Unix True64, Linux) wächst der Bedarf an Optimierung. Außerdem werden Verbindungen mit einer Reihe von

LIBRARY

The Library provides the scientists with media and scientific information in many forms. While the collections of printed material (books, journals) remain a valuable source of information, the importance of electronic media (especially online journals) has been steadily increasing in recent years. Literature databases (Georef, Web of Science etc.) represent another important source of information, as do various document delivery services.

The library collections cover various subject areas (physics, chemistry, biology, mathematics, meteorology, geosciences, astronomy, ecology, nuclear physics) and contain approximately 28.000 volumes (periodicals, monographs, reports, theses), as well as various microforms, CDs and video tapes.

ELECTRONIC DATA PROCESSING (EDP) GROUP

The provision of a modern and problem-oriented EDP-infrastructure is the main task of the EDP-group. This includes the server area with central services (e-mail, internet access, data storage, PC services, print services) as well as securing of the local area network (LAN). In this context operational reliability and data security are of special importance. Particularly the protection of resources and sensitive data becomes more and more complex and gains significance. These demands therefore also include the sensitisation of the users to the challenges associated with modern communication.

The heterogeneous structure of the terminals being used (Windows, Mac OS, Unix True64, Linux) requires increased optimisation. Furthermore, connections with supercomputers (massive parallel and vector machines) are maintained. Due to the visits of the scientists at other institutions, conferences or field measurements, the use of mobile terminals becomes increasingly significant.

ZENTRALE EINRICHTUNGEN SERVICE UNITS

Großrechnern (Massiv-Parallel- und Vektorrechner) bereitgestellt. Durch die häufigen Aufenthalte der Wissenschaftler an anderen Institutionen, bei Tagungen oder Messkampagnen nehmen Problemstellungen im Zusammenhang mit der Nutzung mobiler Endgeräte einen immer größeren Raum ein.

ELEKTRONIKGRUPPE

Der Schwerpunkt der Arbeitsgruppe ist die Instandhaltung des umfangreichen elektronischen Geräteparks sowie zunehmend die Entwicklung von Hard- und Software zur Durchführung oder Unterstützung von wissenschaftlichen Experimenten. Die kommerziell erhältlichen Geräte sind nur in Ausnahmefällen für die speziellen Anwendungen z.B. bei Atmosphärenmessungen geeignet. Vielfach müssen zusätzliche Prozessregler für Temperaturen, Drücke oder Flüsse implementiert werden, um die Prozessparameter der Geräte trotz Änderung der Umgebungsparameter konstant zu halten.

Da es sich bei solchen Systemen meist um Neuentwicklungen handelt, die im Verlauf ihrer Entstehung vielen Änderungen unterworfen werden müssen, nahm in den letzten Jahren die Nachfrage nach modularen, hochgradig flexiblen und skalierbaren Prozesssteuerungen zur Regelung, Datenerfassung, Archivierung und Visualisierung stark zu. Nach Bedarf müssen diese Prozesssteuerungen auch ohne den Operator den sicheren Ablauf von Prozessen steuern und

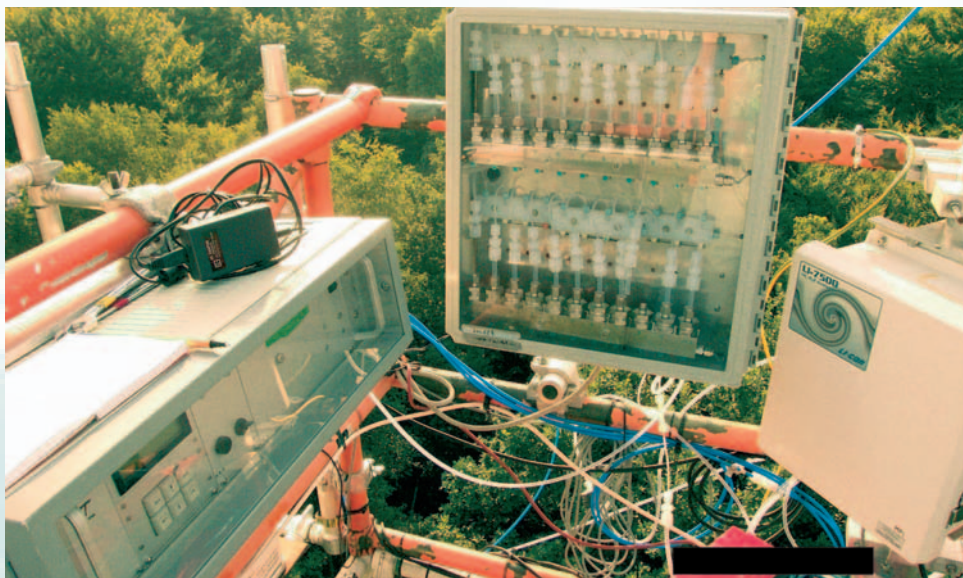
ELECTRONICS GROUP

The main task is the maintenance of various instruments. In addition, the group increasingly deals with hard- and software development needed to support the realisation of scientific experiments. Commercially available equipment rarely meets the special demands of scientific work, e.g., of field measurements. To stabilise the instruments' process parameters, despite of changing environmental conditions, additional process controls for temperature, pressure or flux have to be implemented.

Since these systems are often newly developed and modified, there has been an increasing demand for highly flexible and scalable process control hard- and software. Although primarily needed for control, data management, archiving and visualisation, the equipment is also used in a automated process control, i.e. without the operator. The realisation of such applications is based on a modular system consisting of various processors, input/output modules and software modules.

WORKSHOPS

Many of the measurement devices needed for the institute's research are not commercially available. Therefore, they must be produced in the institute, requiring well-equipped workshops. In the workshop for fine mechanics, new instruments are designed and built in cooperation with scientists. These instruments have to comply with stringent



ZENTRALE EINRICHTUNGEN SERVICE UNITS

überwachen können. Solche Anwendungen werden mit Hilfe eines modularen Baukastensystems – bestehend aus unterschiedlichen Prozessoren, Ein-/Ausgabekomponenten und Softwaremodulen – realisiert.

WERKSTÄTTEN

Viele Messapparaturen, die für die Forschungsvorhaben des Instituts benötigt werden, sind nicht auf dem Markt erhältlich. Sie müssen also selbst gebaut werden, dazu sind gut ausgerüstete Werkstätten notwendig. So besitzt das Institut eine feinmechanische Werkstatt, in der in Zusammenarbeit mit den Wissenschaftlern Messinstrumente entstehen, die auch spezielle Anforderungen, wie sie beispielsweise durch die Verwendung in Satelliten, Flugzeugen oder Schiffen auftreten, erfüllen. Ein breites Tätigkeitsspektrum, vom Schweißen spezieller Werkstoffe, Schneiden großer Eisenmeteorite, Verspannen aller gängigen Metalle bis zur Galvanik, wird von den Mitarbeitern dieser Werkstatt gefordert.

Die zum Teil sehr komplizierten Glasapparaturen werden in der glastechnischen Werkstatt gefertigt. Graphische und fotografische Arbeiten für die wissenschaftliche Dokumentation werden im Zeichenbüro durchgeführt.

Das Institut beteiligt sich seit 1949 auch an der Lehrlingsausbildung. Die Ausbildung zum Maschinenbaumechaniker erfolgt heute in der separaten Mechaniklehrwerkstatt. Im Rahmen der Ausbildung werden Übungswerkstücke angefertigt und institutsinterne Auftragsarbeiten ausgeführt. Die Auszubildenden erhalten weiterhin Fachausbildungen in CNC-Technik, Pneumatik/Hydraulik und Schweißtechnik, zum Teil in überbetrieblichen Lehrgängen.

Kommunikationselektroniker, die in der Elektronikgruppe ausgebildet werden, erhalten in der mechanischen Lehrwerkstatt die metalltechnische Grundausbildung. Des Weiteren werden in der Lehrwerkstatt Betriebspraktika für Schüler und Grundpraktika für verschiedene Studiengänge durchgeführt.

requirements, such as usage on board of satellites, aeroplanes or ships. The employees of this workshop perform a wide range of operations, such as welding specific materials, cutting big iron meteorites or bracing metals and electroplating.

Complex instruments involving glass are produced in the glass-technical workshop. Graphic and photo-optical work for scientific documentation is carried out in the drawing office.

The institute has been training apprentices since 1949. The training for mechanics is currently done in a separate workshop. The apprentices not only craft practice pieces, they also carry machining tasks for the scientific departments. In addition, the apprentices are specially trained in CNC-technique, pneumatics/hydraulic systems and welding technology, partly in interplant courses.

IT-technicians, who are qualified in the electronics group, are provided with basic education in metal-technique as well. In addition, the training workshop offers industrial courses for schools and various types of education.

Nils Stöhr, der am Institut den Beruf des Maschinenbaumechanikers erlernte, ging aus den Leistungswettbewerben der Handwerkerjugend 2005 als Kammer-, Landes- und Bundessieger hervor.

Nils Stöhr, who served his apprenticeship at the institute's mechanics-training workshop, has been especially successful in the 2005 competitions of the Handwerkerjugend, winning the contests on regional, state, as well as federal level.



PERSONAL UND BUDGET

STAFF AND BUDGET

Anfang 2006 waren insgesamt 225 Mitarbeiter am Institut tätig, darunter 50 Wissenschaftler, 61 Nachwuchswissenschaftler und 13 Auszubildende; hinzu kamen 28 Drittmittelbeschäftigte.

Early 2006 a total of 225 persons were employed at the institute, among them 50 scientists, 61 junior scientists and 13 apprentices; furthermore 28 scientists with third-party funding were hosted.

ABKÜRZUNGEN

ABBREVIATIONS

APXS	Alpha-Particle-X-Ray-Spectrometers
CARIBIC	Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container
CCN	Cloud Condensation Nuclei
CLACE	Cloud and Aerosol Characterisation Experiment
COACH	Cooperation on Oceanic, Atmospheric and Climate Change studies
ECHAM5	European Centre Model Hamburg, version 5
ECHO (AFO 2000)	Emission und Chemische Umwandlung biogener flüchtiger Organischer Verbindungen (AtmosphärenForschung 2000)
ENVISAT	ENVironmental SATellite
FACE	Feldberg Aerosol Characterisation Experiments
GABRIEL	Guyanas Atmosphere-Biosphere exchange and Radicals Intensive Experiment with the Learjet
GEOROC	GEOChemistry of Rocks of the Oceans and Continents
GFMC	Global Fire Monitoring Centre
GRAEGOR	Gradient Analyser for Aerosols and Gases
HALO	High Altitude – Long Range Research Aircraft
ICE-CVI	ICE Counterflow-Virtual Impactor
IDPs	Interplanetary Dust Particles
ILEAPS	Integrated Land Ecosystem Atmospheric Processes Study
IN	Ice Nuclei
ITCZ	InnerTropical Convergence Zone
LA-ICP-MS	Laser Ablation Inductively Coupled Plasma Mass Spectrometry
LBA	Large Scale Biosphere Atmosphere Experiment in Amazon
MESSy	Modular Earth Submodel System
METEOSAT	METEORological SATellite
MINOS	Mediterranean INTensive Oxidant Study
NAVDAT	North American Volcanic and Intrusive Rock Database
PAHs	Polycyclic Aromatic Hydrocarbons
PetDB	Petrological DataBase of the Ocean Floor
SCOUT-O3	Stratosphere–Climate Links with Emphasis on the Upper Troposphere and Lower Stratosphere
SOA	Secondary Organic Aerosol
SODAR-RASS	SONic Detection And Ranging - Radio Acoustic Sound System
TROCCINOX-2	Tropical Convection, Cirrus and Nitrogen Oxides Experiment
UTLS	Upper Troposphere and Lower Stratosphere
VOCs	Volatile Organic Compounds

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DER WEG ZUM INSTITUT HOW TO REACH THE INSTITUTE

PER AUTO

Von Süden über die Autobahn A 60, Ausfahrt Mainz-Lerchenberg. Von dort rechts in die Koblenzer Straße, auf der linken Spur bleiben. Direkt vor der 5. Ampel nach rechts zur Haupteinfahrt der Universität.

Von Norden über die Autobahn A 60, Ausfahrt Mainz-Finthen. Folgen Sie der Hinweisbeschilderung „Innenstadt“. Nach dem „Europaplatz“ nach rechts Richtung „Bretzenheim“ und „Universität“. An den beiden nächsten Ampeln jeweils links abbiegen zur Haupteinfahrt der Universität.

PER FLUGZEUG

Von Frankfurt Flughafen mit IC/ICE (Fernbahnhof) oder mit der S-Bahn (S 8) Richtung Wiesbaden bis Mainz Hauptbahnhof.

PER BAHN

Es verkehren pro Tag mehrere IC-, EC- und ICE-Züge über Mainz Hauptbahnhof.

PER BUS

Vor dem Mainzer Hauptbahnhof, an der Bushaltestelle „G“ Nr. 54, 55, 58 oder 68 bis Haltestelle „Friedrich-von-Pfeiffer-Weg“, dann über die Fußgängerbrücke auf den Campus, geradeaus den Pfeifferweg und Strassmannweg entlang bis Johann-J. Becher-Weg, dann links zum Institut.

BY CAR

From the south via the *Autobahn* A60. Take the exit Mainz-Lerchenberg, turn right onto *Koblenzer Straße* and keep the left lane. Before the fifth traffic light, turn right in the direction *Universität* to arrive at the main entrance of the university.

From the north via the *Autobahn* A60. Take the exit Mainz-Finthen and follow the sign *Innenstadt*. After passing the roundabout *Europaplatz* take the next left in the direction of *Bretzenheim* and *Universität*. Turn left at the traffic light and again at the next traffic light to arrive at the main entrance of the university.

BY PLANE

From Frankfurt Airport, take the S 8 train (*S-Bahn*) heading towards Wiesbaden until Mainz Central Station (*Mainz Hauptbahnhof*). From the station take a taxi or a bus to the institute.

BY TRAIN

Mainz Hauptbahnhof is serviced daily by many Intercity (IC), Eurocity (EC) and Intercity Express (ICE) trains.

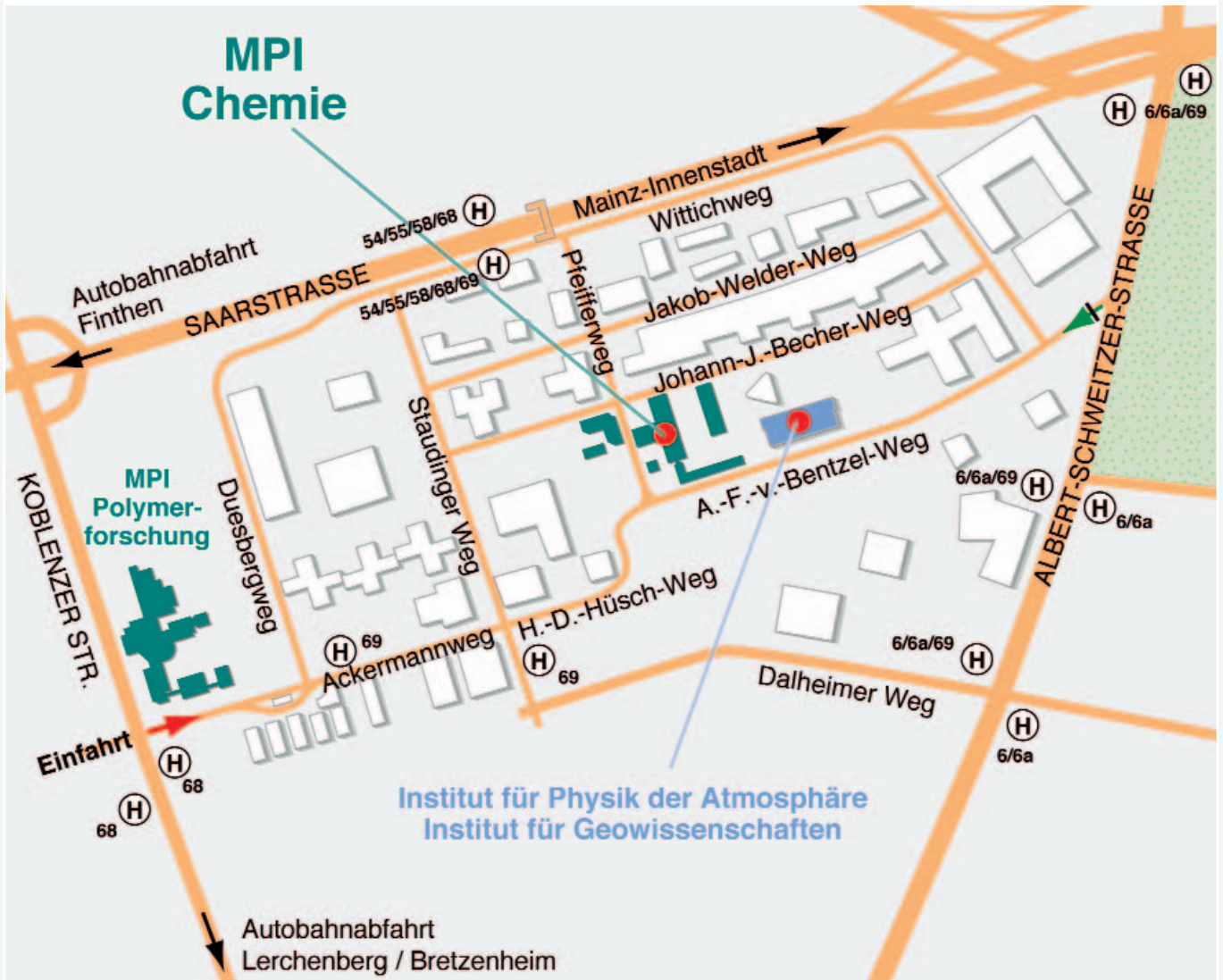
BY BUS

Exit the Mainz Hauptbahnhof through the main hall and go to the right. At bus stop "G", take bus line 54, 55, 58, or 68 to the third stop *Friedrich-von-Pfeiffer-Weg*. Cross the pedestrian bridge and follow the *Friedrich-von-Pfeiffer-Weg* and the *Strassmannweg* to the *Joh.-J.-Becher-Weg*. Turn left and you will see the main building of the institute on your right.



Das Institut liegt auf dem Gelände der Johannes Gutenberg-Universität.

The institute is located on the campus of the Johannes Gutenberg University in Mainz.



IMPRESSUM

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FOTOS

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MAX-PLANCK-INSTITUT FÜR CHEMIE



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