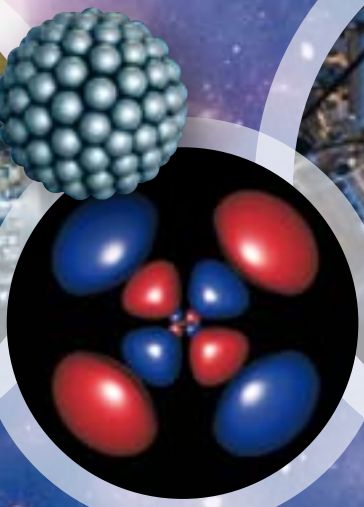
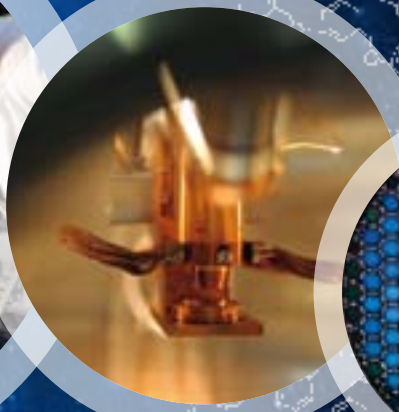
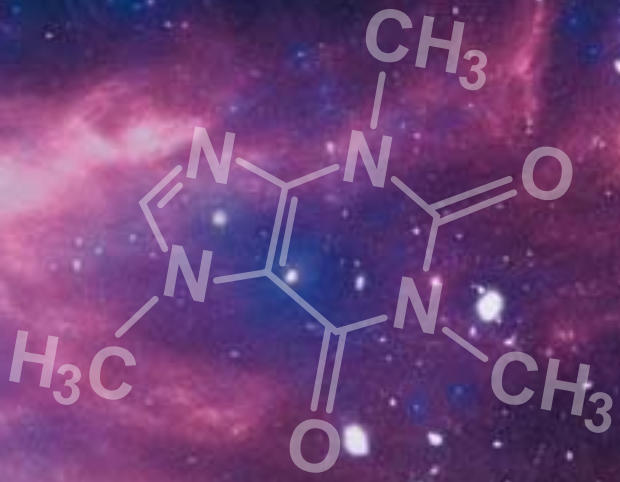
Department
Chemie und Pharmazie




DEPARTMENT OF CHEMISTRY AND PHARMACY

PROFILE 2010



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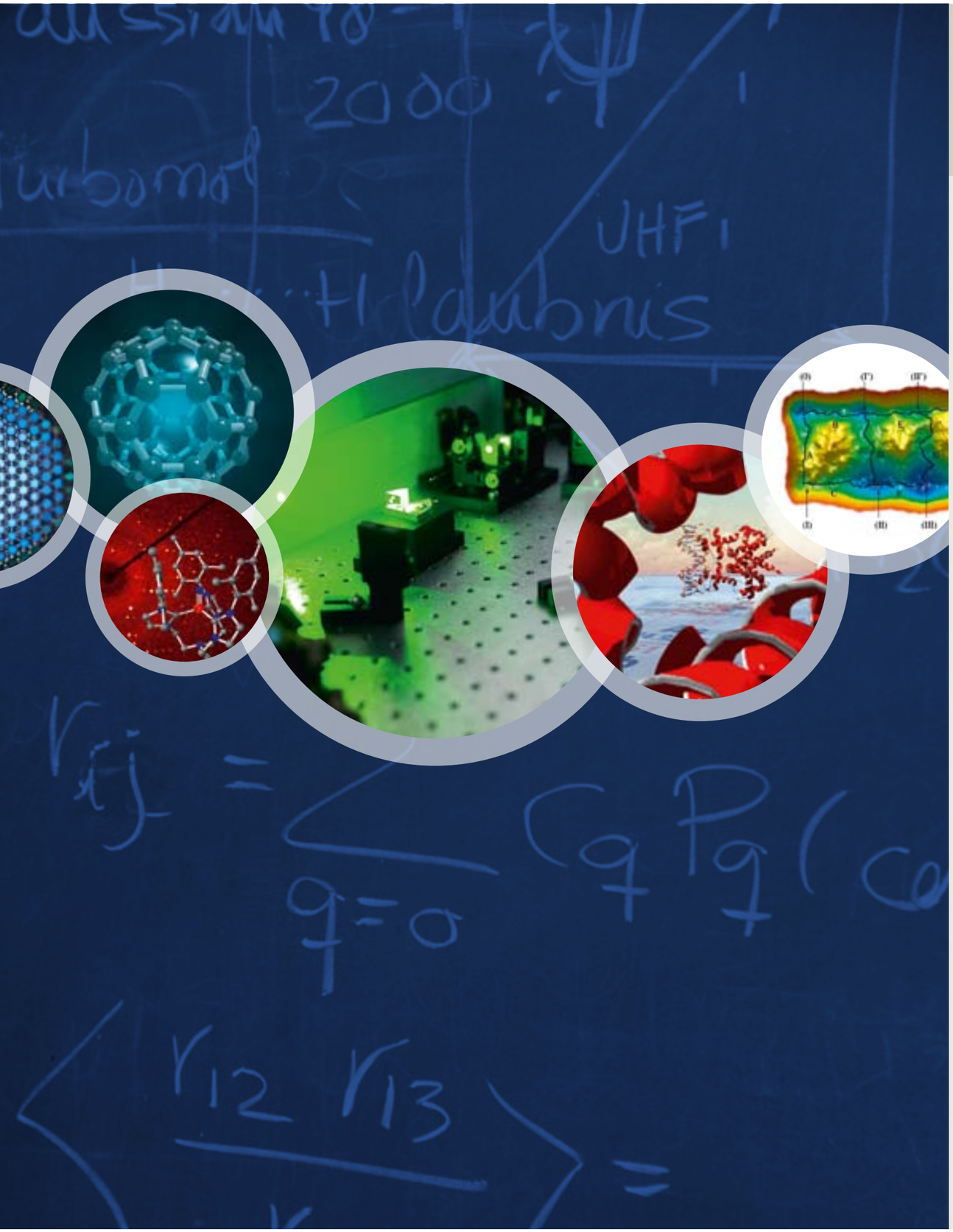


Department
Chemie und Pharmazie

DEPARTMENT OF CHEMISTRY AND PHARMACY – MISSION AND VISION

Chemistry plays an integral role in today's scientific endeavors. It is situated at the intellectual heart of many scientific disciplines. As science has transformed into an increasingly interdisciplinary test bed, we are strongly committed to excellence in education and research. To this end, we are dedicated to the fundamental chemical sciences as well as to exploring fundamental scientific problems related to the chemical nature of matter.

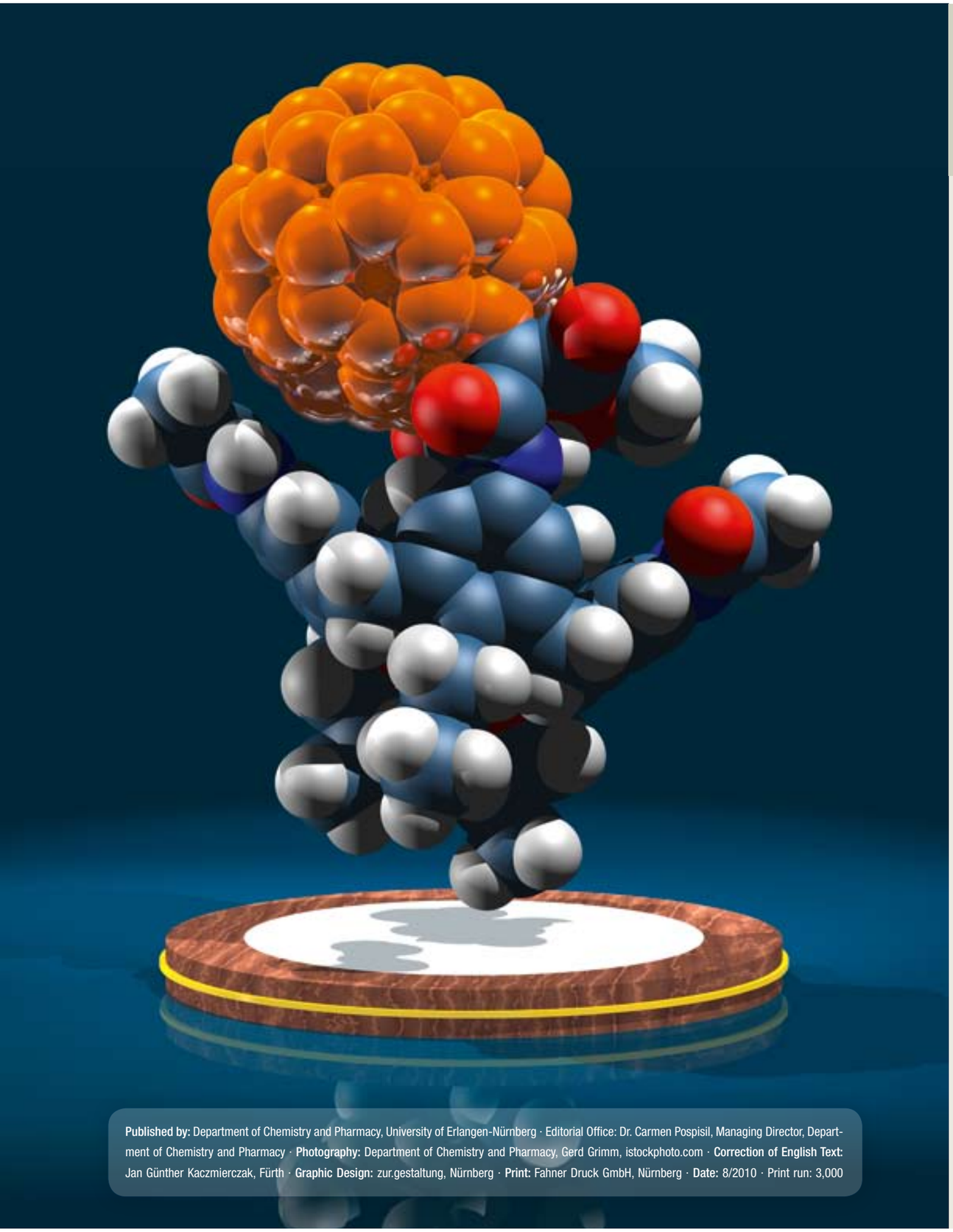
The Department of Chemistry and Pharmacy has a long standing tradition of excellence – because of our vast resources, cutting-edge facilities, and outstanding faculty – and is ranked among the best in the country. This is documented by the quality of its programs, the caliber of its faculty, and the excellence of its students.

The faculty and staff of the Department of Chemistry and Pharmacy provide an environment, where students at all levels explore, discover, and learn chemistry through coursework and research. In fact, undergraduate, graduate, and post-graduate students / research associates join the Department of Chemistry and Pharmacy from across the country and a number of foreign countries to study in specific research programs directed by the University of Erlangen-Nürnberg's chemistry professors.

The Department employs 26 professors pursuing research in all areas of chemistry and pharmacy. The goals of exciting and well-funded research programs include molecular materials and catalysis as well as bioactive molecules. Modern research cuts across traditional disciplinary boundaries, and our faculty plays key roles at the forefront of multiple interdepartmental research units at the University of Erlangen-Nürnberg including the Cluster of Excellence, several Collaborative Research Centers, etc.

Our motto:
"A dedication to promote excellence and innovation in chemistry through education and research."

Dirk M. Guldi
Head of the Department of Chemistry and Pharmacy



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Department
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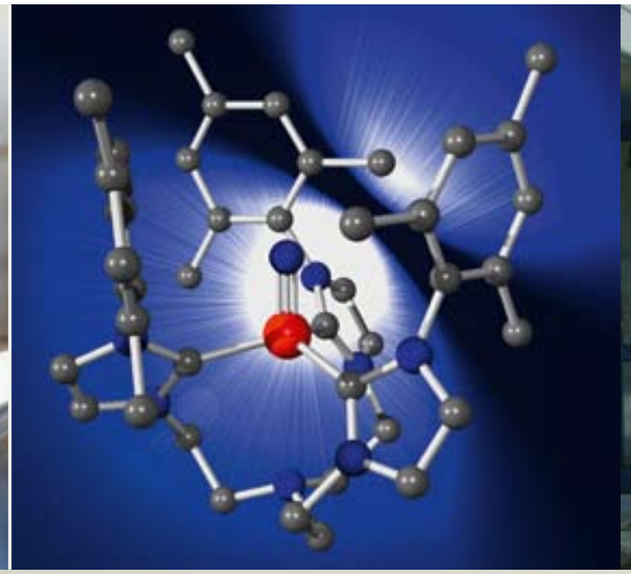


DEPARTMENT OF CHEMISTRY AND PHARMACY

PROFILE

The Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) was founded in 1743. Its mission *"Advance through Networks"* reflects FAU's comprehensive networks of interdisciplinary collaborations at the highest level that are based on excellence in a wide range of research areas. On average 590 professors, 296 chairs, and 1,750 teaching staff educate 27,300 students (2009). Among the five FAU Schools the School of Sciences features five Departments – *Biology, Mathematics, Geography and Geosciences, Physics as well as Chemistry and Pharmacy.*

The *Department of Chemistry and Pharmacy* is home to the two separate research and teaching units Chemistry and Pharmacy. Both are cooperating closely with other Schools within the University, especially with the Schools of Engineering and Medicine as well as with other departments within the School of Sciences. The cooperations range from joint research projects and interdisciplinary research centers to extensive exchange of undergraduate and graduate students.

The organization chart summarizes the structure of the *Department of Chemistry* – with chairs in Inorganic Chemistry, Organic Chemistry, Physical, and Theoretical Chemistry – and Pharmacy with chairs in Medicinal Chemistry, Pharmaceutics and Food Chemistry. To this end, 26 University Professors hold appointments in the diverse areas of Chemistry / Molecular Science and Pharmacy / Food Chemistry. Additional support comes from 24 permanent and 55 non-permanent scientific staff members. External research funds that total up to an average of approximately 6 Million Euro per year finance more than 75 additional scientists. Annually, the members of the Department of Chemistry and Pharmacy publish more than 200 peer reviewed articles in high impact scientific journals.

MAJOR RESEARCH ACTIVITIES

Neighbouring disciplines in the Schools of Sciences, Engineering, and Medicine provide a superb infrastructure and incentives for fostering interdisciplinary research of the *Department of Chemistry and Pharmacy.* Research activities within the *Department of Chemistry and Pharmacy* cover a wide spectrum that ranges from basic to applied research in the areas of chemistry, biology, pharmacy, and pharmaceutical science. The strongly interwoven and multiple interaction nature of these research activities are the inception to a myriad of interdisciplinary collaborative research projects within the university (Collaborative Research Centres (SFB), Research Training Groups (GRK)) and with other nationally and internationally leading institutions (DFG Priority Programs, EU, BMBF, Volkswagenstiftung, DAAD, Humboldt-Foundation, Bayerische Forschungsförderung, etc.). As a matter of fact, the *Department of Chemistry and Pharmacy* creates the molecular bridge between the School of Medicine, on one hand, and the Schools of Engineering and Sciences, on the other hand.

The compelling research at the *Department of Chemistry and Pharmacy* has received top rankings in national and international surveys. For example, the recent survey coordinated and conducted by the German Science Council (e.g. www.forschungsrating.de) rates the Department as "world class". The latter is based on a recommendation prepared by international panel of 15 chemists and underscores that strength of the Chemistry in Erlangen builds on the performance in research quality, the impact, and the effectiveness of research. All of these criteria were rated five out of five stars. Most notable is among other rankings, the number one position in DFG funding (2009). Top marks for excellent research have also been given to the Collaborative Research Centre 583 "Redox-Active Metal Complexes: Control of Reactivity via Molecular Architecture", with its core of principal investigators from the Department of Chemistry and Pharmacy. The five principal investigators from the *Department of Chemistry and Pharmacy* form one of the strongest contributions to the Cluster of Excellence "Engineering of Advanced Materials". In short, research in Chemistry and Pharmacy in Erlangen is excellent. Nevertheless, another milestone toward further securing and extending the leading role is the opening of the new "Chemikum", in 2013.

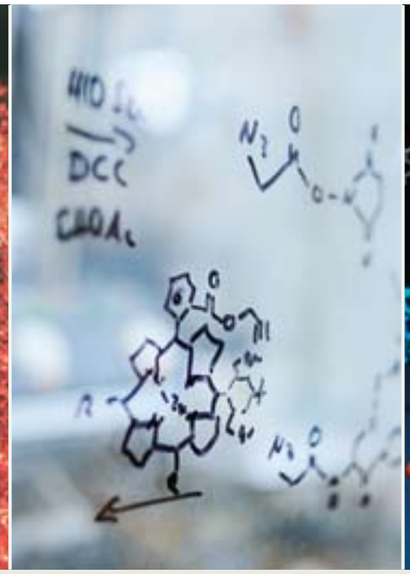
Current research objectives of the *Department of Chemistry and Pharmacy* concentrate on two major areas:

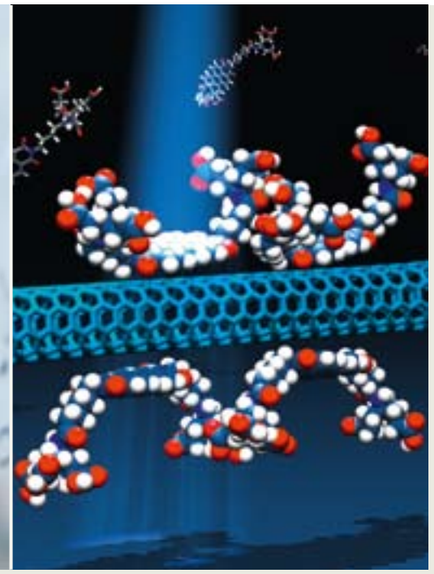
MOLECULAR MATERIALS AND CATALYSIS – METAL COMPLEXES, ELECTRON TRANSFER, NANOSTRUCTURES, AND MODELING

The synthesis and characterization of molecular materials are of core interest to the research activities in the various research groups of *Chemistry.* One important class of materials is redox-active metal complexes (SFB 583), which are used, for example, to catalyze chemical reactions. Also, carbon-rich conjugated π-systems, which exhibit unprecedented materials properties, such as mechanical strength, molecular magnetism and electrical conductivity, are of interest. Additional incentives in the studies of metal complexes and alternative molecular architectures are their supramolecular assembly and integration into hierarchically ordered nanostructures (EAM). Many of these tailored materials undergo photoinduced charge separation processes between redox-active subunits. Consequently, new systems are developed, which will help to solve fundamental challenges of the future, such as the shortage of energy and other resources. A specific strength of the chemical research in Erlangen is the computer assisted determination and modeling of molecular architectures.

BIOACTIVE MOLECULES – NEUROTROPIC AGENTS, BIOLOGICAL SYNTHETIC PEPTIDES AND PROTEIN CONJUGATES

Within the context of the subject Bioactive Molecules, novel neurotropic agents are designed, synthesized and examined for their activity towards signaling proteins. As target proteins, G-protein coupled neuroreceptors, Tet-repressors (SFB 473) as well as prion proteins are addressed. Bioactive food components are studied with a focus on non-enzymatic posttranslational protein modifications and processed food on the one hand, and flavor compounds on the other hand. For profiling of bioactive food components, serveral targeted and non-targeted bionalytical methods are applied. Novel synthetic immunogens are designed and generated based on complex peptides that mimic the binding sites of viral proteins for their cellular receptors (SFB 796, GRK 1071). For the understanding of effects of large-scale processes during the preparation of therapeutic proteins on protein folding and aggre-





gation, stabilization, particle formation, and drying rate of biotechnologically obtained proteins are explored.

RESEARCH NETWORKS

The research activities of the *Department of Chemistry and Pharmacy* are highly interdisciplinary involving not only paramount contributions from chemists but also the close interactions with physicists, material scientists, and engineers as well as medicinal chemists, biologists, and physicians. As a consequence, the *Department of Chemistry and Pharmacy* plays a leading role in cooperative research projects such as

- Cluster of Excellence Engineering of Advanced Materials (EAM),
- Computer-Chemistry-Center (CCC),
- Emil Fischer Center (EFC),
- Erlangen Catalysis Resource Center (ECRC),
- Interdisciplinary Center for Interface-controlled Processes (ICICP),
- Interdisciplinary Center for Molecular Materials (ICMM),
- Institute of Advanced Materials and Processes (ZMP) and the Graduate Schools,
- Graduate School Advanced Materials and Processes,
- Graduate School Emil Fischer,
- Graduate School Molecular Science.

Based on the unique combination of the top-ranked Schools of Sciences and Engineering at the University of Erlangen-Nürnberg, a unique environment in terms of cutting-edge research is provided by the newly established *Cluster of Excellence "Engineering of Advanced Materials"* (www.eam.uni-erlangen.de). Bridging the gap between fundamental research and real-world applications of modern high-performance materials in key scientific and engineering areas the scientific concept of the Cluster of Excellence focuses on the science and engineering of hierarchical materials organized from the molecular to the macroscopic levels. The close collaboration of chemists, physicists, materials scientists, and engineers in the field of advanced materials was the key for the success in the Excellence Initiative by the German Federal and State Governments, where the University was awarded with the Cluster of Excellence: Engineering of Advanced Materials (EAM), which received a budged of more than 60 million Euro.

The *Department of Chemistry and Pharmacy* is the founding institution of SFB 583 "Redox-active Metal Complexes", and its members participate in SFB 796 "Reprogramming of host cells by microbial effectors", and in the Research Training Groups (postgraduate programmes) GRK 1161 "Disperse Systems for Electronic Applications" and 1071 "Viruses of the Immune System". Technology transfer takes place within the framework of frequent research projects and industrial cooperations as well as jointly funded projects (BMBF, EU, DFG).

INTERNATIONALIZATION OF RESEARCH

Internationality is a key character of the *Department of Chemistry and Pharmacy* in Erlangen. A steadily increasing number of foreign scholars and exchange programs – funded through DAAD/RISE, SCS-IREU/DAAD, and ERASMUS – are a clear documentation for the internationalization for undergraduate and graduate studies. The latter complemented by international doctoral and post-doctoral students at the highest international level – funded through DAAD, Alexander von Humboldt Foundation, and EU programs. Cooperation with, for example, Osaka University in Japan and/or the University of Wollongong in Australia are initiated by excellence in research and teaching and are often built up by committed members of the *Department of Chemistry and Pharmacy.* They include frequent exchanges of students and researchers. Since 2004 the *Department of Chemistry and Pharmacy* has appointed four professors from USA, UK, and Canada and five out of the eleven chairs have an international background.

DEPARTMENT OF CHEMISTRY AND PHARMACY

INORGANIC CHEMISTRY	ORGANIC CHEMISTRY	PHYSICAL/THEORETICAL CHEMISTRY	PHARMACY AND FOOD CHEMISTRY
Inorganic and Analytical Chemistry **Prof. Dr. R. van Eldik** Prof. Dr. N. Burzlaff	**Organic Chemistry I** **Prof. Dr. R. Tykwinski** Prof. Dr. J. Schatz Prof. Dr. S. Tsogoeva	**Physical Chemistry I** **Prof. Dr. D. M. Guldi** Prof. Dr. C. Kryschi Prof. Dr. T. Drewello	**Medicinal Chemistry** **Prof. Dr. P. Gmeiner** Prof. Dr. J. Eichler Prof. Dr. M. Heinrich
Inorganic and General Chemistry **Prof. Dr. K. Meyer** Prof. Dr. S. Rau Prof. Dr. U. Zenneck	**Organic Chemistry II** **Prof. Dr. A. Hirsch** Prof. Dr. H. Gröger Prof. Dr. W. Bauer PD Dr. N. Jux	**Physical Chemistry II** **Prof. Dr. H.-P. Steinrück** Prof. Dr. R. Fink Prof. Dr. J. Libuda PD Dr. J. M. Gottfried PD Dr. H. Marbach	**Food Chemistry** **Prof. Dr. M. Pischetsrieder** PD Dr. A. Büttner
Bioinorganic Chemistry **Prof. Dr. I. Ivanović-Burmazović**		**Theoretical Chemistry** **Prof. Dr. A. Görling** Prof. Dr. D. Zahn PD Dr. M. Belén Ruiz PD Dr. W. Hieringer	**Pharmaceutics** **Prof. Dr. G. Lee**

COMPUTER CHEMISTRY CENTER (CCC)
Techn. Director: Prof. Dr. T. Clark

INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS (ICMM)
Prof. Dr. F. Gröhn Prof. Dr. B. Meyer

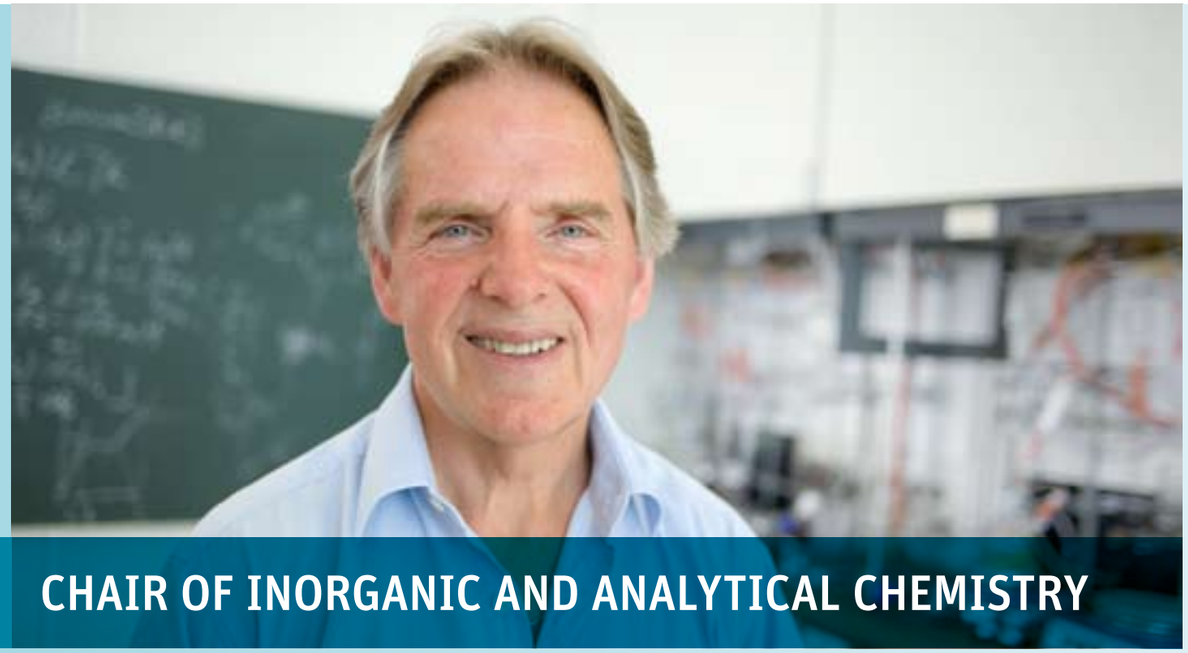
DIDACTICS OF CHEMISTRY
Prof. Dr. A. Kometz

INTERDISCIPLINARY CENTERS
- Emil Fischer Center (EFC)
- Erlangen Catalysis Resource Center (ECRC)
- Institute of Advanced Materials and Processes (ZMP)
- Interdisciplinary Center for Interface-Controlled Processes (ICICP)
- Cluster of Excellence: Engineering of Advanced Materials (EAM)

DEGREE PROGRAMS

CHEMISTRY	MOLECULAR SCIENCE NANOSCIENCE/LIFE SCIENCE	CHEMISTRY TEACHING DEGREE	PHARMACY	FOOD CHEMISTRY
(B.Sc. / M.Sc.)	(B.Sc. / M.Sc.)	(State Examination)	(State Examination)	(State Examination)

GRADUATE SCHOOLS
- Emil Fischer Graduate School
- Graduate School Advanced Materials and Processes
- Graduate School Molecular Science



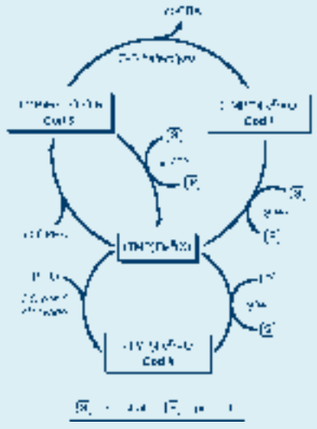
CHAIR OF INORGANIC AND ANALYTICAL CHEMISTRY

PROF. DR. DR. h. c. mult. RUDI VAN ELDIK

vaneldik@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/vaneldik

CURRICULUM VITAE

2008 – 2011	Visiting Professor, Sun Yat-Sen University, Guangzhou, China
2003	Wilsmore Visiting Professor, University of Melbourne, Australia
1999 – 2000	Dozor Visiting Professor, Ben Gurion University, Beer Sheva, Israel
1993 – 1998	Visiting Professor, University of Utah, Salt Lake City, USA
1994 – 2010	University Full Professor, Chair of Inorganic and Analytical Chemistry at the University of Erlangen-Nürnberg, Germany
1987 – 1994	Professor of Inorganic Chemistry, University of Witten/Herdecke, Germany
1982	Habilitation in Physical Chemistry from the J. W. Goethe University of Frankfurt, Germany
1971	DSc from the Potchefstroom University, South Africa



OBJECTIVES

To contribute to the mechanistic understanding of inorganic/bioinorganic reactions that involve the interaction with transition metal centers in solution. These include ligand substitution reactions, the activation of small molecules, and electron transfer processes.

SCIENTIFIC BACKGROUND

I was educated in South Africa as a Physical Chemist and studied the mechanisms of thermal and photochemical reactions of transition metal complexes in solution. During my post-doc years in the US and Germany, I was involved in projects dealing with the catalytic hydration of CO_2/dehydration of HCO_3^-, and the application of high pressure kinetic techniques to assist the elucidation of inorganic reaction mechanisms. This formed the basis for my habilitation in Physical Chemistry, during which time I could supervise a team of researchers specializing on the development and application of high pressure thermodynamic and kinetic techniques. These included UV-Vis, stopped-flow, temperature-jump and photochemical instrumentation to study the reactions of transition metal complexes in solution at pressures up to 200 MPa. The mechanistic studies dealt mostly with inorganic systems, with the result that I accepted Chairs for Inorganic Chemistry at the University of Witten/Herdecke and later at the University of Erlangen-Nürnberg. During this time we extended our experimental capabilities to electrochemical and NMR measurements under high pressure. Our interest changed steadily from inorganic to more bioinorganic systems, focusing on the activation of small molecules and electron transfer processes.

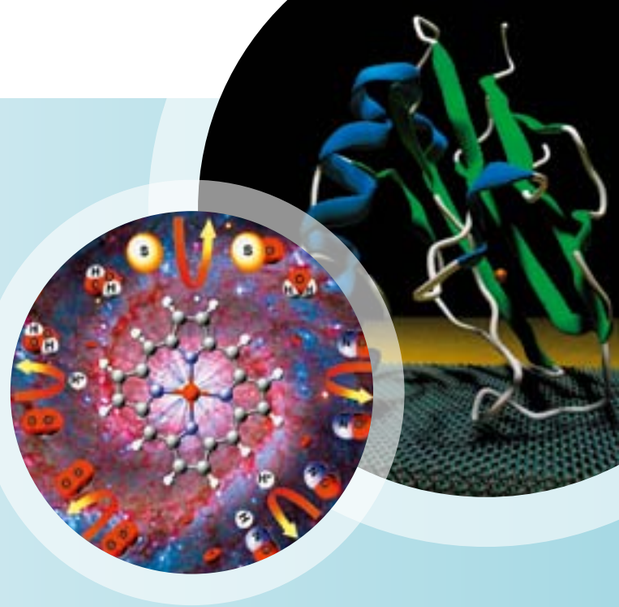
RESEARCH HIGHLIGHTS

The application of high pressure thermodynamic and kinetic techniques has contributed to the clarification of many solvent exchange and ligand substitution reactions of transition metal complexes of industrial, environmental and biological interest. These studies laid the basis for studies on more complex systems that involve the activation of small molecules. It is especially the activation of NO by aquated metal ions and model porphyrin complexes that showed how the underlying reaction mechanism is controlled by the pH of the solution. Furthermore, the non-innocent nature of NO allowed us to distinguish between the reversible binding of NO and the formal charge-transfer process by which the metal center can either be oxidized or reduced by coordinated NO. A similar behavior was studied for the reversible binding of NO to cytochrome P450 and functional models. In all cases volume profiles constructed from the pressure dependence of these reactions revealed unequivocal evidence for the suggested reaction mechanism. On the basis of the gained mechanistic insight, we studied the activation of H_2O_2, ROOH and RC(O)OOH by functional model iron porphyrin complexes. The application of low-temperature rapid-scan techniques allowed us for the first time to selectively prepare, characterize and study the reactivity of functional models for Compounds 0, I and II, which play a vital role in biological oxidation processes.

PERSPECTIVES

Our ability to spectroscopically follow the formation and subsequent reactions of functional models for Compounds 0, I and II with different substrates, now allow us to perform more detailed kinetic studies including systematic solvent, temperature, and pressure dependencies. It should also now be possible to study kinetic isotope effects for the oxygen transfer reactions induced by these different compounds. This should in turn allow us to gain further insight in the underlying reaction mechanisms involved in the oxygen transfer process, which is of fundamental importance for the understanding of biological oxidation processes.

Most of the highlights mentioned above involve reactions that occur either in aqueous solution or in conventional organic solvents. The challenge now is to extend these studies to similar reactions in ionic liquids in order to be able to account for the effect ionic liquids have on the mechanism of chemical processes. In this respect the role of trace impurities and the potential coordination ability of the anionic component of ionic liquids can play an important role and even control the nature of the reaction mechanism. The activation of small molecules such as O_2, NO and CO_2 by transition metal complexes will form the focus of our studies in ionic liquids.



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- A. Franke, C. Fertinger, R. van Eldik, *Angew. Chem. Int. Ed.* **2008,** 47, 5238 – 5242

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- C. D. Hubbard, R. van Eldik, Application of high pressure in the elucidation of inorganic and bioinorganic reaction mechanisms, *Physical Inorganic Chemistry. Principles, Methods, and Models* **2010,** A. Bakac (Ed.), Wiley, 269 – 365
- I. Ivanović-Burmazović, R. van Eldik, Metal complex-assisted activation of small molecules. From NO to superoxide and peroxides, *Dalton Trans.* **2008,** 5259 – 5275

SELECTED AWARDS

- 2010 Honorary Doctor of Science, University of Pretoria, South Africa
- 2010 Honorary Doctor of Science, Jagiellonian University, Krakow, Poland
- 2009 Inorganic Mechanisms Award, Royal Society of Chemistry, London
- 2009 Federal Cross of Merit ('Bundesverdienstkreuz') awarded by the Federal President of Germany
- 2006 Honorary Doctor of Science, Kragujevac University, Serbia
- 1997 Honorary Doctor of Science, Potchefstroom University, South Africa
- 1997 Raikes Medal of the South African Chemical Institute
- 1977 Alexander von Humboldt Fellowship

PROFESSOR OF INORGANIC CHEMISTRY

PROF. DR. NICOLAI BURZLAFF

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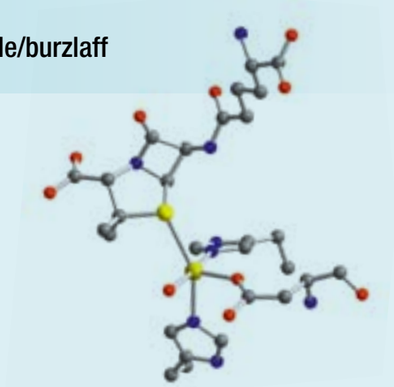

CURRICULUM VITAE

Since 2004	University Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
1999 – 2004	Habilitation at the University of Konstanz, Germany
1997 – 1999	Postdoctoral Fellow at the Dyson Perrins Laboratory, Oxford, Great Britain
1997	PhD from the University of Würzburg, Germany

OBJECTIVES

To design innovative heteroscorpionate ligands as a toolbox for metalloenzyme models, organometallics, supramolecular chemistry, and hybrid materials.

SCIENTIFIC BACKGROUND

In the past decade protein structures of several 2-oxoglutarate dependent iron oxygenases have been reported by various groups. Two iron binding histidines and one aspartate or glutamate – the so called 2-His-1-carboxylate facial triad – are conserved throughout the whole family of enzymes. This *N,N,O* binding motif, which is also found in some zinc peptidases, is the key research target of the Burzlaff group. Thus, to mimic this motif is the task of most of our model complexes for these iron and zinc dependent enzymes. Small heteroscorpionate ligands such as κ^3-N,N,O coordinating ligands are applied for this purpose. These ligands can be tailored with bulky substituents to modify their sterical hindrance and with linker groups for solid phase fixation or copolymerization. One future goal of such hybrid materials is to develop artificial enzymes e.g. by applying imprinted polymer techniques.

RESEARCH HIGHLIGHTS

Bioinorganic model complexes of various bis(pyrazol-1-yl)acetato or bis(imidazol-2-yl)propionato ligands mimic the 2-His-1-carboxylate facial triad of mononuclear non-heme iron oxygenases. With iron and ruthenium models bearing such ligands our group tries to mimic certain steps in the catalytic cycle and the biosynthesis catalyzed by the enzymes. Some model complexes show catalytic activity in peroxide shunt type reactions. Coordination of substrates or substrate analogues and inhibitors to the models are investigated.

Analog zinc complexes are structural models for the active sites of gluzincins that are useful tools to develop and test new zinc binding groups (ZBGs) to identify new lead structures for peptidase inhibitors. This concept was also extended to models for peptide deformylases (PDFs). Several ligands have been grafted on Merrifield resins or on silica. Moreover copolymers of several scorpionate ligands with MMA/EGDMA have been synthesized. By varying the amount of crosslinker control of the coordination geometry can be achieved. Ongoing work focuses on the generation of *imprinted polymers* by template complexes to generate artificial enzymes. Furthermore, various coordination polymers and metal organic frameworks (MOFs) are accessible with the heteroscorpionates as well as with new bidentate ligands.

The heteroscorpionate ligands are also quite useful in organometallics and coordination chemistry and allow a chemistry comparable to that of cyclopentadienyl (Cp) or hydrido(trispyrazol-1-yl)borato ligands (Tp). Several transition metal oxo, carbonyl, carbene, vinylidene, allenylidene, dinitrogen, hydrido and hydrogen complexes have been synthesized so far.

Besides coordination polymers and MOFs also supramolecular assemblies of nanoscaled dimension have been gained with the ligand library.

New chiral enantiopure tripod ligands are designed from cheap compounds of the *chiral pool* such as (+)-camphor or (-)-menthone, which are suitable for transition metal mediated enantioselective catalysis. So far *ee* values up to 68 % have been obtained for the Cu(I) mediated cyclopropanation of styrene.

PERSPECTIVE

In the future, we will intensify the ongoing projects but we would also like to extend our efforts on five new topics.

First, variation of the amount of EGDMA crosslinker in MMA/EGDMA copolymers containing scorpionate ligands allows controlling the coordination geometry of the metal center. Such polymers might have self-healing properties either by photoinduced or heat-induced bisligand moiety formation and will be tested in this regard.

Second, the synthesis of one-dimensional coordination polymers that might show conducting or semi-conducting properties.

Third, the cation induced self assembly of tri- and tetranuclear manganese complexes that might establish a route to models for the oxygen evolving center (OEC) of the photosystem II (PSII).

Fourth, we will investigate the catalytic properties of complexes bearing our new ligands. Ruthenium Tp complexes for example show catalytic activity for the conversion of CO_2 into formic acid. Similar ruthenium heteroscorpionate complexes might have advantages in this reaction due to a possible cooperative effect of the carboxylate donor with H_2 and will thus be tested for their catalytic properties. Furthermore, chromium complexes bearing *N,N,N*-ligands recently showed interesting catalytic activity in alkene polymerisation. Thus, we are interested in chromium complexes with enantiopure heteroscorpionate ligands.

Finally, in cooperation with the university hospital, we will search for small molecules that control the erythropoetin (EPO) formation by stabilization of the hypoxia inducible transcription factor HIF. New inhibitors will be identified by coordination studies with ferrous model complexes, by in silico docking and by in vitro and in vivo bioassays.

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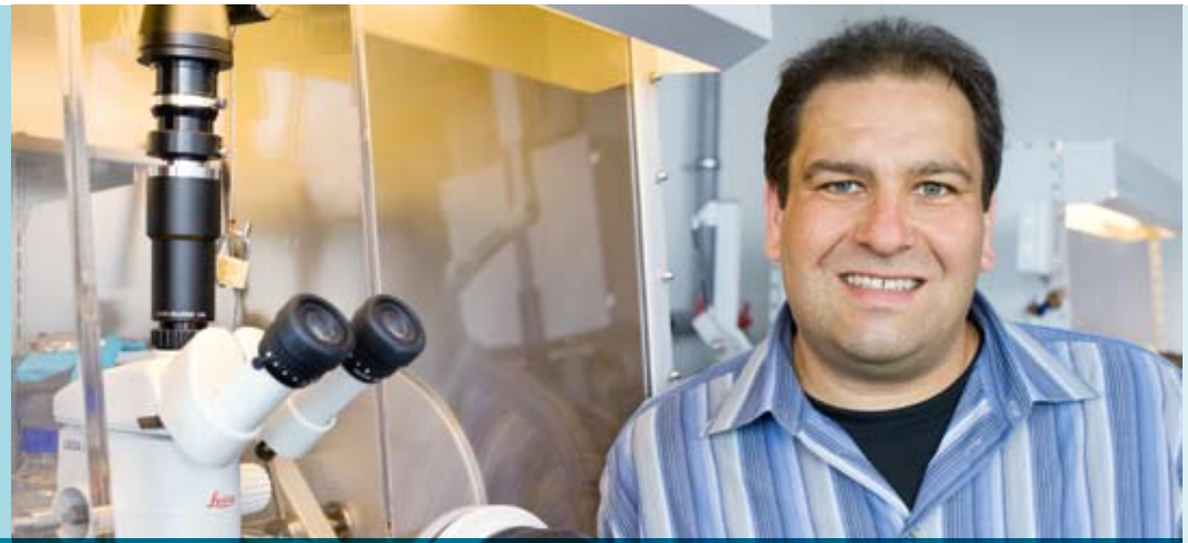

CHAIR OF INORGANIC AND GENERAL CHEMISTRY

PROF. DR. KARSTEN MEYER

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CURRICULUM VITAE

Since 2009	Visiting Professor at the University of Manchester, UK
Since 2006	University Full Professor, Chair of Inorganic and General Chemistry at the University of Erlangen-Nürnberg, Germany
2001 – 2005	Assistant Professor at the University of California, San Diego (UCSD), USA
1998 – 2000	Postdoctoral Studies at the Massachusetts Institute of Technology (MIT), USA
1995 – 1998	PhD, Max Planck Institute (MPI) for Radiation Chemistry (now MPI for Bioinorganic Chemistry), Mülheim / Ruhr, Germany
1989 – 1995	Study of Chemistry at the Ruhr-University of Bochum, Germany; Diploma (Ruhr-University of Bochum)

OBJECTIVES

General objectives of our research are the syntheses of new chelating ligands and their transition and actinide metal coordination complexes. These complexes often exhibit unprecedented coordination modes and unusual electronic structures, which result in enhanced reactivities towards small molecules of industrial and biological relevance such as organic azides and H_2, H_2O, N_2, CH_4, CO, CO_2, NO, O_2, O_3, P_4 etc. Whereas synthetic chemistry is at the heart of the Meyer group research, high-level spectroscopy is applied to help understand the molecular and electronic structure as well as the basis for reactivity of the newly synthesized reactive metal complexes.

SCIENTIFIC BACKGROUND

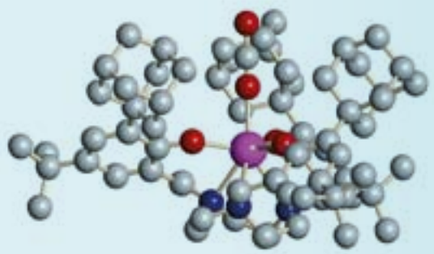
Small molecules such as alkanes, carbon dioxide, and water are attractive natural resources for the synthesis of fine chemicals and fuels. This is particularly true for the greenhouse gases CO_2 and CH_4. Functionalization of CH_4 and CO_2, however, is difficult due to their thermodynamic stabilities. One approach to circumvent this limitation is to coordinate the inert C1 molecules to a redox-active metal ion, which can serve as an electron source to reduce strong bonds. Based on the versatile reactivity of uranium and transition metal complexes it is expected that novel complexes are capable of unprecedented coordination of small molecules opening opportunities for activation and functionalization of chemical feedstock.

RESEARCH HIGHLIGHTS

The Meyer research program is focused on the activation of small molecules of biological and industrial interest using redox-active uranium and transition metal complexes in molecularly engineered ligand environments. Highlights of this work include the activation, cleavage, and multiple-bond metathesis of carbon dioxide at uranium complexes and the synthesis of reactive peroxo-, imido-, and nitrido-complexes for the functionalization of organic molecules via atom and group transfer chemistry. The series of actinide and transition metal complexes are unique as they are isostructural with varying oxidation states, e.g. Fe(I) to Fe(V) and U(III) and U(VI), enabling a complete and systematic analysis of the structure-reactivity relationships. This analysis presents a distinct benefit for the understanding of fundamental transition metal and uranium coordination chemistry. Topics such as the nature of f-orbital covalency in uranium complexes and the role of electronic structure in coordination complex reactivity are under continuous investigation.

PERSPECTIVES

Future research will focus on the advancement of novel actinide and transition metal chemistry and unprecedented transformations involving simple chemical feedstock, such as carbon dioxide, nitrogen, and water that are the key to sustainable energy resources.



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- O. P. Lam, C. Anthon, K. Meyer, Influence of steric pressure on the activation of carbon dioxide and related small molecules by uranium coordination complexes, *Dalton Trans.* **2009,** 9677 – 9691
- S. C. Bart, K. Meyer, Highlights in Uranium Coordination Chemistry, *Structure & Bonding* **2008,** 127, 119 – 176
- S. C. Bart, K. Meyer, Tripodal Ligands for Electron-Rich Transition and Actinide Metal Complexes. *Advances in Inorganic Chemistry* **2008,** 60, 1 – 30
- C. Hauser, K. Meyer, Uranchemie zwischen Phobie und Begeisterung, *Nachr. Chem.* **2007,** 55, 1195 – 1199
- I. Castro-Rodríguez, K. Meyer, Small Molecule Activation at Uranium Coordination Complexes: Control of Reactivity via Molecular Architecture, *Chem. Commun.* **2006,** 1353 – 1368

SELECTED AWARDS

- 2010 Dalton Transactions European / African Lectureship Award
- 2010 Japanese Society for the Promotion of Science (JSPS) Fellowship
- 2009 Israel Chemical Society Lifetime Honorary Membership
- 2004 / 2005 Alfred P. Sloan Award
- 2003 Faculty Career Development Award, Academic Senate
- 2002 Hellman Fellow, Chris & Warren Hellman Young Faculty Award
- 1999 / 2000 DFG Postdoctoral Fellowship

PROFESSOR OF INORGANIC CHEMISTRY

PROF. DR. SVEN RAU

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CURRICULUM VITAE

Since 2008	University Professor of Inorganic Chemistry II at the University of Erlangen-Nürnberg, Germany
2003 – 2007	Habilitation at the Friedrich Schiller University Jena, Germany
2000 – 2002	Postdoctoral Fellow, Inorganic Chemistry at the Friedrich Schiller University Jena, Germany
1997 – 2000	PhD at the Friedrich Schiller University Jena, Germany

OBJECTIVES

The research concept of the Rau group evolves around photoactive metal complexes. These metal complexes are developed for three different areas. Solar energy conversion in the form of light driven catalysis for water splitting is the central area of our activities. In addition we develop novel dyes for dye sensitized solar cells and potential biosensors and photodynamic therapeutics. For the area of solar energy conversion we develop novel multinuclear metal catalysts and investigate their photo catalytic reactions with spectroscopic techniques to improve their performance.

SCIENTIFIC BACKGROUND

Sven Rau has started his career in Jena at the Friedrich Schiller University in 1993. After obtaining his Vordiplom in 1994 he moved to the Dublin City University under the Erasmus Scheme returned in 1995 to Jena and performed his Diplom project under guidance from Prof. Dr. D. Walther, Jena and Prof. Dr. J. G. Vos, Dublin. After completing his degree in 1997 he worked with a scholarship of the "Studienstiftung des Deutschen Volkes" for his PhD at the Inorganic Chemistry in the area of carbon dioxide detection and activation. He obtained his PhD in 2000 and continued at the Friedrich Schiller University Jena where he started his independent career in 2002. From 2003 till 2006 he was a projectleader in the collaborative research center 436 in Jena. He finished his habilitation in 2007 and joined the Department of Chemistry and Pharmacy in Erlangen in 2008. Since 2010 he is elected member of the managing committee of the photochemistry division of the German Chemical Society (GDCh).

RESEARCH HIGHLIGHTS

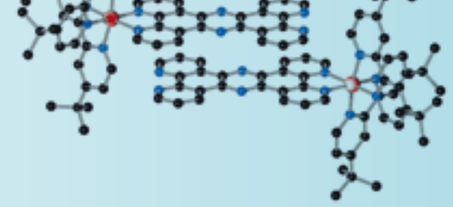
The Rau group has shown that heterodinuclear complexes composed of a ruthenium polypyridine unit, a bridging ligand and a palladium centre function as photochemical molecular device for the light driven hydrogen formation (*Angew. Chem.* **2006**). The function of these supramolecular complexes can be best described by a photo-redoxactive ruthenium unit which transfers an electron over the bridging ligand to the palladium catalytic centre. This process is with 316 ps extremely fast (*Chemistry Eur. J.* **2009**). The reductive quenching of this state with triethylamine under continuous irradiation leads to the formation of an active catalyst not only for hydrogen formation but also for hydrogen free hydrogenation of unsaturated substrates. The detailed analysis of the initial charge transfer processes showed that the location of the first excited state determines the fate of the photocatalyst (*Angew. Chem.* **2010**). Therefore, optimization of the catalytic efficiency is possible using tailor-made catalysts. Based on these results intramolecular photocatalysis might form the basis of a full photocatalytic water splitting reaction highly relevant for solar energy conversion.

Synthetic concepts have been developed which enable the efficient and high yielding production of ruthenium complexes with different substation patterns (*ICA* **2004**). The microwave assisted reactions are not only reducing reaction times by more than 90 %, increased yields are also observed. This concept can be extended to heterosupramolecular building blocks, where varying amounts of anchoring groups can be incorporated (*EUJIC* **2008**). In cooperation with the Vos research group from Dublin concepts for the efficient synthesis of ruthenium complexes with three different bipyridine ligands could be developed (*Dalton* **2006**). This synthetic expertise forms the basis for the successful implementation of the other research areas.

Ruthenium complexes with extended pi-conjugated ligands can intercalate into DNA which switches their emission behaviour. We could show that this switching can be tuned by substitution at all ligands (*Dalton* **2010**, *PCCP* **2009**). Even more interesting is the potential application of ruthenium complexes for the development of novel anti-cancer drugs. The selectivity of the cellular uptake can be determined by the nature of the sugar substituent, in other words the sugar substituent serves as an address code for the metal complex. These ruthenium complexes still show long lived triplet excited states which are quenched by oxygen, leading to the formation of cytotoxic singlet oxygen. (*Chem. Bio. Chem.* **2010**)

PERSPECTIVES

The focus of the future development will address solar energy questions. The discovery that electron transfer processes within one molecule can be utilized for catalytic activation enables us to use a vast array of spectroscopic techniques for elucidating the mechanisms of light induced electron transfer processes. With this knowledge we will expand to new catalytic reactions and concepts, like light driven CO_2 utilization. The detailed synthetic expertise generated by us will enable us to further investigate biomedical applications of metal complexes within interdisciplinary cooperations.



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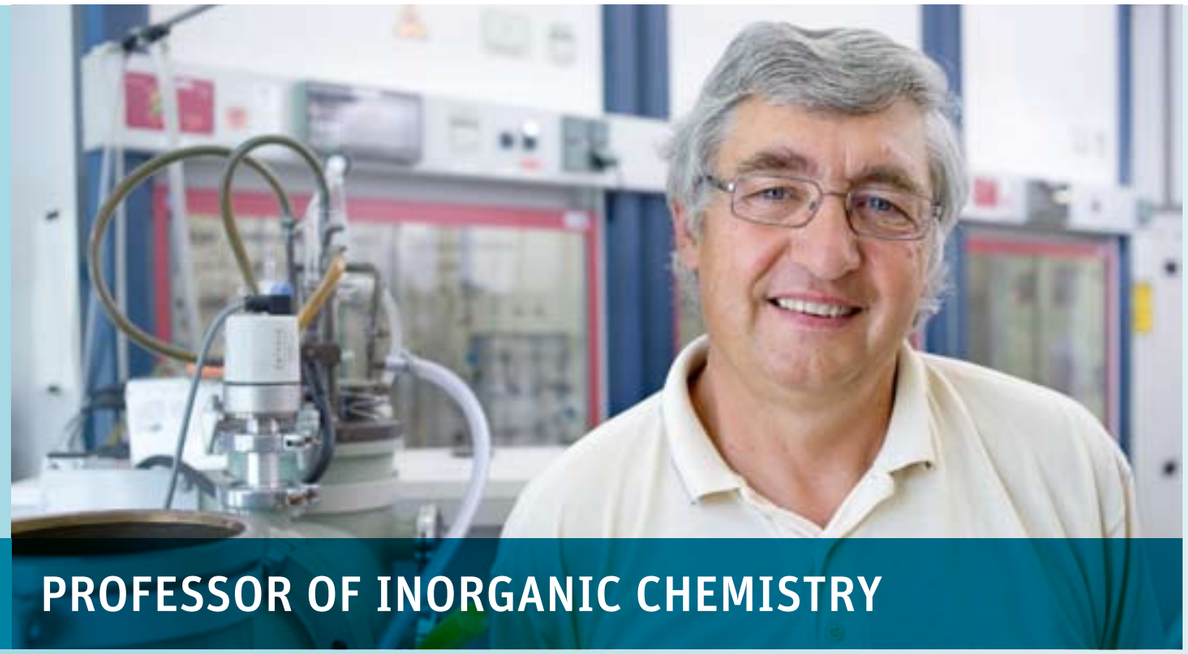
- M. Gottschaldt, U. S. Schubert, S. Rau, S. Yano, J. G. Vos, T. Kroll, J. Clement, I. Hilger, *ChemBioChem* **2010,** 11, 649 – 652
- S. Rau, B. Schäfer, D. Gleich, E. Anders, M. Rudolph, M. Friedrich, H. Görls, W. Henry, J.G. Vos; *Angew. Chem. Int. Ed.* **2006,** 45, 6215 – 6218

SELECTED REVIEWS

- S. Losse, J. G. Vos, S. Rau, Catalytic hydrogen production at cobalt centres, *Coord. Chem. Rev.* **2010,** DOI:10.1016/j.ccr.2010.06.004
- S. Rau, D. Walther, J. G. Vos, Inspired by Nature: Light Driven Organometallic Catalysis by Heterooligonuclear Ru(II) Complexes, *Dalton Transactions* **2007,** 915 – 919

SELECTED AWARDS

- 2001 "Promotionspreis", CGF, Friedrich Schiller University Jena, Germany
- 1998 "Fakultätspreis", CGF, Friedrich Schiller University Jena, Germany
- 1998 PhD – Scholarship Studienstiftung des Deutschen Volkes



PROFESSOR OF INORGANIC CHEMISTRY

PROF. DR. ULRICH ZENNECK

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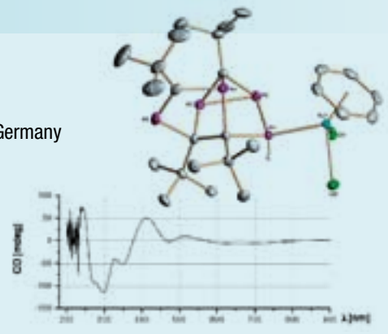


CURRICULUM VITAE

Since 1991	Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
1988	Habilitation at the University of Heidelberg, Germany
1981 – 1990	Research Associate at the University of Heidelberg, Germany
1980 – 1981	Postdoctoral Fellow at the University of Bristol, UK
1980	PhD University of Marburg, Germany

OBJECTIVES

Transition metal complex design for the targeted preparation of metallic nanoparticles or thin films, and for homogeneous and heterogeneous catalysis.

Preparation and investigation of chemical, structural, and chiroptical properties of cage-chiral organophosphorus cage compounds.

Characterization of redox process by electrochemistry and spectroscopy of paramagnetic redox products, including short-lived intermediates.

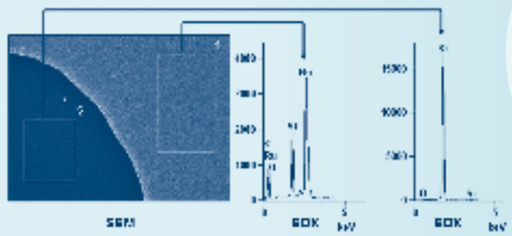
SCIENTIFIC BACKGROUND

Preparative organometallic and organophosphorus chemistry form the basis of most of our research projects. They are combined with electrochemistry to characterize the redox properties of the compounds including EPR and NMR spectroscopy of paramagnetic redox products. Short-lived redox intermediates are characterized by in situ EPR spectroscopy at the surface of a working electrode. A specific approach on organometallic chemistry deals with the preparation of transition metal π-complexes with designed melting, evaporation and thermal decomposition properties which include a completely controllable follow-up chemistry of the decomposition products. Metal vapor chemistry – a speciality of our group – allows the most effective access to iron(0) π-complexes. Such compounds are very useful as precursors for the preparation of metallic nanoparticles and thin films and those are of interest as functional materials and heterogeneous catalysts.

Transition metal chemistry is combined with the chemistry of unsaturated organophosphorus compounds like P-alkenes and P-alkynes. This fruitful field of research led to the investigation of novel structural motifs and chemical reactivity including high-yield routes to asymmetric P-C cage compounds.

RESEARCH HIGHLIGHTS

Isolation of enantiopure P_5-deltacyclenes opened the gate for the first time to cage-chiral P-C cage compounds, whose chemistry we are developing now. The class of compounds is characterized by remarkable CD-spectra. Cage formation and cage rearrangement reactions of P_5-deltacyclenes and related asymmetric P-C cage compounds are highly diastereoselective or enantioselective, depending on the stereo-chemical constellation of the process under investigation. (*Chem. Eur. J.* **2009,** 15, 5998) Chirally modified stannyl P-heterocycles give detailed insight into the molecular dynamics of those compounds. (*Eur. J. Inorg. Chem.* **2008,** 2225) Iron and molybdenum π-complexes with unsaturated P-heterocyclic ligands such as 1,3-diphosphetes and 1,3,5-triphosphinines allow the observation of novel intramolecular reaction pathways for π-ligands that include low-activated hydrogen transfer processes, ring-element exchange reactions, and the formation of completely unprecedented structural motifs. (*Comptes Rendus Chimie* **2010,** *Angew. Chem.* **2002,** 114, 4221)



[(Benzene)(1,3-cyclohexadiene)Ru] was identified as an excellent chemical vapor deposition precursor compound which allows to control the purity of the resulting thin ruthenium films by the inherent properties of both, the precursor complex itself and the freshly formed ruthenium thin layer. (*Chem. Vap. Deposition* **2007,** 13, 389) Methylation of one or both ligands allow the preparation of liquid precursor complexes while maintaining good vapor pressures and moderate decomposition temperatures and a complete control of the follow-up chemistry of the ligands. (Submitted) Surface deposited iron nanoparticles from [(aren)(diene)Fe] precursor complexes haven been proven to be highly efficient carbon nanotube catalysts. (*Powder Technology,* **2010**)

PERSPECTIVES

We are developing the chemistry of optically active cage-chiral P-C cage compounds and their metal complexes. The cages are of interest for the preparation of chemically robust new materials with pronounced chiroptical properties and as highly space filling ligands in enantioselective transition metal complex catalysis.

A series of actual interdisciplinary research projects deal with applications of our new-developed Fe, Ru, and W π-complexes as chemical vapour deposition (CVD) precursor complexes. Together with partners in physics, physical chemistry, chemical engineering, materials sciences, and industry we aim for a complete control of the metallic nanoparticle (NP) and thin film forming processes by highly advanced surface analysis. We contribute our specific competence to preparing designed CVD precursor complexes together with a solid know-how for the deposition of nanoparticles and thin films on several sorts of substrates to that multi-sided cooperation project. Our close scientific information exchange with surface and materials specialists and technical users for advanced materials aims for structure-property-relations of the precursor complexes that allow designing optimal precursor complexes for specific applications. Target properties of the NP and thin films include heterogeneous reduction and carbon nanotube catalysts, superparamagnetic NP for the control of ferromagnets, chemically inert, but redox-active NP for enhancing the quality of electrodes, and surface protection with respect to chemical and mechanical stress by well-adhered metal and metal carbide thin layers.

SELECTED PUBLICATIONS

- K. Eggers, F. W. Heinemann, M. Hennemann, T. Clark, P. Binger, U. Zenneck, *Comptes Rendus Chimie* **2010**
- K. Danova, I. Jipa, U. Zenneck, N. Popovska, *Powder Technology* **2010**
- M. Hofmann, C. Höhn, F. W. Heinemann, U. Zenneck, *Chem. Eur. J.* **2009,** 15, 5998 – 6007
- J. Panhans, F. W. Heinemann, U. Zenneck, *J. Organometal. Chem.* **2009,** 694, 1223 – 1234
- M. Hofmann, T. Clark, F. W. Heinemann, U. Zenneck, *Eur. J. Inorg. Chem.* **2008,** 2225 – 2237
- A. Schneider, N. Popovska, I. Jipa, B. Atakan, M. A. Siddiqi, R. Siddiqi, U. Zenneck, *Chem. Vap. Deposition* **2007,** 13, 389 – 395
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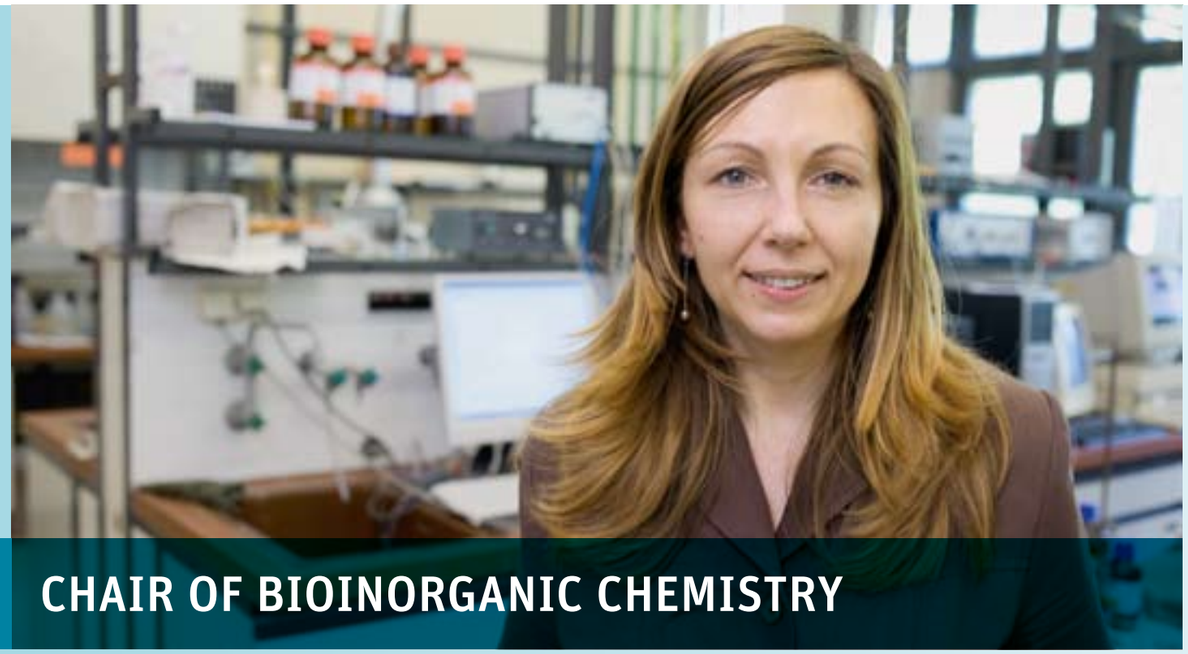
SELECTED REVIEWS

- M. Hofmann, U. Zenneck, Four-Membered Rings with Two Heteroatoms Including Phosphorus to Bismuth, *Comprehensive Heterocyclic Chemistry III* **2008,** Vol. 2, 875 – 905
- U. Zenneck, A. M. Trzeciak, Arene Ruthenium Complexes: Highly Enantioselective Catalysts and Excellent Precursors for MOCVD Deposition of Thin Ruthenium Films, *Education in Advanced Chemistry* **2005,** 9, 73 – 92
- U. Zenneck, B. Pietsch, Ionenfreie Nanometall-Polymerverbunde, Verfahren zu ihrer Herstellung und Verwendung, *Deutsches Patent DE 196 39 632 A1,* **2005**

SELECTED AWARDS

- 2001 Guest Professorship at the University Rennes 1, France
- 1991 Guest Professorship at the University of Pisa, Italia



CHAIR OF BIOINORGANIC CHEMISTRY

PROF. DR. IVANA IVANOVIĆ-BURMAZOVIĆ

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CURRICULUM VITAE

Since 2008	University Full Professor, Chair of Bioinorganic Chemistry at the University of Erlangen-Nürnberg, Germany
2008	Offer for a professorship of Bioinorganic Chemistry at the University of Texas at Arlington, USA
2008	Habilitation in Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
2001 – 2003	Alexander von Humboldt Postdoctoral Fellow at the University of Erlangen-Nürnberg, Germany
2000 – 2003	Assistant Professor of General and Inorganic Chemistry at the University of Belgrade, Serbia
1996 – 2000	Research and Teaching Assistant of Inorganic Chemistry at the University of Belgrade, Serbia
1999	DSc Faculty of Chemistry, University of Belgrade, Serbia

OBJECTIVES

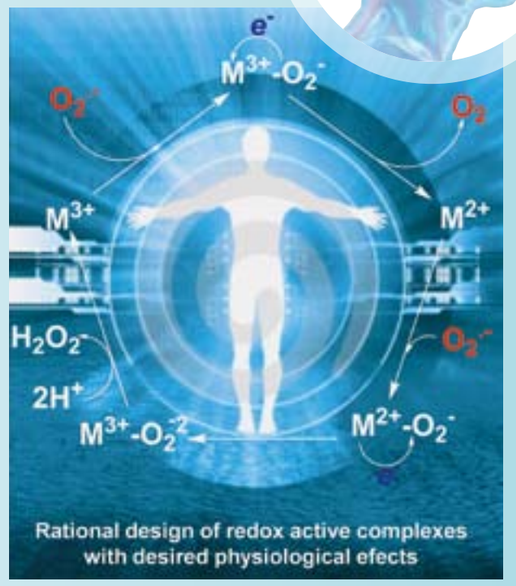
The general goal of our Chair for Bioinorganic Chemistry is elucidation of the metal-tuned redox processes of biological and catalytic relevance at the molecular level. In a focus is the activation of small molecules (superoxide radical anion (O_2^-), nitric oxide (NO), peroxynitrite ($ONOO^-$), hydrogen sulphide (H_2S)) by redox-active metal complexes, which can have physiological or pathophysiological consequences in biological systems, but at the same time can find application in bioinspired catalysis and biotechnology. We study reaction mechanisms to understand elementary reaction steps of complex bioinorganic processes and design efficient enzyme mimetics, metal based human pharmaceuticals and chemical catalysts. The approach is to rationally design bio-active metal complexes with desirable physiological effects based on understanding of their kinetic, thermodynamic, redox and mechanistic behavior.

SCIENTIFIC BACKGROUND

Syntheses of redox-active transition metal complexes of different coordination geometry and their versatile solution/reaction behavior are the general interests of our research group. We explore a wide range of intermolecular interactions in solutions (multiple proton-coupled electron transfer processes, week secondary interactions and host-guest chemistry in solution, interactions with solvent molecules, solvent exchange processes, stabilization of reactive superoxide via electrostatic interaction in ionic liquids) and reaction mechanisms in order to predict a potential application of metal based structures and tune their desirable activity. We apply a wide range of instrumentation methods in our research: time-resolved UV/vis low-temperature (down to -90 °C) and high-pressure stopped-flow measurements, high-pressure fluorescence stopped-flow measurements, high-pressure NMR measurements, temperature and pressure dependent electrochemical measurements, cryo time-resolved preparative spectroelectrochemistry, time-resolved solution IR, high-resolution tandem mass spectrometry with nano- and cryo-spray ionization.

RESEARCH HIGHLIGHTS

Our studies on seven-coordinate superoxide dismutase (SOD) mimetics that entered clinical trials shed new light on their catalytic mechanism, showing that the acyclic and rigid ligand systems can also be considered as structural motifs for the design of SOD mimetics. Methodologically we have further developed direct measurements of the catalytic superoxide decomposition in aqueous media by establishing a fast time-resolved UV/vis detection for obtaining highly reliable catalytic rate constants. In the area of SOD mimetics we went even further beyond the state of the art demonstrating their new type of reactivity towards nitric oxide (NO) and peroxynitrite ($ONOO^-$). Generation of NO^- by SOD mimetics can be even more beneficial than O_2^- removal, since our results (in vivo studies) suggest that NO^- is involved in activation of the gene and antioxidant enzymes expression enabling self-defense and regeneration of damaged tissues. An additional novelty in the suproxide chemistry was our demonstration that O_2^- can react with a metal center in a reversible manner forming quite stable M(III)-peroxo species, which can release superoxide to form an M(II) species by fine tuning of the proton concentration. Even more we have shown that M(III)-peroxo complexes are in general in equilibrium with corresponding M(II)-superoxo species. These findings show a new dimension of the reactivity of M-peroxo species in oxidative nucleophilic reactions and in metalloenzyme-catalyzed O_2 activation, where such complexes have been invoked as key intermediates. Our newest results point out that such species have a crucial role in the very efficient catalytic removal of H_2S.



Rational design of redox active complexes with desired physiological efects

PERSPECTIVES

Our efforts are directed to conceive the basic chemical processes behind the pharmacological treatment of oxidative and nitrosative stress, which are generators of aging and pathophysiological processes. In a time ahead of us we see utilization of redox-active metal complexes in regulation of the cells redox status, activation of immune system mechanism and as pharmaceuticals for treating the disease states related to immunodeficiency, inflammation/infection and neuropathology. With the same goal we will work on the effects of H_2S, which is a very potent reductant, in triggering beneficial physiological mechanisms in the cells with an extreme redox status. Thus, development of new compounds that will at the same time act as SOD mimics, H_2S and/or NO^- donors as potential pharmaceuticals is challenging for us and can help on elucidation of the elementary reaction steps that accompany inflammation processes and consequent immune-response.

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- D. Lieb, A. Zahl, T. E. Shubina, I. Ivanović-Burmazović, *J. Am. Chem. Soc.* **2010,** 132, 7282 – 7284
- M. R. Filipović, R. Miloš, A. C. W. Koh, S. Arbault, V. Niketić, A. Debus, U. Schleicher, Ch. Bogdan, M. Guille, F. Lemaître, Ch. Amatore, I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2010,** 49, 4228 – 4232
- M. R. Filipović, K. Duerr, M. Mojović, V. Simeunoviić, R. Zimmermann, V. Niketić; I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2008,** 47, 8735 – 8739
- G.-F. Liu, M. Filipović; I. Ivanović-Burmazović, F. Beuerle, P. Wittek, A. Hirsch, *Angew. Chem. Int. Ed.* **2008,** 47, 3991 – 3994
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- Liu, Gao-Feng, Filipović, Miloš, Heinemann, Frank W., I. Ivanović-Burmazović, *Inorg. Chem.* **2007,** 46, 8825 – 8835

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- I. Ivanović-Burmazović, Metal complex-assisted activation of small molecules. From NO to superoxide and peroxides, *Adv. Inorg. Chem.* **2008,** 60, 59 – 100
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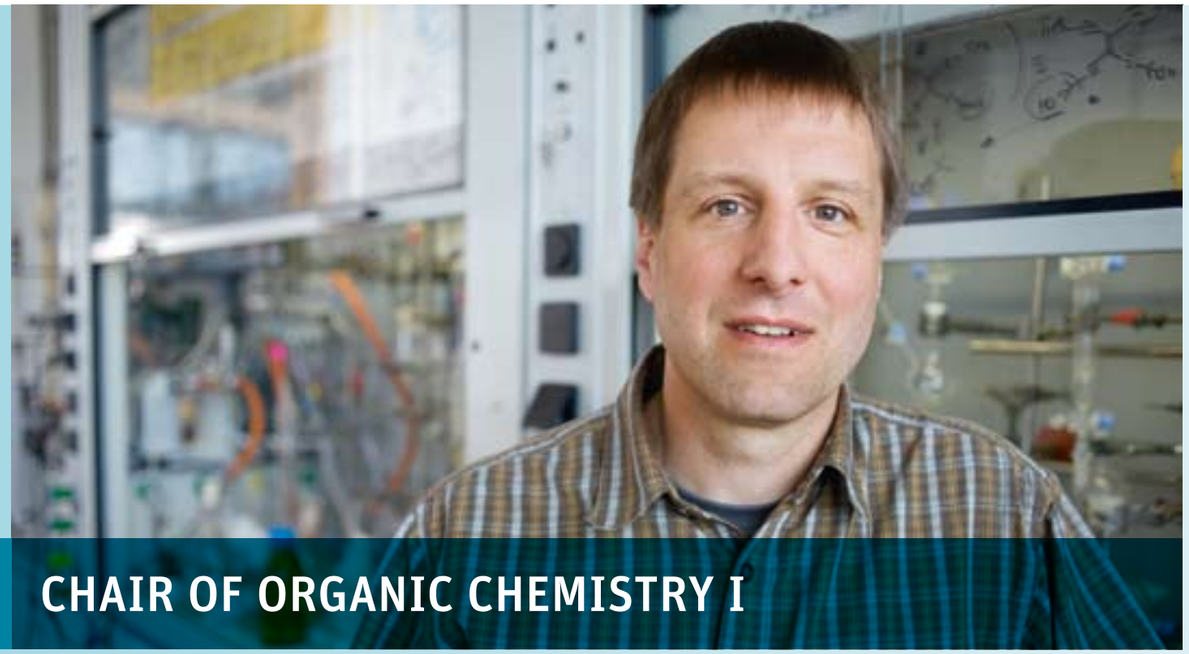

CHAIR OF ORGANIC CHEMISTRY I

PROF. DR. RIK R. TYKWINSKI

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CURRICULUM VITAE

Since 2009	University Full Professor, Chair of Organic Chemistry I at the University of Erlangen-Nürnberg, Germany
2005 – 2009	Professor of Chemistry, Department of Chemistry, University of Alberta, Edmonton, Canada
2002 – 2005	Associate Professor of Chemistry, Department of Chemistry, University of Alberta, Edmonton, Canada
1997 – 2002	Assistant Professor of Chemistry, Department of Chemistry, University of Alberta, Edmonton, Canada
1996 – 1997	Postdoctoral Fellow, Swiss Federal Institute of Technology (ETH), Zürich, Switzerland
1994 – 1996	U.S. ONR PDF Swiss Federal Institute of Technology (ETH), Zürich, Switzerland
1989 – 1996	PhD Organic Chemistry, University of Utah, Salt Lake City, Utah, USA

OBJECTIVES

- To develop new synthetic methods for the optimized formation of conjugated organic molecules, oligomers, and polymers with diverse structures.
- To understand the subtle interconnections between molecular structure and the electronic and optical properties that these materials display.
- To integrate our study of molecules with the goals of physicists and engineers toward the development of technologically useful materials and devices.

SCIENTIFIC BACKGROUND

Over the past decade or so, organic materials have become one of the most promising avenues toward the realization of a new generation of inexpensive, lightweight, and efficient optical and electronic devices. The realization of such materials requires a combination of efficient synthetic methods and a fundamental understanding of molecular properties. Our work in this area typically begins with the design of a new class of organic molecules that might solve a particular problem in molecular electronics. In some cases this problem might concern device operation, such as conductivity or solid-state molecular order. In other instances, however, it can be a more practical issue such as increasing solubility or stability. In either case, we then use our synthetic strengths to form specific members of this class, often developing new methodology along the way. Finally, our attention turns toward the exploration of molecular and materials properties as a function of structure. While we often do much of this molecular characterization within our own laboratory, many of the most exciting results come through close collaborations with physicists, engineers, and materials scientists who share our goals.

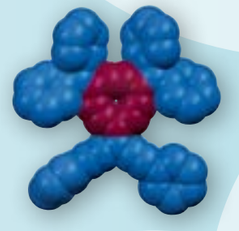
HIGHLIGHTS

Using a structure-function approach to molecular materials, our major discoveries have come through the synthesis of conjugated molecules, oligomers, and polymers based on acetylenic scaffolding. Within the series of carbon allotropes beginning with diamond and graphite (sp^3- and sp^2-carbon, respectively), our study of (sp-carbon) provides the foremost insight into the quest for the final member of this progression, carbyne. For example, we have recently synthesized the longest known polyynes, constructed of 44 consecutive sp-hybridized carbons. Our studies of polyynes also reveal some of the potential properties of carbyne, including: 1) The first crystallographic study of reduced bond length alternation that confirms Peierls distortion in these molecules, 2) The first experimental proof that polyynes are not linear in solution, as might be expected, but rather they are bent, and 3) Confirmation that polyynes are amongst the most efficient organic NLO materials. In addition to molecules composed almost completely of acetylenic building blocks, we have worked extensively in the synthesis of conjugated macrocycles with unique structures and properties, including porous solids and chiral host systems. Finally, our efforts to form new organic semiconductors offer the first oligomeric systems based on pentacene, some of which show unprecedented photoconducting properties.

PERSPECTIVES

One of our primary goals is to extend Nature's diversity beyond the known carbon allotropes, e.g., fullerenes, nanotubes, graphite, and diamond. This is accomplished via the rational synthesis of new 1- and 2-dimensional carbon molecules (e.g., carbyne and graphyne). We are intrigued by the fact that polyynes can serve as an ideal, 1-D molecular wire since their conjugated framework is essentially unaffected by bond rotation. Current synthetic methods are not likely suitable for polyynes longer than those known, and innovative routes toward encapsulation of the polyyne skeleton are a challenging goal, as are methods toward incorporating endgroups to allow polyynes to serve as molecular wires.

The future of many aspects of molecular electronics requires the design and discovery of new classes of molecules with, for example, enhanced solid-state order and more effective inter-molecular communication via pi-stacking. To meet these demands, we are exploring modular and divergent synthetic routes to new polycyclic aromatic hydrocarbons (PAHs). For example, PAHs (acenes) containing strategically placed heteroatoms offer a wealth of possibilities, and these systems can be optimized for integration into devices such as organic field effect transistors. Alternatively, we target segments of graphyne, a 2-D carbon material arrived at via the formal insertion of alkyne segments into the framework of graphene. Similar to fullerenes and nanotubes, one fascinating aspect of graphyne is the ability to form curved all-carbon surfaces with unique properties.



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- M. Gholami, F. Melin, R. McDonald, M. J. Ferguson, L. Echegoyen, R. R. Tykwinski, *Angew. Chem. Int. Ed.* **2007,** 46, 9081 – 9085
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- K. Campbell, C. A. Johnson II, R. McDonald, M. J. Ferguson, M. M. Haley, R. R. Tykwinski, *Angew. Chem. Int. Ed.* **2004,** 43, 5967 – 5971
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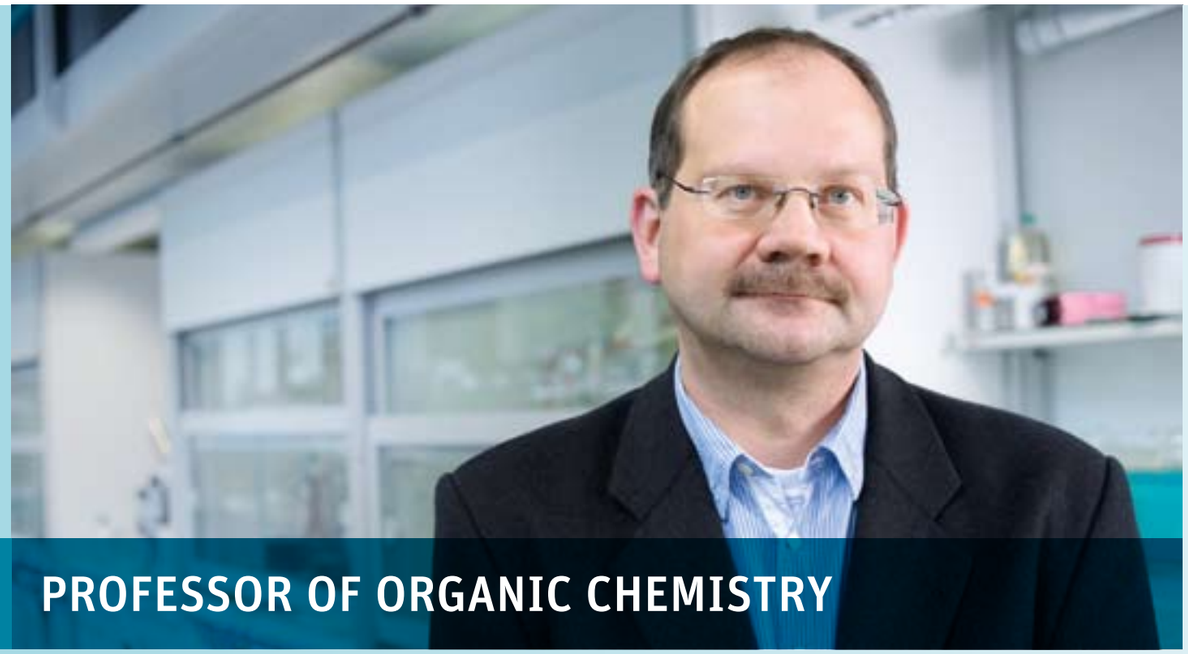
- M. Gholami, R. R. Tykwinski, Oligomeric and Polymeric Systems with a Cross-conjugated π-Framework, *Chem. Rev.* **2006,** 106, 4997 – 5027
- A. L. K. Shi Shun, R. R. Tykwinski, Synthesis of Naturally Occurring Polyynes, *Angew. Chem. Int. Ed.* **2006,** 45, 1034 – 1057

SELECTED AWARDS

- 2004 Faculty of Science Research Prize, University of Alberta
- 2003 Martha Cook Piper Research Prize
- 2001 PetroCanada Young Innovator Award



PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. JÜRGEN SCHATZ

schatz@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/schatz

CURRICULUM VITAE

Since 2007	University Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
2007	Lecturer, Department of Chemistry and Pharmacy, Ludwig-Maximilians-Universität München (LMU), München, Germany
2002 – 2007	Privatdozent, University of Ulm, Germany
1995 – 2002	Habilitation, University of Ulm, Germany
1994 – 1995	Postdoctoral Fellow, Department of Chemistry, Imperial College, London, UK
1994	PhD in Organic Chemistry at the University of Regensburg, Germany

OBJECTIVES

To use (pure) water as an medium for organic and supramolecular chemistry. Here, we want to design molecular systems based on weak (supramolecular) interactions and to exploit such arrays for catalysis, biological applications or as sensors.

SCIENTIFIC BACKGROUND

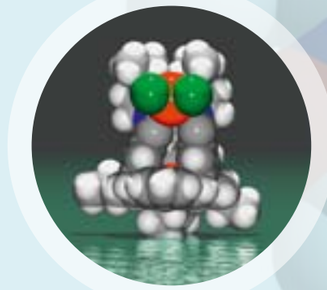
Organic Chemistry is usually performed in its corresponding environment – organic solvents. However, the interest in environmentally friendly ("green") and sustainable processes has recently increased dramatically.

Here, our general interest in organic chemistry which uses pure water as a solvent can help to develop methodologies which allow organic transformations in aqueous media. We focus on the use of water-soluble macrocycles, e.g. calixarenes, cyclodextrins, cyclophanes, or cucurbiturils, to adjust the solubility of both reagents and catalysts by supramolecular, non-covalent interactions. However, on the way to catalysis using self-assembled, non-covalently linked catalysts in water, many fundamental scientific problems have to be tackled: The supramolecular interactions between all components have to be elucidated both structurally and quantitatively. Therefore, we study the host-guest chemistry of artificial receptor molecules with cations, anions, or neutral molecules as guests.

Supramolecular interactions are also the underlying theme of a second research topic: The use of calixarene-based gadolinium complexes for applications in magnetic resonance imaging (MRI).

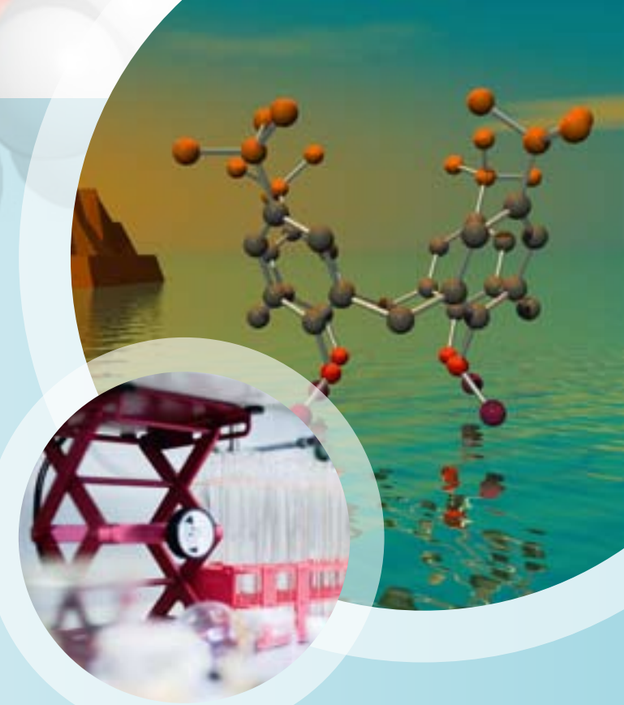
RESEARCH HIGHLIGHTS

Over the last 3 years, after relocating the research group to Erlangen, we developed methods to perform standard organometallic reactions in pure water. Suzuki cross coupling as well as Grubbs-type metathesis reactions can now be realized in pure aqueous solution. The design, syntheses, and optimisation of water-soluble macrocycles, which can be used as additives in these reactions, proved to be decisive. Especially, imidazolium salt based systems were very successful. This class of compounds can also act as precursors for N-heterocyclic carbenes (NHCs) which are ligands for both Palladium and Ruthenium used in Suzuki couplings and Grubbs metathesis reactions, respectively. In this way, both solubility and catalysis could be addressed using the same type of compounds.



Imidazolium salts were also extremely useful in the recognition of small inorganic and organic anions. Recently, we succeeded in developing a naked-eye detection of small amounts of fluoride, acetate or benzoate using a calixarene-based anion receptor molecule.

In the supramolecular chemistry of cations Gadolinium-azacrownether-calixarene hybrids were synthesized which exhibit an outstanding performance in MRI applications.



PERSPECTIVES

In future, we want to pursue three main areas of research: organometallic catalysis in water, anion recognition especially in polar environment, and novel MRI contrast agents.

In the first area, we want to develop efficient, tailor-made catalysts for applications in aqueous solution as medium. Additionally, we are working on the combination of various methods available in the "catalysts tool box". Multi-step, one-pot procedures exploiting transition metal-, organo- and biocatalysis – all disciplines well represented here in Erlangen– are here an appealing target. The quest for "naked-eye" receptors which detect anions with high efficiency and selectivity in pure water as an environment can be regarded as a holy grail in supramolecular chemistry. We want to address the challenge using organic cations as molecular platforms for anion receptors because these building blocks provide both colour, necessary for the optical read-out, and increased binding strength. Chiral discrimination in non-covalent recognition processes will also be a attractive issue for further research. Third, we will incorporate MRI contrast agents in biological structures such as liposomes, vesicles, or membranes.

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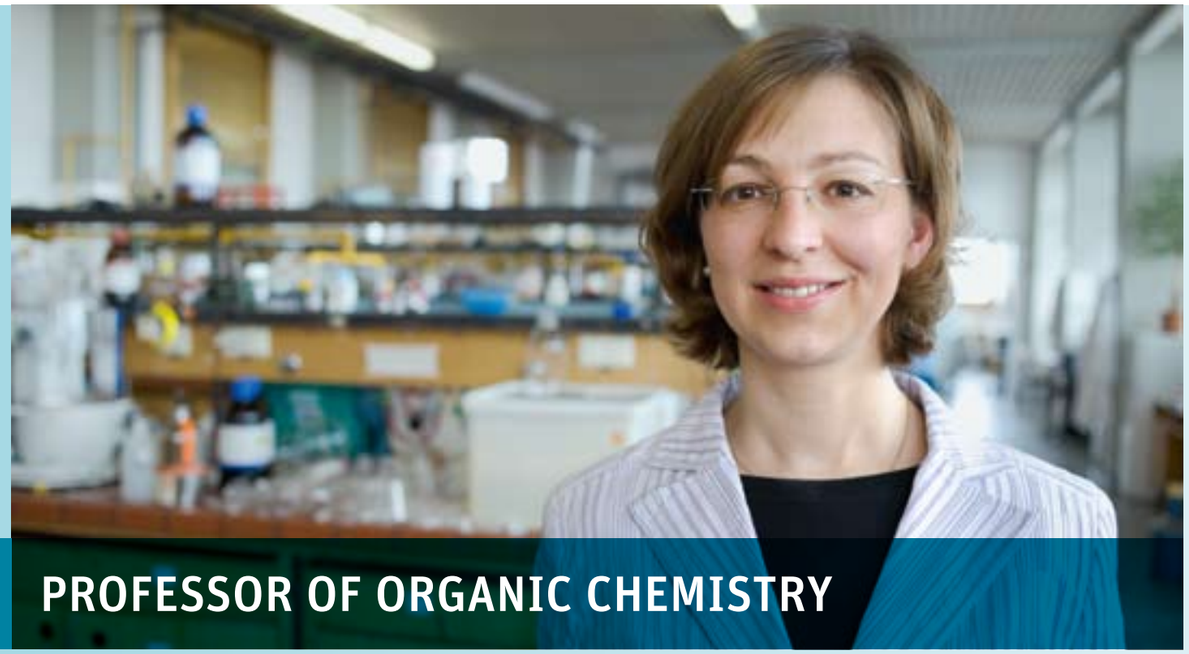
- D. T. Schühle, M. Polásek, I. Lukes, T. Chauvin, É Tóth, J. Schatz, U. Hanefeld, M. C. A. Stuart, J. A. Peters, *Dalton Trans.* **2010,** 39, 185 – 191
- T. Fahlbusch, M. Frank, G. Maas, J. Schatz, *Organometallics* **2009,** 28, 6183 – 6193
- Th. Bredgen, T. Fahlbusch, M. Frank, D. T. Schühle, M. Seßler, J. Schatz, *Adv. Synth. Catal.* **2009,** 351, 303 – 307
- S. Bartz, B. Blumenröder, A. Kern, J. Fleckenstein, S. Frohnapfel, J. Schatz, A. Wagner, *Z. Naturforsch.* **2009,** 64b, 629 – 638
- M. Rehm, M. Frank, J. Schatz, *Tetrahedron Lett.* **2009,** 50, 93 – 96

SELECTED REVIEWS

- J. Schatz, M. Seßler, Product Class 10-12: Thiophenes, Thiophene 1,1-Dioxides, and Thiophene 1-oxides, Selenophenes, and Tellurophenes, in: *Science of Synthesis* (Houben-Weyl Methods of Molecular Transformations), Thieme Verlag, Stuttgart, New York, **2010**
- Th. Brendgen, J. Schatz, D. Schühle, Thiophenes and their Benzo Derivatives: Applications, Chapter 3.12. in Comprehensive Heterocyclic Chemistry-III (CHEC-III), Eds. A. Katritzky, Ch. Ramsden, E. F. V. Scriven, R. J. K. Taylor, G. Jones, **2008**
- J. Schatz, Ab initio calculations on supramolecular systems, *Encycl. Supramol. Chem.* **2006,** 1 – 8
- J. Schatz, Recent Application of ab initio Calculations on Calixarenes and Calixarene Complexes, *Coll. Czech. Chem. Commun.* **2004,** 69, 1169 – 1194

SELECTED AWARDS

- 2008, 2009, 2010 Teaching Awards, University of Erlangen-Nürnberg, Medical School
- 2002 Lehrbonus University of Ulm (Teaching Award)
- 1994 E.ON Bayern – Kulturpreis Ostbayern (PhD Award)



PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. SVETLANA B. TSOGOEVA

tsogoeva@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/tsogoeva

CURRICULUM VITAE

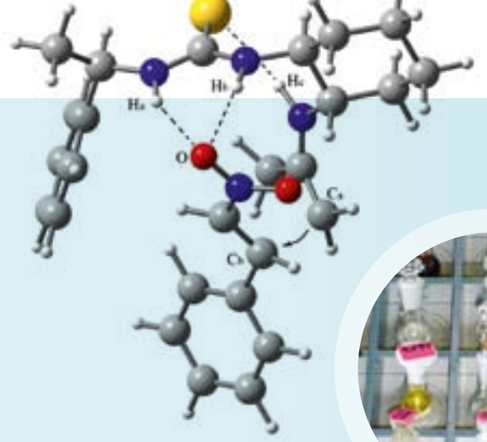
Since 2007	University Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
2002 – 2007	Juniorprofessor at the Institute of Organic and Biomolecular Chemistry, University of Göttingen, Germany
2000 – 2002	Postdoctoral Research Fellow at the Fine Chemicals Division of Degussa AG, Hanau-Wolfgang, Germany
1998 – 2000	Postdoctoral Research Fellow at the Johann Wolfgang Goethe University, Frankfurt am Main, Germany
1995 – 1998	PhD. at the St.-Petersburg State University, St.-Petersburg, Russia

OBJECTIVES

The development, application, and teaching of modern synthetic methods in asymmetric catalytic synthesis and chiral resolution is a central goal in our group. Computations and experiment are often both employed to address specific problems and in the same project. State-of-the-art analytical techniques and skills are used to carry out experiments, notably for design and evaluation of chiral organocatalysts and metal-catalysts. Interdisciplinary and international collaborations round off our profile, where both sides mutually profit from the synergy of the expertises existing in different research groups.

SCIENTIFIC BACKGROUND

Many bioactive compounds are chiral and there is an ever-growing demand in contemporary pharmaceutics or material science for compounds with high enantiopurity, e.g. for single enantiomer chiral drugs and their precursors. Stereochemistry therefore aims at introducing chiral centers of defined absolute configuration at desired positions into molecules and with high conversion rates from prochiral reactants. Hence, there is a continued need to design more active, more versatile and more enantioselective catalysts. In addition, we endeavour to find successful new synthetic methods and/or catalytic systems in enantioselective organocatalysis, aiming at high throughput, high enantioselectivity and diastereoselectivity, a wide substrate or reaction scope and use of environmentally benign solvents (e.g. water). To achieve this goal, computational methodologies and tools are employed to predict enantioselectivities or for finding clues for improved catalyst lead structures. Novel organic process techniques are being developed in our lab, accessing autocatalysis and crystal engineering. A further area of research interest is the design of synthetic hybrids of natural bioactive compounds with potential applicability in medicinal chemistry. Further, non-heme iron complexes with peptide-based ligands are employed in asymmetric oxidation reactions.



RESEARCH HIGHLIGHTS

Research in our group is centered around *Asymmetric Organocatalysis, Chiral Autocatalysis; Asymmetric Oxidations with Redox-Active Metal Complexes and Natural Product Hybrids for Medicinal Chemistry.*

In the flourishing research area of *Asymmetric Organocatalysis* we focused early on the design, synthesis and application of novel *chiral bifunctional organocatalysts* for different organic transformations. We found and applied the first primary amine containing *unmodified dipeptides and thiourea-amine organocatalysts* for highly enantioselective C-C bond formation reactions (e.g. nitro-Michael, Mannich, aldol reactions). We discovered lately the first *organo-autocatalytic reactions.* Combining the novel concept of product catalysis with that of asymmetric amplification, we first demonstrated spontaneous enantioenrichment in fully organic reactions.

Recently we extended the spectrum of our research to *redox-active non-heme iron complexes* as mimics of non-heme iron enzyme and their potential synthetic application in asymmetric oxidation reactions, and using hydrogen peroxide as an environmentally friendly oxidant.

Medicinal chemistry involves the identification, synthesis and development of promising new compounds suitable for therapeutic use. It also includes the study of existing drugs, their biological properties, and their structure activity relationships. *Hybridization of bioactive natural and unnatural compounds* rates among the most promising recent approaches in this field. Our interest focuses on the development of new lead structures and the design of promising candidates for potent drugs in the field of medicinal chemistry.

PERSPECTIVES

The future of asymmetric catalysis and of the technologies used in generation of enantiomerically pure compounds in the industry might look rather different from what we know today. The discovery of organoautocatalysis is evidence that seemingly already well-understood organic reactions might possess much more complicated mechanisms than hitherto believed. To uncover the exact nature of stereoselective reactions could offer new opportunities for catalyst design and process development in catalytic asymmetric synthesis, e.g. in more efficient reactions that are more atom-economical or which produce less waste. In this context, one-pot multicomponent reactions in which different catalytic steps proceed successively and without the need of intermittent product extraction, catalyst retrieval and purification steps plays a promising role for the future development of asymmetric synthesis. The exploitation of novel chiral resolution techniques like crystal engineering in combination with conventional asymmetric synthesis has a high potential for future optimizations to attain high-throughput and efficient production of single enantiomer compounds, which have a tremendous economic potential.

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- A. Zamfir, S. B. Tsogoeva, *Org. Lett.* **2010,** 12, 188 – 191.
- S. B. Tsogoeva, S.-W. Wei, M. Freund, M. Mauksch, *Angew. Chem. Int. Ed.* **2009,** 48, 590 – 594, *Angew. Chem.* **2009,** 121, 598 – 602.
- D. A. Yalalov, S. B. Tsogoeva, T. E. Shubina, I. M. Martynova, T. Clark, *Angew. Chem. Int. Ed.* **2008,** 47, 6624 – 6628; *Angew. Chem.* **2008,** 120, 6726 – 6730
- C. Baudequin, A. Zamfir, S. B. Tsogoeva, *Chem. Commun.* **2008,** 4637 – 4639
- M. Mauksch, S. B. Tsogoeva, I. M. Martynova, S.-W. Wei, *Angew. Chem. Int. Ed.* **2007,** 46, 393 – 396, *Angew. Chem.* **2007,** 119, 397 – 400
- S. B. Tsogoeva, S.-W. Wei, *Chem. Commun.* **2006,** 1451 – 1453

SELECTED REVIEWS

- S. B. Tsogoeva, Organo-Autocatalysis: Challenges for Experiment and Theory, *Journal of Systems Chemistry* **2010**
- S. B. Tsogoeva, Recent Progress in the Development of Synthetic Hybrids of Natural or Unnatural Bioactive Compounds for Medicinal Chemistry, *Mini Rev. Med. Chem.* **2010,** 10(9), 773 – 793
- S. B. Tsogoeva, Recent Advances in Asymmetric Organocatalytic 1,4-Conjugate Additions, *Eur. J. Org. Chem.* **2007,** 1701 – 1716
- S. B. Tsogoeva, Short Peptides and Peptide-Like Enzyme Mimics – Efficient Organic Catalysts in Asymmetric Synthesis, *Lett. Org. Chem.* **2005,** 2, 208 – 213

SELECTED AWARDS

- 2008 Tetrahedron: Asymmetry “Most Cited Paper 2005 – 2008 Award”
- 2007 Thieme Journal-Preis

CHAIR OF ORGANIC CHEMISTRY II

PROF. DR. ANDREAS HIRSCH

hirsch@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/hirsch

CURRICULUM VITAE

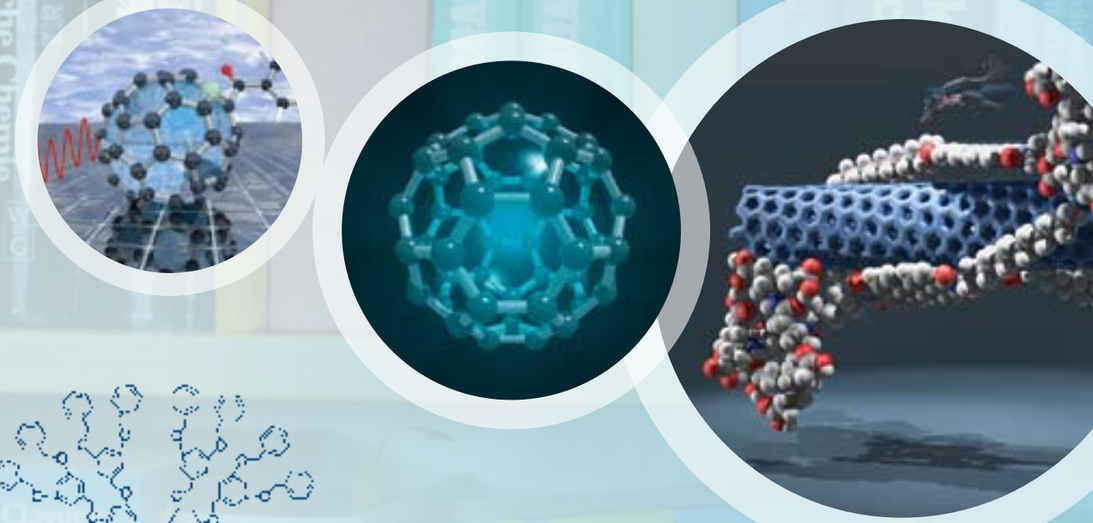
Since 1995	University Full Professor, Chair of Organic Chemistry II at the University of Erlangen-Nürnberg, Germany
1995	Professor for Organic Chemistry at the University of Karlsruhe, Germany
1991 – 1995	Habilitation at the Institute of Organic Chemistry, University of Tübingen, Germany
1990 – 1991	Postdoctoral research with Prof. Fred Wudl at the Institute for Polymers and Organic Solids, Santa Barbara, USA
1987 – 1990	PhD under the supervision of Prof. Hanack at the Institute of Organic Chemistry at the University of Tübingen, Germany

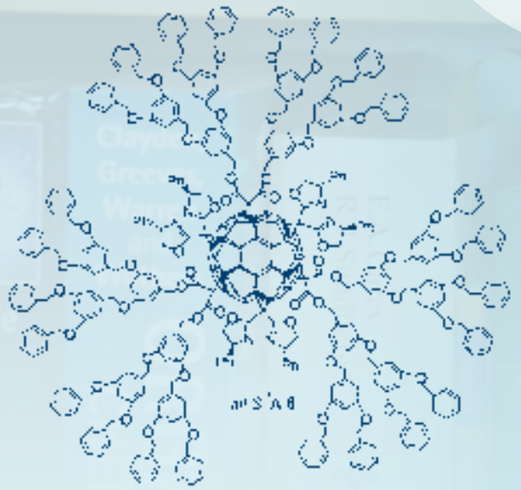
OBJECTIVES AND SCIENTFIC BACKGROUND

Hirsch's laboratory has been pioneering and is at the forefront of carbon allotrope chemistry and is well-known for the investigations of basic principles for the functionalization of the 0-dimensional fullerenes, the 1-dimensional carbon nanotubes and the 2-dimensional graphene, which lead to synthesis of numerous examples of derivatives with tailor-made structural, electronic, photophysical and biomedical properties. Andreas Hirsch's work in synthetic organic chemistry includes synthesis of oligoynes, development of new covalent, ionic and H-bonded dendrimers, porpyrines, calixarenes, perylenes and redox-active ionic liquids.

RESEARCH HIGHLIGHTS

The research of the Hirsch group is characterized by its uncompromising commitment to *interdisciplinarity.* Among the most important achievements are: control over the regiochemistry of multiple addition reactions, the shape dependent difference of endohedral and exohedral functionalization, the $2(n+1)^2$-rule for the description of spherical aromaticity of fullerenes, which is namedas Hirsch rule, the introduction of water solubility into these carbon rich systems and the first p-type doping of carbon nanotubes, the synthesis of self-assembled dendrimers, the generation of shape persistent micelles and switchable Buckysomes, the synthesis and investigation of well defined monodisperse polyelectrolytes, the retrofunctionalization of carbon nanotubes and finally the first systematic investigation on the covalent and non-covalent functionalization of graphene. Numerous examples of fullerene, nanotube and graphene derivatives with tailor-made properties such as a) donor-acceptor hybrids suitable to undergo photoinduced energy and electron transfer, b) synthetic mimics for globular hemeproteins, c) dendrizymes, d) heterofullerenes, e) cluster opened fullerenes, f) the largest polyelectrolytes with completely defined and monodisperse structures, g) nanotube based carriers for gene delivery, h) giant bis-fullerene dipoles, i) the first example of fullerene amphiphiles that aggregate completely in shape persistent micelles, whose structure could be determined with molecular precision and j) water soluble fullerene derivatives that act as very potent superoxide dismutase models in the field of biomedical chemistry. The PI's work in synthetic chemistry includes synthesis of acetylenic compounds such as polyynes and stabilized oligoynes which are of interest in approaching a new hypothetical allotrope of carbon, the one-dimensional carbine sp-C_∞.





PERSPECTIVES

The systematic investigation of the carbon allotrope chemistry and the development of new concepts in supramolecular chemistry will pave the way to high performance applications as molecular materials. Examples are printable electronics, organic photovoltaic devices, redox-active as potent neuro-protective drugs.

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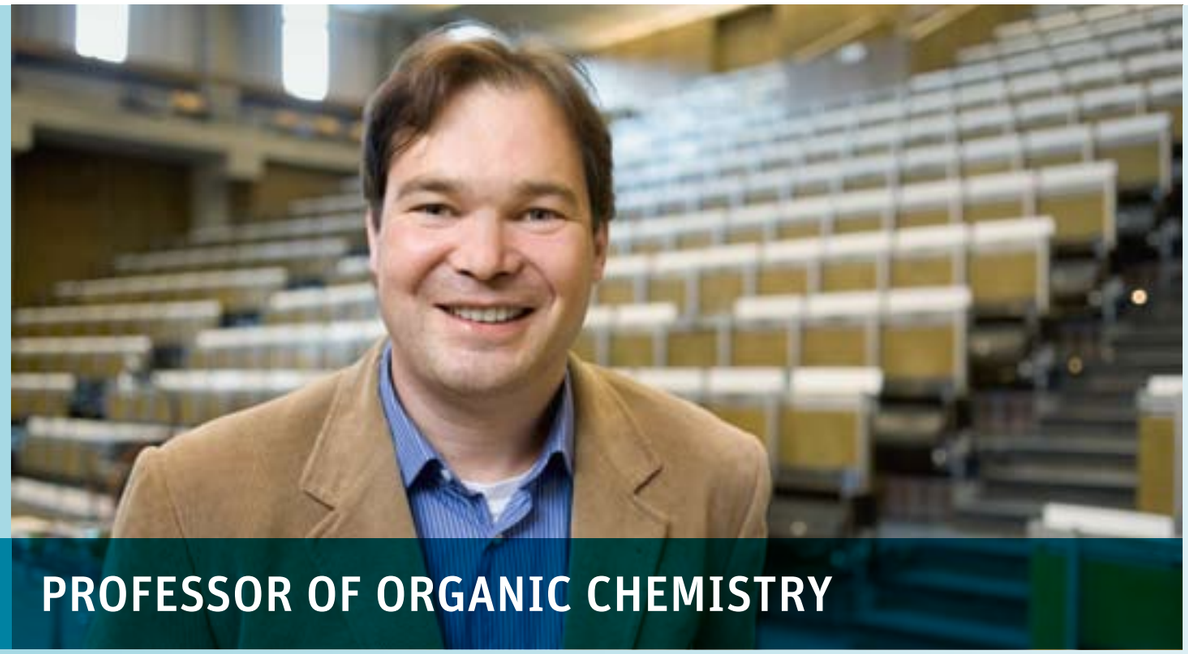
- Z. Syrgiannis, B. Gebhardt, C. Dotzer, F. Hauke, R. Graupner, A. Hirsch, *Angew. Chem. Int. Ed.* **2010,** 49, 3322 – 3325, *Angew. Chem.* **2010,** 122, 3394 – 3397
- C. Ehli, C. Oelsner, D. M. Guldi, A. Mateo-Alonso, M. Prato, C. D. Schmidt, C. Backes, F. Hauke, A. Hirsch, *Nature Chemistry* **2009,** 1, 243 – 249
- C. Backes, C. D. Schmidt, F. Hauke, C. Böttcher, A. Hirsch, *J. Am. Chem. Soc.* **2009,** 131, 2172 – 2184
- G.-F. Liu, M. Filipović, I. Ivanović-Burmazović, F. Beuerle, P. Witte, A. Hirsch, *Angew. Chem. Int. Ed.* **2008,** 47, 3991 – 3994, *Angew. Chem.* **2008,** 120, 4055 – 4058
- B. Schade, K. Ludwig, C. Böttcher, U. Hartnagel, A. Hirsch, *Angew. Chem. Int. Ed.* **2007,** 46, 4393 – 4396, *Angew. Chem.* **2007,** 119, 4472 – 4475
- R. Graupner, J. Abraham, D. Wunderlich, A. Venvelova, P. Lauffer, J. Röhrl, M. Hundhausen, L. Ley, A. Hirsch, *J. Am. Chem. Soc.* **2006,** 128, 6683 – 6689

SELECTED REVIEWS

- A. Hirsch, Unzipping Carbon Nanotubes: A Peeling Method for the Formation of Graphene Nanoribbons, *Angew. Chem. Int. Ed.* **2009,** 48, 6594 – 6596, *Angew. Chem.* **2009,** 121, 6718 – 6720
- O. Vostrowsky, A. Hirsch, Heterofullerenes, *Chem. Rev.* **2006,** 106, 5191 – 5207
- A. Hirsch, Functionalization of Single-wall Carbon Nanotubes, *Angew. Chem. Int. Ed.* **2002,** 41, 1853 – 1859, *Angew. Chem.* **2002,** 114, 1933 – 1939
- M. Bühl, A. Hirsch, Spherical Aromaticity of Fullerenes, *Chem. Rev.* **2001,** 101, 1153 – 1183

SELECTED AWARDS

- 2009 ERC Advanced Grant
- 2007 Professor of the Year (Unicum Beruf)
- 2006 Elhuyar-Goldschmidt-Prize
- 1994 ADUC Award for Habilitands
- 1994 Otto-Röhn-Award



PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. HARALD GRÖGER

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CURRICULUM VITAE

Since 2006	University Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
2004 – 2006	Senior Project Manager at the Service Center Biocatalysis of Degussa AG
2001 – 2003	Project Manager at the Project House Biotechnology of Degussa AG
1998 – 2001	Head of Laboratory at the Research Department "Chemische Forschung" of SKW Trostberg AG
1997 – 1998	Postdoctoral Fellow at the University of Tokyo in the research group of Prof. Dr. Shibasaki, Japan
1994 – 1997	Doctoral thesis at the University of Oldenburg in the research group of Prof. Dr. Martens
1994	Diploma thesis at the University of Oldenburg in the research group of Prof. Dr. Martens
1988 – 1994	Study of Chemistry (Diplom-Chemie) at the Universities of Erlangen-Nürnberg and Oldenburg

OBJECTIVES

The research activities of the Gröger group center around the application of enzymes as valuable and environmental friendly catalysts in organic synthetic transformations. A particular goal of the highly interdisciplinary research projects is the development of synthetic processes which fulfil the criteria of high efficiency, sustainability as well as scalability. To realize such processes we focus on (1) the development of efficient biocatalytic reactions (biotransformations) and technical applications thereof, (2) the combination of biocatalysis with chemocatalysis in one-pot multi-step syntheses in water, and (3) target driven synthesis based on the use of biocatalysts in synthetic key steps. A key feature of the research activities in the Gröger group at the interface between biology and organic chemistry is the high degree of interdisciplinarity, underlined by numerous collaborations with academic and industrial partners.

SCIENTIFIC BACKGROUND

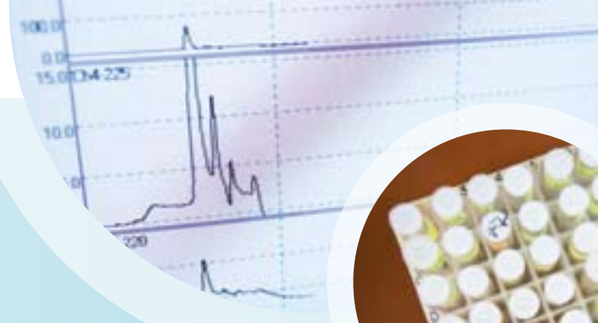
Applied enzyme catalysis (biocatalysis), also nowadays known as "white biotechnology" is considered to represent one of the key technology areas of the 21th century. In spite of the potential and importance of enzymes as catalysts in organic chemistry, however, the number of efficient industrially applied processes is still limited in comparison to "classic" chemical or chemocatalytic syntheses. At first, this might surprise when considering the obvious advantages of biocatalysis such as high enantio-, diastereo-, regio-, and chemo-selectivity, the use of water as a reaction medium, and the potential to realize environmentally friendly processes. On the other hand, however, the use of enzymes in organic synthesis is still often limited, e.g., by the incompatibility of enzymes with an organic solvent environment, narrow substrate range as well as the typical separation of biocatalytic reactions from "classic chemical" types of reactions. Overcoming these limitations represents a major challenge in biocatalysis in order to fully benefit from the tremendous catalytic potential of enzymes and to develop efficient, environmentally friendly *and* technically feasible biocatalytic organic synthetic transformations.

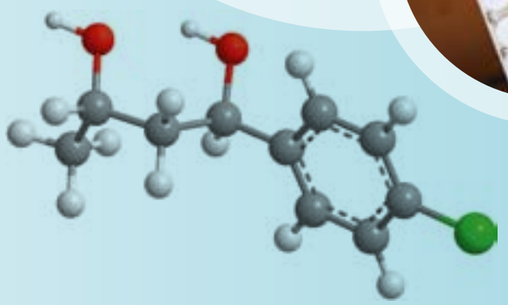
RESEARCH HIGHLIGHTS

In the research area of bioprocess development Gröger and his teams (in industry until 2006, and at the University of Erlangen-Nürnberg since 2006) developed successfully many new biocatalytic processes applying, e.g., innovative biocatalyst concepts. Notably, within these interdisciplinary projects jointly with collaboration partners several industrially applied processes have been realized. A particular highlight is the developed highly efficient asymmetric biocatalytic reduction and reductive amination technology based on the use of recombinant whole cell catalysts. Both types of processes run at high substrate loading of typically >100 g/L and give the desired products with >99 % ee. Recently, jointly with collaboration partners new biocatalytic processes have been developed based on the use of enoate reductases (for C= C-bond reduction) and L-threonine aldolases (for aldol reactions). A further research highlight is the successful development of various chemoenzymatic one-pot multi-step processes in water. Notably, "classic" chemical reactions, metal-catalyzed reactions and organocatalytic reactions, respectively, have been combined with enzymatic transformations, leading to the formation of the desired products in an efficient fashion and with excellent enantioselectivity. These research achievements underline that such combinations of the two "worlds of catalysis", chemocatalysis and biocatalysis, are possible, enabling advantageous synthetic processes, which avoid solvent-intensive and waste-generating process steps. Furthermore, we could successfully apply biocatalysts in the enantioselective (multi-step) synthesis of pharmaceutically relevant molecules. By means of different types of biotransformations as key steps, novel synthetic approaches towards non-natural α-amino acids, β-amino acid derivatives and specific chiral alcohols have been realized.

PERSPECTIVES

Among major challenges of our current and future work are the development of efficient biocatalytic oxidation and carbon-carbon bond forming processes as well as the expansion of the existing chemoenzymatic one-pot processes in water towards novel tandem processes and the combination of three or more synthetic steps including at least one biotransformation. In addition, expanding the range of chemocatalytic and biocatalytic reactions applicable for modular one-pot multi-step syntheses is a further goal. In the field of target driven synthesis, novel retrosynthetic approach towards pharmaceutically relevant molecules based on the use of enzymatic key steps, which fulfil the criteria of both high efficiency and sustainability, is a further challenge.





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- M. Kraußer, W. Hummel, H. Gröger, *Eur. J. Org. Chem.* **2007,** 5175 – 5179
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- H. Gröger, O. May, H. Hüsken, S. Georgeon, K. Drauz, K. Landfester, *Angew. Chem.* **2006,** 118, 1676 – 1679; *Angew. Chem. Int. Ed.* **2006,** 45, 1645 – 1648

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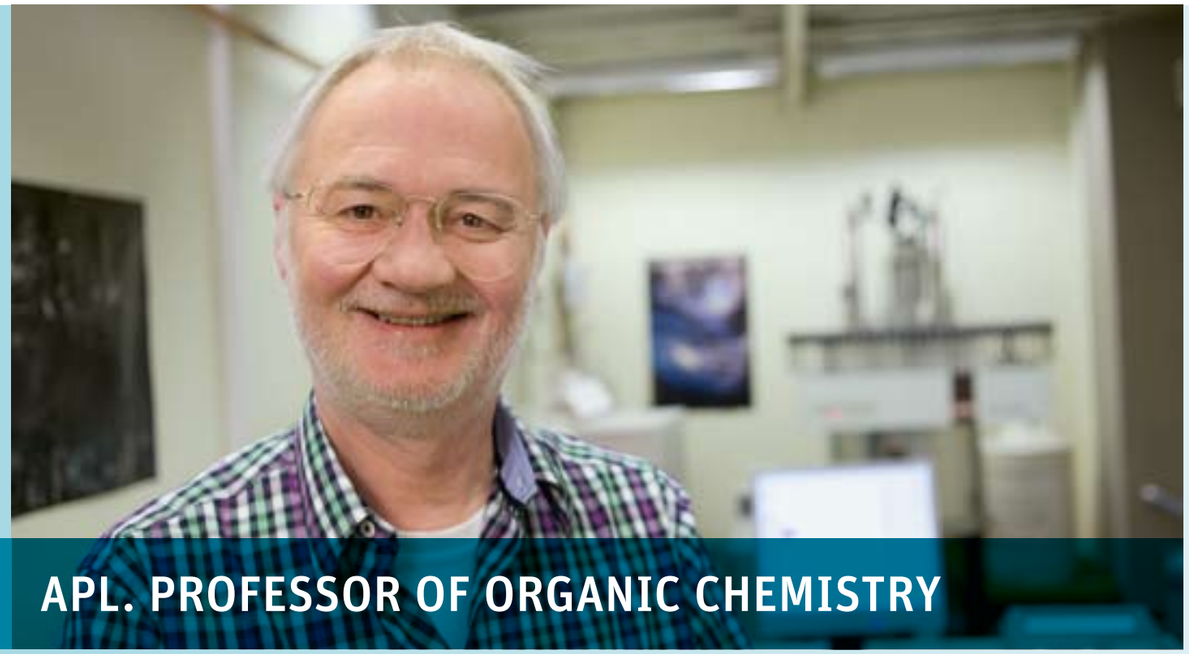
- H. Gröger, Enzyme-Catalyzed Asymmetric Synthesis, in: *Catalytic Asymmetric Synthesis* (Ed.: I. Ojima), 3. ed., John Wiley & Sons, Hoboken, New Jersey **2010,** chapter 6, 269 – 341
- H. Gröger, F. R. Dietz, Biocatalytic Synthesis of Natural and Non-Natural α-Amino Acids, in: *Wiley Encyclopedia of Chemical Biology* (Ed.: T. P. Begley), vol. 1, John Wiley & Sons, Hoboken **2009,** 191 – 204
- S. Buchholz, H. Gröger, Enantioselective Biocatalytic Reduction of Ketones for the Synthesis of Optically Active Alcohols, in: *Biocatalysis in the Pharmaceutical and Biotechnology Industries* (Hrsg.: R. N. Patel), CRC Press, New York **2006,** chapter 32, 757 – 790
- A. Berkessel, H. Gröger, *Asymmetric Organocatalysis,* Wiley-VCH, Weinheim **2005**

SELECTED AWARDS

- 2008 Carl-Duisberg-Memorial-Prize 2008 from the German Chemical Society (GDCh)
- 2007 Thieme-Journal Prize 2007
- 2005 Degussa Innovation Award 2005 in the Category "New or Improved Processes"
- 2005 Final Round at the "Innovation Award of the German Industry 2004"
- 2003 Degussa Innovation Award 2003 in the Category "New Products"
- 1997 Scholarship of the Japan Science and Technology Corporation (JST)
- 1996 Scholarship of the Heinz-Neumüller-Stiftung



APL. PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. WALTER BAUER

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CURRICULUM VITAE

Since 2006	Akademischer Direktor at the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
Since 2005	Director of the Mass Spectrometry Section of the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
Since 2003	ApI. Professor at the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
1995 – 2003	Privatdozent at the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
1994	Habilitation in Organic Chemistry, University of Erlangen-Nürnberg, Germany
1993	Akademischer Oberrat at the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
Since 1984	Director of the NMR Section of the Organic Chemistry division, University of Erlangen-Nürnberg, Germany
1983 – 1984	Postdoctoral Fellow at the ETH Zürich (Prof. Seebach), Switzerland
1982	PhD in Organic Chemistry at the University of Regensburg (Prof. Daub), Germany

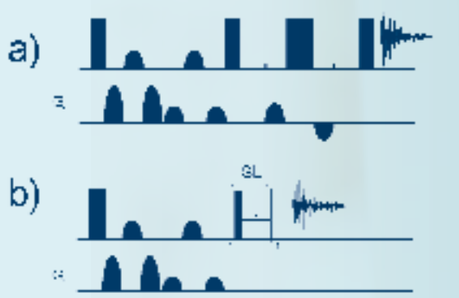
OBJECTIVES

NMR is one of the most versatile methods in structural analysis of organic compounds, indispensible in chemistry research. In the Erlangen Organic Chemistry division, a 500 MHz spectrometer is the instrument of choice for undertaking NMR studies which are more than routine. Here, applications are done which involve both own research as well as sophisticated analyses for research groups inside and outside the building. International cooperations open up new insights into unusual structures of various classes of compounds by simultaneous development of adequate new pulse sequences.

SCIENTIFIC BACKGROUND

The nuclear Overhauser effect (NOE) exploits spatial relationships of nuclei based on cross relaxation. Both homonuclear (e.g., $^{1}H,^{1}H$-NOESY) and heteronuclear (e.g., $^{1}H,^{31}P$; HOESY) variants may be applied. Inherently, the NOE is related to the inverse 6th power of the internuclear distances. Thus, the NOE offers a powerful tool for structural analysis of, e.g., proteins or organolithiums.

Diffusion ordered spectroscopy (DOSY) is a highly valuable tool for exploiting diffusion constants of unknown compounds. Thus, sizes of molecules may be determined and the aggregation behaviour of e.g. organolithiums may be studied in solution. Along with other analytical methods (X-ray, solid state NMR) similarities and differences in solution and in the solid state give interesting insights into organolithium structures.



RESEARCH HIGHLIGHTS

NOE methods based on pulsed field gradients and on gradient echoes (“excitation sculpting”) have become popular in recent years (DPFGSE-NOE). However, the well-known problem of “NOE zero-crossing” for $\omega\tau_c = 1.12$ still persists for DPFGSE-NOE. We have described the application of the rotating frame analogue, DPFGSE-ROE for such cases. The corresponding pulse sequences are shown in the figure above. By using DPFGSE-ROE, all direct NOEs are positive, irrespective of the molecular correlation time.

We have applied DPFGSE-ROE to a variety of organolithiums, calixarene inclusion compounds and other “normal” organic molecules. Though DPFGSE-ROE is inherently less sensitive than its analogue in the laboratory frame (DPFGSE-NOE), in the regime of the NOE zero crossing valuable insights have been gained. Typically, for small molecules this condition is met at low temperatures with accordingly long correlation times. Here, the rotating frame variant is the only method for the assignment of spatial relationships. In many cases, low temperatures must be maintained in order to avoid decomposition of organolithiums or to slow down dynamic processes within these compounds. For example, DPFGSE-ROE has been successfully applied for the assignment of diastereotopic protons, one of which is selectively metalated by treatment with n-butyllithium.

Solid state NMR is the link between X-ray structure analysis and solution state NMR. For cyclopentadienyl lithium (CpLi), a monomer-sandwich dimer equilibrium has been established in THF solution. However, we were able to show by NMR that CpLi is an endless polymer in the solid state. These results have been confirmed by simulations of the relevant carbon and lithium solid state NMR spectra, as well as by theoretical calculations.

PERSPECTIVES

A current DFG project is based on a continuation of the chemistry of retired Prof. Rolf W. Saalfrank. Many X-ray structures have been determined in Saalfrank’s group, involving multinuclear clusters with various metals. In solution, many of these compounds exhibit highly interesting dynamic phenomena. NMR is the ideal tool for the study of these processes. Thus, in combination with solid state NMR, the “static” crystal structures may be linked to structures in solution. First results have revealed very interesting exchange processes of cesium ions inside and outside a cluster. Moreover, exchange between contact ion paired cesium and cesium in solvent separated ion pairs are observed. By using ^{133}Cs, ^{1}H-HOESY, an assignment of the ^{133}Cs signals has been achieved for the first time. It is planned to further extend our heteronuclear NMR studies on the ^{133}Cs isotope. A number of papers related to this chemistry are listed below.

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- R. W. Saalfrank, N. Mooren, A. Scheurer, H. Maid, F. W. Heinemann, F. Hampel, W. Bauer, *Eur. J. Inorg. Chem.* **2007,** 4815 – 4822
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- J. Betz, F. Hampel, W. Bauer, *J. Chem. Soc., Dalton Trans.* **2001,** 12, 1876 – 1879
- C. Gaul, P. I. Arvidsson, W. Bauer, D. Seebach, *Chemistry Eur. J.* **2001,** 7, 4117 – 4125

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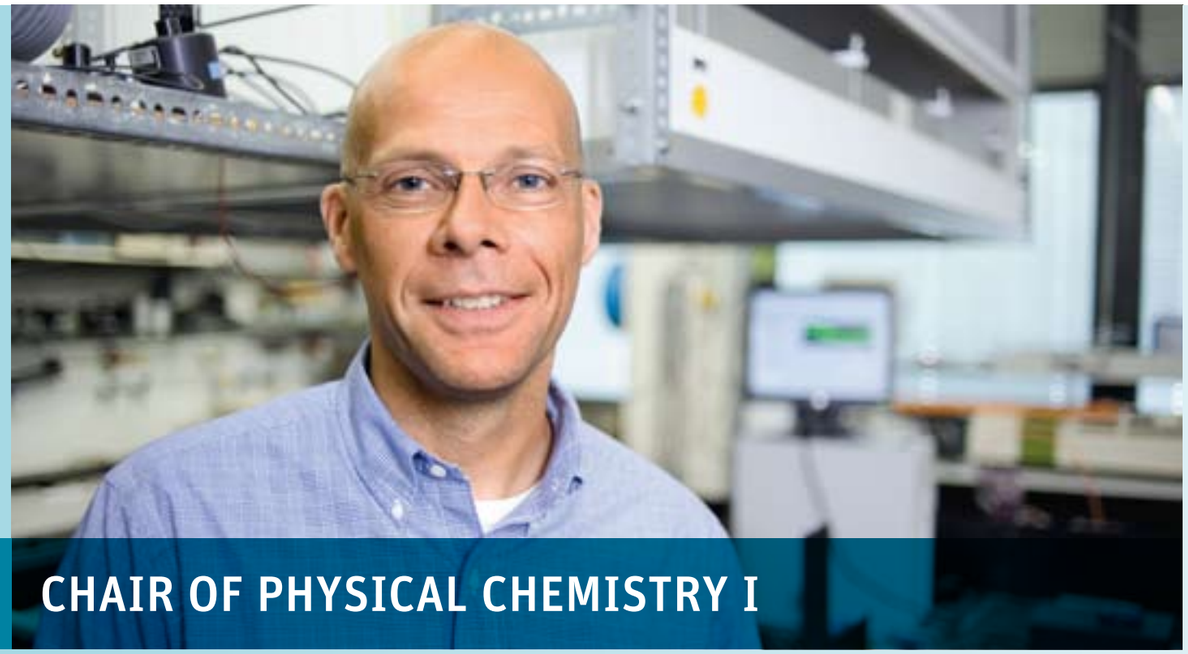
- W. Bauer, NMR of Organolithium Compounds: General Aspects and Application of Two-Dimensional Heteronuclear Overhauser Effect Spectroscopy (HOESY), in: A.-M. Sapse, P. v. R. Schleyer (Eds.), *Lithium Chemistry: A Theoretical and Experimental Overview* **1995,** 125 f
- W. Bauer, P. v. R. Schleyer, Recent Results in NMR Spectroscopy of Organolithium Compounds, in: V. Snieckus (Ed.), *Advances in Carbanion Chemistry* **1992,** vol. 1, Jai Press, Greenwich (Connecticut), 89

SELECTED AWARDS

- 1983 Dissertation prize, University of Regensburg, Germany



CHAIR OF PHYSICAL CHEMISTRY I

PROF. DR. DIRK M. GULDI

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CURRICULUM VITAE

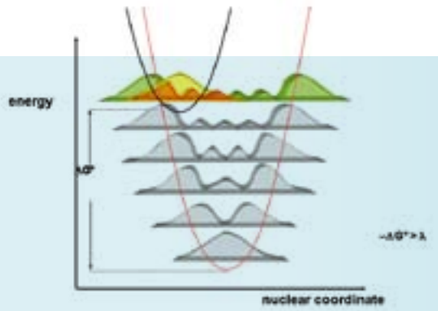
Since 2007	Head of Department, Department of Chemistry and Pharmacy at the University of Erlangen-Nürnberg, Germany
Since 2007	Distinguished Scientist in COE Program, Osaka University, Japan
Since 2004	University Full Professor, Chair of Physical Chemistry I at the University of Erlangen-Nürnberg, Germany
1995 – 2004	Faculty, University of Notre Dame, Radiation Laboratory, Notre Dame, USA
1992 – 1995	Researcher, Hahn-Meitner-Institute, Physical Chemistry, Berlin, Germany
1991 – 1992	Postdoctoral Fellow, National Institute of Standards & Technology, Gaithersburg, MD, USA
1988 – 1990	PhD, University of Köln, Germany

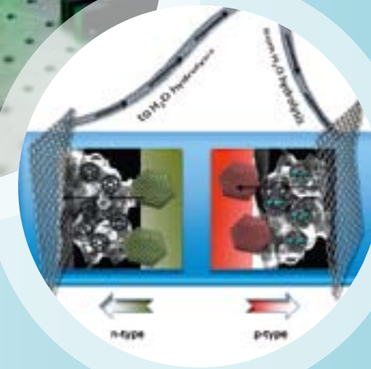
OBJECTIVES

The research activities of the Guldi group cover the timely topic of designing, devising, synthesizing, and testing novel nanometer scale structures as integrative components for solar energy conversion. Nanocarbon materials are at the forefront of our studies by probing them in solution, in transparent films and at electrode surfaces. Our experimental tools span from ultrafast spectroscopy and vibrational spectroscopy to electrochemistry and microscopy. Such conception is extremely valuable for the realization of solar energy conversion, photovoltaics, and catalytic reactivity, specifically to novel chemical and light driven systems.

SCIENTIFIC BACKGROUND

Dirk M. Guldi is one of the world-leading scientists – currently ranked No 63 in the scientist ranking in chemistry with an H-index > 60 – in the field of charge transfer/nanocarbons. In particular, he is well-known for his contributions to the areas of charge-separation in donor-acceptor materials and construction of nanostructured thin films for solar energy conversion. His scientific career has begun at the University of Köln, where he graduated in Chemistry (1988) and from where he received his PhD (1990). After a postdoctoral stay at the National Institute of Standards and Technology in Gaithersburg/USA (1991/1992), he took a position at the Hahn-Meitner-Institute Berlin (1992 – 1994). Following a brief stay as a Feodor-Lynen Fellow at Syracuse University/USA he joined the faculty of the Notre Dame Radiation Laboratory/USA (1995). Then, after nearly a decade in the USA, the University of Erlangen-Nürnberg succeeded in attracting Dirk M. Guldi back to Germany, despite major efforts by the University of Notre Dame (2004) and the University of Bowling Green (2005).





RESEARCH HIGHLIGHTS

A first highlight is that the Guldi group was among the first to demonstrate the outstanding electron acceptor properties of fullerenes in a set of donor-acceptor materials (*JACS* **1997**) that give rise to photoinduced charge transfer events. Almost simultaneously with this pioneering work, they illustrated (*JACS* **1997**) the beneficial features of fullerenes in artificial photosynthesis, that is, charge-recombination is located deep in the „inverted region" of the Marcus parabola (*JACS* **2006/2008**). This paved the way to their champion systems (*JACS* **2001/2004**), in which all the primary events of photosynthesis are successfully mimicked. Impressive are the lifetimes of the spatially-separated radical ion pair states, the product of a sequence of energy and multi-step charge transfer reactions, which reach 1.6 s – a time domain that has never been accomplished so far in a molecular mimic of the photosynthetic reaction center.

The incentives for their ground-breaking work on carbon nanotubes were taken from using them as a versatile platform for charge management, namely charge transfer, charge transport, and charge storage (*Nature* **2007)**. A first breakthrough in the field of functional carbon nanotubes (*Angewandte Chemie* **2003**/*Nature Chemistry* **2010**) was the manifestation of an intramolecular charge transfer event triggered by light, which led to radical ion pair lifetimes in the range of several µs. To this end, a tremendous challenge is the characterization of radical ion pair states that involve different redox states of carbon nanotubes. Here, the Guldi group was first to succeed in establishing conclusively the spectroscopic signatures of reduced (*JACS* **2007**) and oxidized forms (*Nature Chemistry* **2009**) of carbon nanotubes, which evolve from donor-acceptor interactions. The outstanding tensile strength of carbon nanotubes is also notable. They realized values of 220 ± 40 MPa in a revolutionary composite material (*Nature Materials* **2002**).

In general, the charge separation in any of the highlighted materials has a lifespan long enough to dissipate and then utilize the charge carriers. The Guldi group makes use of this and focuses on the systematic and molecularly controlled integration/organization of fullerenes (*Angewandte Chemie* **2000**) and carbon nanotubes (*Angewandte Chemie* **2005**) into photovoltaic devices, where again photoinduced charge transfer in the photoactive layers is the modus operandi. Key to accomplish device performances as remarkably high as >4 % are for the first time in situ measurements (*Nature Materials* **2009**). These allow charge carrier formation, geminate recombination, etc. to be visualized spectroscopically and kinetically.

PERSPECTIVES

The major thrust of current and future work addresses the expanding global need for energy by developing a groundbreaking platform of different forms of nanocarbons to produce chemical fuels using solar energy. To advance to such a level of sophistication, future research in our group centers on constructing all nanocarbon based optoelectronic devices that make use of the unique and outstanding features of carbon allotropes ranging from fullerenes and carbon nanotubes to carbon nanohorns and graphene, which will power the electrolytic formation of H_2 and its conversion into a portable fuel-formic acid.

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- A. A. Mamedov, N. A. Kotov, M. Prato, D. M. Guldi, J. P. Wicksted, A. Hirsch, *Nature Materials* **2002,** 1, 190 – 194

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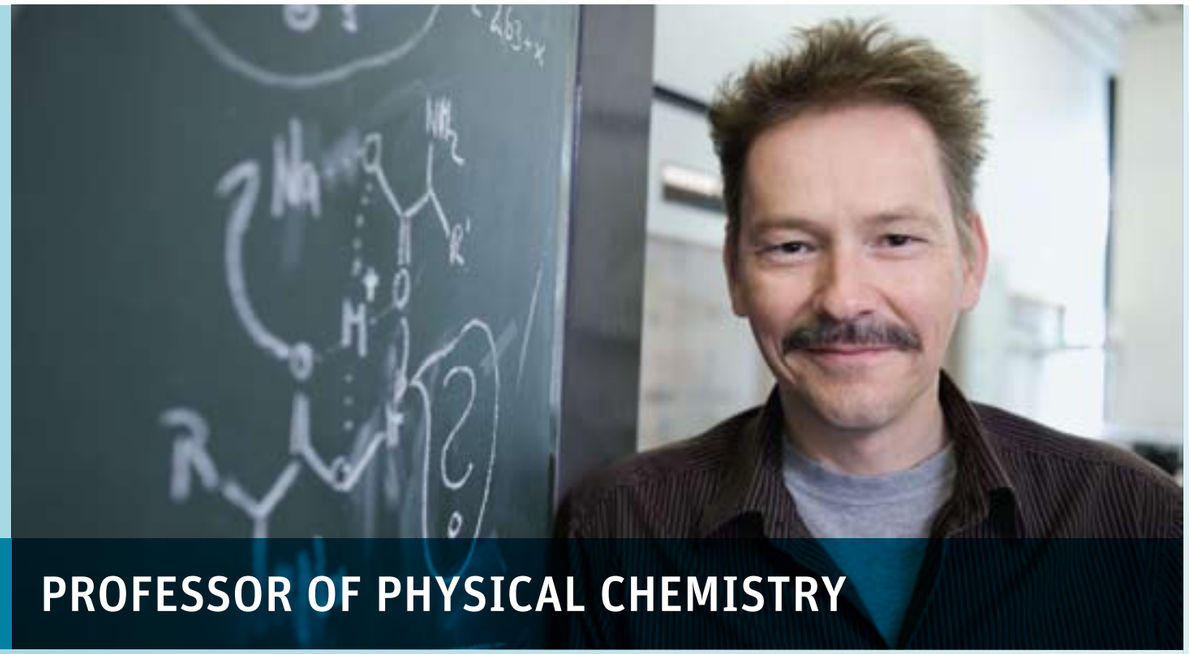
- G. Bottari, G. de la Torre, D. M. Guldi, T. Torres, Covalent and Noncovalent Phthalocyanine Carbon Nanostructure Systems: Synthesis, Photoinduced Electron Transfer, and Application to Molecular Photovoltaics, *Chem. Rev.* **2010,** DOI: 10.1021/cr900254z
- D. M. Guldi, G. M. A. Rahman, F. Zerbetto, M. Prato, Carbon Nanotubes: Electron Donor Acceptor Nanocomposites, *Acc. Chem. Res.* **2005,** 38, 871 – 878

SELECTED AWARDS

- 2009 Elhuyar-Goldschmidt Award (Spanish Chemical Society)
- 2004 JPP Award (Society of Porphyrins & Phthalocyanines)
- 2003 JSPS Award (Japan Society for the Promotion of Science)
- 2000 Grammaticakis-Neumann Prize (Swiss Society of Photochemistry)
- 1999 Heisenberg Prize (DFG)



PROFESSOR OF PHYSICAL CHEMISTRY

PROF. DR. THOMAS DREWELLO

drewello@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/drewello

CURRICULUM VITAE

Since 2008	University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1995 – 2007	Associate Professor at the University of Warwick, UK
1990 – 1995	Researcher, Hahn-Meitner-Institute, Berlin, Germany
1989 – 1990	Postdoctoral Fellow, University of Amsterdam, NL
1989	PhD, Technische Universität Berlin, Germany

OBJECTIVES

Research in this group is concerned with the development of mass spectrometry-based methods for the improved characterisation of modern materials. Investigations into the mechanisms of gentle ionisation methods such as (Matrix-assisted) laser desorption / ionisation [(MA)LDI] and Electrospray ionisation [ESI] are essential in this context. Of major interest is the behaviour of cluster ions in the gas phase, which involves the production, reactivity (kinetics) and thermochemistry of different kinds of clusters, ranging from the loosely bound van der Waals-type to strongly connected, covalent architectures. Modern mass spectrometry is developed and applied partly as an analytical tool and partly as a reaction vessel for the elucidation of geometries, energetics, and reactivities of gas phase species, aiming at the translation of these findings into the macroscopic world.

SCIENTIFIC BACKGROUND

Our research activities have always employed mass spectrometry as a tool in one form or another. Early investigations focussed on the use of large scale multi-sector instrumentation for the study of the fragmentation behaviour of organic and organometallic species. The emphasis in these studies was on the thermochemical requirements connected with the formation of multiply charged ions in the gas phase and on the elucidation of metal induced reactivity. We have been also involved in the application of synchrotron radiation to strictly single-photon-ionisation, studying inner shell excitation of different types of clusters and obtaining ionisation and appearance energies. The more recent activities focussed on reactivity studies of size-selected metal clusters with small molecules. For these investigations a metal cluster source was coupled with Fourier transform-ion cyclotron resonance (FT-ICR) mass spectrometry. We have, also, developed interest in the area of laser desorption ionisation both as an approach towards gentle ion formation and as a means to fuse and aggregate tailor-made precursors into larger architectures. Further recent interest is in mechanistic aspects of electrospray-based ionisation. Current instrumentation is mainly based on quadrupole, time-of-flight and ion trap technologies.

RESEARCH HIGHLIGHTS

Research in this group has a high collaborative component, which consequently extends to the resulting achievements. A main research focus in recent years was on the development of soft ionisation approaches for a meaningful analysis of derivatised fullerenes. The challenge here was to transfer a solid molecule which is clearly thermo-labile into the gas-phase and ionise it while preventing its dissociation during both processes. Key investigations along those lines concerned the observation that C_{60} degrades to $C_{120}O$ on standing (Taylor, Sussex), as well as the development of dissociation-free analyses of fluorinated fullerenes (Boltalina and Strauss, Fort Collins) and of organic fullerene derivatives (Hirsch, Erlangen and Orfanopoulos, Crete) by mass spectrometry.

The use of laser desorption as a tool for harsh activation led to the conversion of a $C_{60}H_{30}$, "PAH-like" non-fullerene precursor into the C_{60} fullerene (Scott, Boston), an observation which helped paving the way to the first rational synthesis of C_{60} by L.T. Scott and co-workers.

Jointly with several groups (Derrick, Warwick / Massey; Woodruff, Warwick; Mackenzie; Warwick / Oxford; Beyer, Munich / Kiel) we were involved in the creation of a laser ablation/expansion source for the efficient production of metal clusters in conjunction with FT-ICR MS which allowed the investigation into the reactivity of selected cluster ions with small molecules.

PERSPECTIVES

An exciting extension of our current activities lies in the area of what could be described more broadly as spectroscopy of ions. Radiation-induced decomposition of size-selected, stored ions can be applied as a powerful tool for structure elucidation and – depending on the quality of the light source – also as a means to obtain thermochemical quantities which would be difficult to establish otherwise.

The further development of soft ionisation methods for the sensitive and informative analysis of new materials continues to be a challenging task. For laser desorption-based methods "imaging" constitutes an important approach. For spray-based methods we see further challenges in the development of protocols towards the effective ion formation of compound classes that are inactive in spray ionisation. In this context, we lay emphasis on the qualitative and thermochemical elucidation of ion/neutral and supramolecular interactions.

Examples of materials under investigation include ligated and open-cage fullerenes, empty and metal-containing macrocycles, dendrimers, pure and modified graphene, ionic liquids and polyoxometalates.

Finally, extending our metal cluster research, future investigations will focus on the formation, characterisation and reactivity of noble metal clusters. Emphasis here will be for instance on the role of molecular additives influencing the cluster formation as (bio)organic mediator promoting cluster growth and as shell in monolayer-protected nanoparticles.

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- I. V. Kuvychko, A. V. Streletskii, N. B. Shustova, K. Seppelt, T. Drewello, A. A. Popov, S. H. Strauss, O. V. Boltalina, *J. Am. Chem. Soc.* **2010,** 132 (18), 6443 – 6462
- M. L. Anderson, A. Lacz, T. Drewello, P. J. Derrick, D. P. Woodruff, S. R. Mackenzie, *J. Chem. Phys.* **2009,**130 (6), 064305/1-064305/8
- M. D. Tzirakis, M. N. Alberti, L. C. Nye, T. Drewello, M. Orfanopoulos, *J. Org. Chem.* **2009,** 74 (15), 5746 – 5749
- C. Bruno, M. Marcaccio, D. Paolucci, C. Castellarin-Cudia, A. Goldoni, A. V. Streletskii, T. Drewello, S. Barison, A. Venturini, F. Zerbetto, F. Paolucci, *J. Am. Chem. Soc.* **2008,** 130 (12), 3788 – 3796
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SELECTED AWARDS

- 1988 "Mattauch-Herzog-Award" by the German Mass Spectrometry Society

PROFESSOR OF PHYSICAL CHEMISTRY

PROF. DR. CAROLA KRYSCHI

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CURRICULUM VITAE

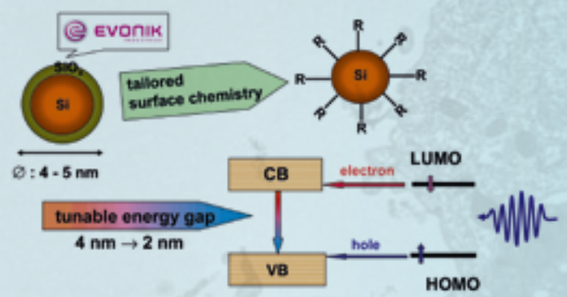
Since 2000	University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1994 – 2000	Assistant Professor, Department of Experimental Physics (Solid-State Spectroscopy) at the University of Düsseldorf, Germany
1993	Habilitation in Experimental Physics: “Relaxation Dynamics in Molecular Crystals”
1988 – 1993	Assistant lecturer at the Department of Experimental Physics, University of Düsseldorf, Germany
1987	Postdoctoral Fellow, Department of Chemistry at Stanford University, USA
1983 – 1986	PhD, Institute of Physical Chemistry at the University of Düsseldorf, Germany

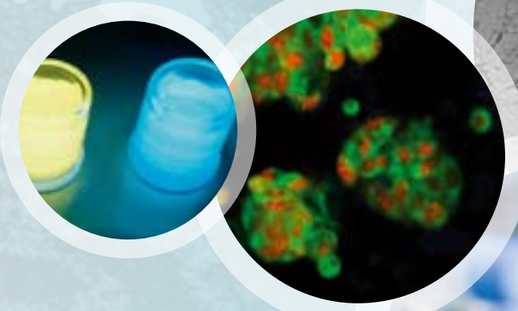
OBJECTIVES

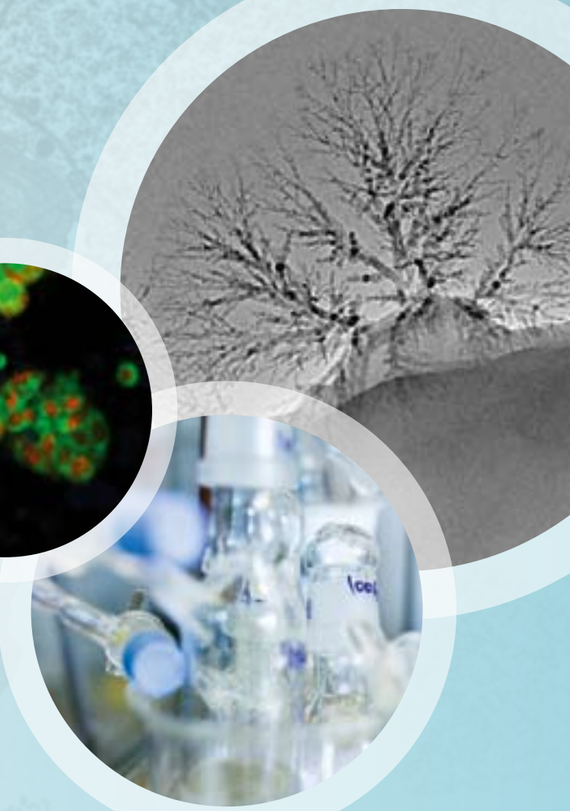
Current and future research activities focus on advanced nonlinear spectroscopic methods and are directed to engineering of functionalized luminescent silicon quantum dots for optoelectronic applications, surface-stabilized metal nanoparticles for catalysis and superparamagnetic iron oxide nanoparticles as transfection reagent for gene therapies.

SCIENTIFIC BACKGROUND

Carola Kryschi started her scientific career in 1987 with a postdoctoral stay at Stanford University/USA (1987) where she achieved expertise on ultrafast laser spectroscopy techniques. Starting 1988 as assistant lecturer and continuing after postdoctoral lecture qualification (1993) as Assistant Professor at the Department of Experimental Physics of the University of Düsseldorf she focussed her research activities on studies of ultrafast excited-states relaxation dynamics, tautomerization reactions and phase transitions in molecular crystals and thin polymer films using ps resolving transient grating and photon echo spectroscopy. In cooperation with Prof. H.-D. Martin (University of Düsseldorf) and Prof. H.-P. Trommsdorff (UJF Grenoble) she successfully carried out a research project on optical switches in liquid and solid phase which are based on photochromic dithienylethene compounds. Another cooperation project with H.-D. Martin resulted into the successful realization of nonlinear optical probes based on hemicyanine dyes which provide direct detection of cell membrane potential changes in living cells. Since 2000 Ms Kryschi is Professor of Physical Chemistry at the University of Erlangen-Nürnberg.







RESEARCH HIGHLIGHTS

Site configurations of tetracene and terrylene guests in p-terphenyl crystals were completely elucidated employing optical high-resolution spectroscopy and molecular packing & dynamics computations. Tetracene was shown to decorate domain walls in the triclinic structure and the guest-site spectra were successfully used to probe the triclinic to monoclinic phase transition (*CPL* **1994,** 227, 13).

Another research highlight was the successful realization of molecular optical switches built on dithienylethene which reversibly operate on the picosecond scale by switching between a transparent and coloured state as well as allow switching on and off the emission of an attached fluorophore (*JPC* **2001**).

In cooperation with Evonik Industries AG we developed a two-step procedure enabling for the first time the fabrication of surface stabilized, oxide-free luminescent silicon quantum dots (EP 2 067743 A1) which were shown to function as transfection reagent for siRNA (BBRC 2009) that initiated RNAi mediated specific gene suppression.

PERSPECTIVES

Our future research is focused on functionalized metal, metal oxide and semiconductor nanoparticles (quantum dots) tailored for catalysis, optoelectronic, or medical application. We will develop functionalized luminescent silicon quantum dots with adjustable sizes and defined surface structures which are processible for optoelectronic applications. The other research objectives are targeted to the processing of noble-metal nanoparticle colloids that catalyze chemical reactions in liquid phase and superparamagnetic ultra-small iron oxide nanoparticles suited for magnetic-field directed transport of cytostatic drugs or siRNA into tumor cells.

SELECTED PUBLICATIONS

- A. Ebbers, C. Kryschi, C. Cimpean, V. Kuntermann, **2009,** EP 2 067743 A1
- S. Klein, O. Zolk, M. F. Fromm, F. Schrödl, W. Neuhuber, C. Kryschi, *Biochemical and Biophysical Research Communications* **2009,** 387, 164 – 168
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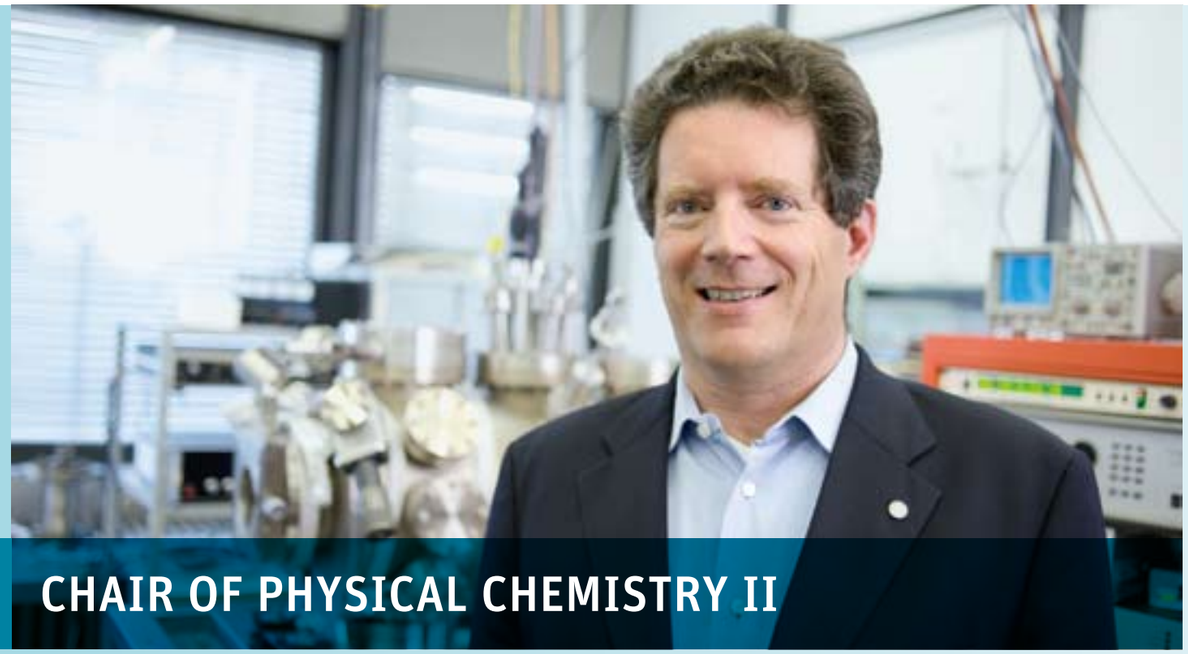
- V. Kuntermann, C. Cimpean, G. Brehm, G. Sauer, C. Kryschi, H. Wiggers, *Phys. Rev.* **2008,** B 77, 115343 – 115343
- A. Bock, D. Schmid, C. Kryschi, *J. Chem. Phys.* **1999,** 111, 1185 – 1190.

SELECTED REVIEWS

- C. Cimpean, V. Groenewegen, V. Kuntermann, A. Sommer, C. Kryschi, Ultrafast Exciton Relaxation Dynamics in Silicon Quantum Dots, *Laser & Photon. Rev.* **2009,** 1

SELECTED AWARDS

- 1989 Benningsen-Foerder (NRW) Award



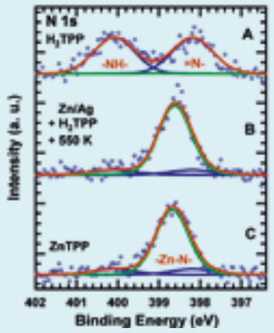
CHAIR OF PHYSICAL CHEMISTRY II

PROF. DR. HANS-PETER STEINRÜCK

steinrueck@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/steinrueck

CURRICULUM VITAE

Since 2006	Vicepresident of the University of Erlangen-Nürnberg, Germany
Since 1998	University Full Professor, Chair of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1994 – 1998	Associate Professor of Experimental Physics at the University of Würzburg, Germany
1993	Visiting Scientist at Rutgers University, USA
1992	Habilitation in Experimental Physics (Dr.rer.nat.habil.)
1986 – 1994	Assistant at Technische Universität München (TUM), Germany
1985 – 1986	Postdoctoral Fellow at Stanford University, USA
1985	PhD (Dr. techn.) at Graz University of Technology, Austria
1983	Diploma in Technical Physics (Dipl.-Ing.) at Graz University of Technology, Austria

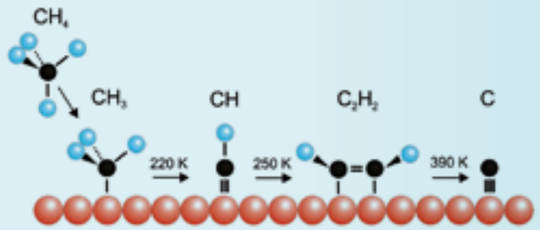


OBJECTIVES

The mission of the Chair of Physical Chemistry II is to provide an optimum of environment to perform surface and interface science at the highest possible level and to create an attractive and international competitive atmosphere for researchers at all stages of their career, from B.Sc., M.Sc. and PhD students to postdocs and junior group leaders. The research activities follow an interdisciplinary approach with numerous local, national and international cooperations with colleagues in physics, chemistry, chemical engineering, and materials science, which are documented in collaborative research projects and publications. Specific emphasis lays, also, on the education of undergraduate students, on lectures, seminars and lab-courses.

SCIENTIFIC BACKGROUND

Surfaces are the outer boundary of any condensed material. They dominate the interaction with the environment and play a decisive role in numerous natural and technological processes, ranging from heterogeneous catalysis, sensor technology and nanotechnology to modern material science. Our activities focus in the area of surface and interface science with main research interests in: 1) Development of new materials with novel electronic, geometric and chemical properties, 2) Investigation of elementary steps of surface reactions and 3) Construction of advanced scientific apparatus. These studies aim at a fundamental physical and chemical understanding of the mechanisms and processes involved, at an atomic level. For these investigations a large variety of



experimental methods is applied, including synchrotron radiation-based photoelectron spectroscopy, scanning electron and scanning tunneling microscopy, and molecular beam methods.

RESEARCH HIGHLIGHTS

Our activities cover a number of different highlight topics: *"Surface Science with porphyrins"* pays specific attention to the synthesis of metallo-porphyrinoids by in situ metallation on a surface, their formation of supramolecular networks, their internal conformation, their electronic interaction with metal substrates and the adsorption of small molecules at their metal center. *"Surface Science with Ionic Liquids"* addresses the systematic study of their surface composition, of enrichment effects and the chemical reactivity of dissolved transition metal complexes. Our *"In situ studies of surface reactions"* aim at the investigation of processes in situ on timescales down to 1 sec by high-resolution XPS or at pressures up to 1 mbar. *"Electron beam induced deposition (EBID)"* of precursor molecules allows to fabricate ultra-clean metal and oxide nanostructures of an arbitrary shape. By *"Nanocalorimetry"* the adsorption enthalpy of irreversibly adsorbing species (metals on polymers or organic molecules) is determined; presently a new nanocalorimeter is built. *"Catalysis with nanosize gold"* addresses the question of the active site in gold catalysis. And finally, *"Ultrathin metal, alloy and oxide films"* deal with the preparation of such systems and the systematic variation of their electronic, geometric, and chemical properties.

PERSPECTIVES

Based on the achieved detailed understanding for simple model systems one of our future goals is to address more complex systems to bridge different gaps, which are present challenges in the science of solid/gas, liquid/gas and solid/liquid interfaces. The *"pressure gap"* concerns model conditions in ultrahigh vacuum systems vs. real world catalysis, the *"materials gap"* defect free single crystal surfaces vs. nanoparticles with facets, kinks and steps, and finally the *"communication gap"* stands for the difficulties one faces when new interdisciplinary collaborations are initiated. In addition, one major driving force is to continue our thorough investigations at the highest experimental level to obtain insight in the fundamental aspects of physical and chemical processes occurring at the surfaces of solids and liquids.

SELECTED PUBLICATIONS

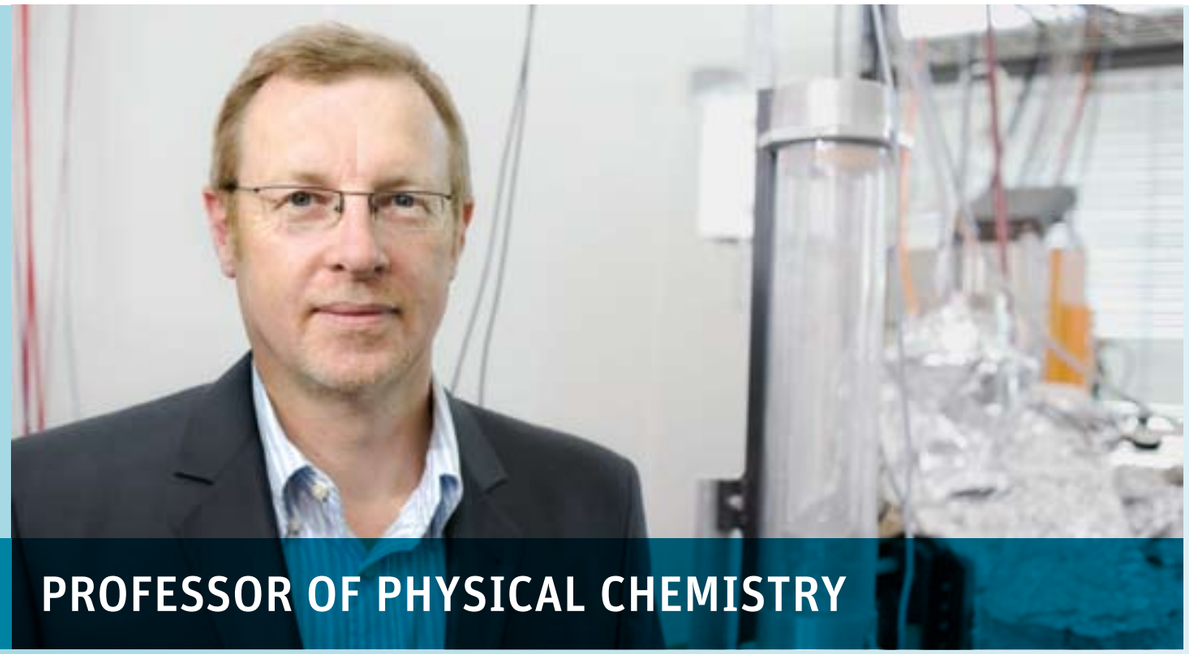
- M.-M. Walz, M. Schirmer, F. Vollnhals, T. Lukasczyk, H.-P. Steinrück, H. Marbach, *Angew. Chem. Int. Ed.* **2010,** 49, 4669 – 4673
- R. Streber, C. Papp, M. P. A. Lorenz, A. Bayer, R. Denecke, H.-P. Steinrück, *Angew. Chem. Int. Ed.* **2009,** 48, 9743 – 9746
- F. Buchner, K. Seufert, W. Auwärter, D. Heim, J. V. Barth, K. Flechtner, J. M. Gottfried, H.-P. Steinrück, H. Marbach, *ACS Nano* **2009,** 3, 1789 – 1794
- K. Flechtner, A. Kretschmann, H.-P. Steinrück, J. M. Gottfried, *J. Am. Chem. Soc.* **2007,** 129, 12110 – 12111
- F. Maier, J.M. Gottfried, J. Rossa, D. Gerhard, P. S. Schulz, P. Wasserscheid, H.-P. Steinrück, *Angew. Chem. Int. Ed.* **2006,** 45, 7778 – 7780
- J. M. Gottfried, K. Flechtner, A. Kretschmann, T. Lukasczyk, H.-P. Steinrück, *J. Am. Chem. Soc.* **2006,** 128, 5644 – 5645

SELECTED REVIEWS

- K. R. J. Lovelock, I. J. Villar-García, F. Maier, H.-P. Steinrück, P. Licence, Photoelectron Spectroscopy of Ionic Liquid Based Interfaces, *Chem. Rev.,* DOI: 10.1021/cr100114t
- H.-P. Steinrück, Surface Science goes liquid! *Surf. Sci.* **2010,** 604, 481 – 485
- G. Held, H.-P. Steinrück, Cyclic hydrocarbons, in: Landolt-Börnstein, *Physics of Covered Solid Surfaces – Adsorbed Layers on Surfaces* **2005,** Vol. III/42, Subvolume A4, 300 – 369
- H.-P. Steinrück, Angle-resolved photoemission studies of adsorbed hydrocarbons, *Journal of Physics: Condens. Matter* **1996,** 8, 6465 – 6509

SELECTED AWARDS

- Since 2009 Guest Professor, University of Science and Technology of China (USTC), Hefei, China
- 1985 "KOHLRAUSCH"-Prize of the Austrian Physical Society



PROFESSOR OF PHYSICAL CHEMISTRY

PROF. DR. RAINER FINK

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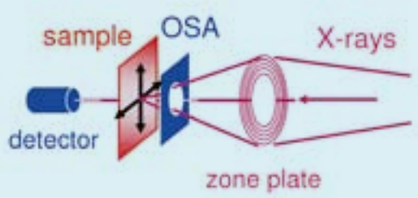
CURRICULUM VITAE

Since 2002	University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1993 – 2002	Researcher at the University of Würzburg (Prof. Umbach), Germany
1992 – 1993	Postdoctoral Fellow, Uppsala Universitet, Sweden
1992	PhD in Experimental Physics at the University of Konstanz (Prof. Schatz), Germany



OBJECTIVES

We aim for the spectroscopic and microscopic characterization of organic nanostructures and thin films mainly using X-ray based analytical tools. The understanding of structure-property relationships is essential to improve organic electronic devices. High-resolution electron spectroscopy and X-ray microscopy shall offer insight into the electronic properties, electronic excitations, intra- and intermolecular interactions in controlled organic structures, hybrid materials and molecular magnets.

SCIENTIFIC BACKGROUND

Ultrathin organics are widely used in various fields, from, e.g., protective polymer films to active layers in organic electronic devices. Their electronic properties largely depend on their structure which may be controlled by growth conditions or the underlying substrate material. We have explored the fundamental growth properties of organic thin films and their electronic structure from the submonolayer regime to thicker films. The impact of intermolecular interactions and the coupling to metal substrates has been studied in detail. In particular, the initial growth process controls the formation of microcrystalline domains. Using surface-sensitive high-resolution spectromicroscopy, the influence of surface defects like e.g. step edges could be explored. High-resolution NEXAFS spectroscopy offers detailed insight into the intramolecular excitation and electronic relaxation effects when comparing the condensed and gas phases. In favourable cases, the coupling of electronic excitations to vibronic modes can be monitored. Thus, structure-property relationships become directly accessible. Present soft X-ray microspectroscopes combine the superior spectroscopic fingerprint behaviour of NEXAFS with ultimate spatial resolutions and offer the chance to investigate more complex structures like multinary materials, polymer blends or hybrid materials.

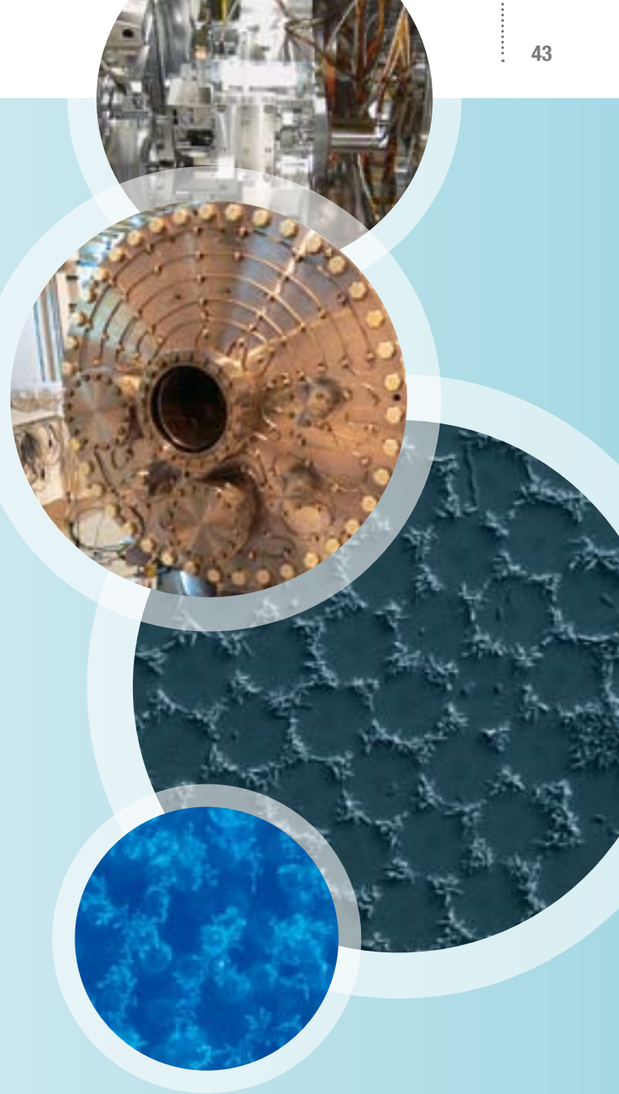
RESEARCH HIGHLIGHTS

During recent experiments in thin film analysis we were able to explore an unusual structural phase transition: upon cooling below a critical temperature of about 160 K, NTCDA monolayers adsorbed on Ag(111) undergo a reversible order-disorder phase transition, i.e., a disordered low-temperature state forms in contrast to conventional phase transitions. This phenomenon is called an inverse-melting process. Inverse melting has so far only been observed in few materials when applying high external pressure. In our case, sufficiently strong interaction of the adsorbed molecules with the underlying surface is considered to induce lateral pressure within the organic film. Thus, the delicate balance of lateral and vertical forces can no longer stabilize the ordered phase.

Using scanning X-ray transmission microspectroscopy (STXM) a variety of different topics have been addressed and studied in detail. E.g., in microparticles stabilized by a polyvinyle alcohol network may serve as gas micro-containers with potential applications in medical analysis and drug delivery. STXM could offer direct insight into the microbubbles to proof the gas enclosure. In some cases we were able to monitor the chemical changes within the shell thus enabling gas permeation. Microspectroscopic thin film analysis focuses on the investigation of functional organic materials like e.g. pentacene-based organic field effect transistors. Using the local NEXAFS probe we were able to monitor the electronic structure within the active area while the OFET is operated.

PERSPECTIVES

There are few ongoing technological developments to improve the resolution in X-ray microspectroscopy. Besides improvements in zone plate technology to produce smaller foci in conventional STXM analysis, lensless imaging is becoming an important tool. Implementation of such techniques into existing zone-plate scanning microscopes will provide access to the phase thus allowing more evolved image reconstruction techniques (ptychography). Aberration-free imaging and improved spatial resolutions may then become available. In addition, modifications of the sample surroundings will offer potential new applications in X-ray microspectroscopy, like, e.g., imaging of biological samples in their natural state without staining or specific sample preparations. Organic thin films and their self-organization mechanism and applications in molecule-based electronics will become another important field in future research studies. The spin of electrons is becoming more important in device technology. Sufficiently strong spin interactions in metalloorganic substances offer large potential in spin-based electronics in case of band transport mechanisms. We aim to employ circular X-ray magnetic dichroism microscopy to study the electronic and spin properties of nanocrystalline samples of such materials. The experiments shall be extended to the ultra-low temperature regime (< 100 mK) to explore correlation phenomena.

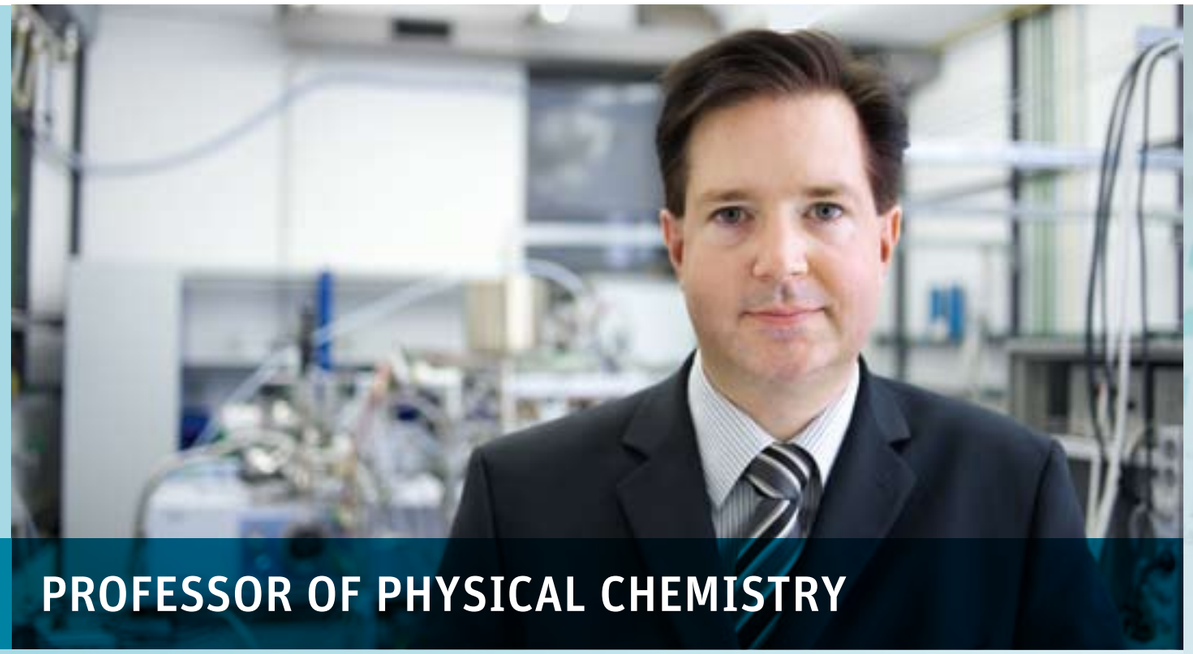


SELECTED PUBLICATIONS

- A. Schöll, L. Kilian, Y. Zou, J. Ziroff, S. Hame, F. Reinert, E. Umbach, R. H. Fink, *Science* **2010,** 329, 303 – 305
- C. Hub, M. Burkhardt, M. Halik, G. Tzvetkov, R. Fink, *J. Mat. Chem.* **2010,** 20, 4884 – 4887
- G. Tzvetkov, P. Fernandes, A. Fery, F. Cavalieri, G. Paradossi, R. Fink, *Soft Matter* **2008,** 4, 510 – 514
- Y. Zou, L. Kilian, A. Schöll, Th. Schmidt, R. Fink, E. Umbach, *Surf. Sci.* **2006,** 600, 1240 – 1251
- D. Hübner, F. Holch, M. L. M. Rocco, K. C. Prince, S. Stranges, A. Schöll, E. Umbach, R. Fink, *Chem. Phys. Lett.* **2005,** 415, 188 – 192
- A. Schöll, Y. Zou, L. Kilian, D. Hübner, D. Gador, C. Jung, S. G. Urquhart, Th. Schmidt, R. Fink, E. Umbach, *Phys. Rev. Lett.* **2004,** 93 (14) 146406

SELECTED REVIEWS

- R. Fink, Chr. Hub, G. Tzvetkov, Zone-plate based nanospectroscopy with soft x-rays at the SLS, *Acta Physica Polonica* **2009,** A 115, 462 – 466
- J. Raabe, R. Fink, G. Tzvetkov, U. Flechsig, M. Böge, A. Jaggi, B. Sarafimov, C. Quitmann, M. Heuberger-Vernooij, T. Huthwelker, H. Ade, D. Kilcoyne, T. Tyliszczak, PolLux: A new Beamline for Soft X-Ray Spectromicroscopy at the SLS, *Rev. Sci. Instrum.* **2008,** 79, 113704



PROFESSOR OF PHYSICAL CHEMISTRY

PROF. DR. JÖRG LIBUDA

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CURRICULUM VITAE

Since 2005	University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1996 – 2005	Group Leader, Dept. of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft (MPG), Berlin, Germany
2003	Habilitation, Humboldt University of Berlin, Germany
1998 – 1999	Postdoctoral Fellow, Dept. of Chemistry, Princeton University, USA
1996	PhD, Ruhr-University Bochum, Germany

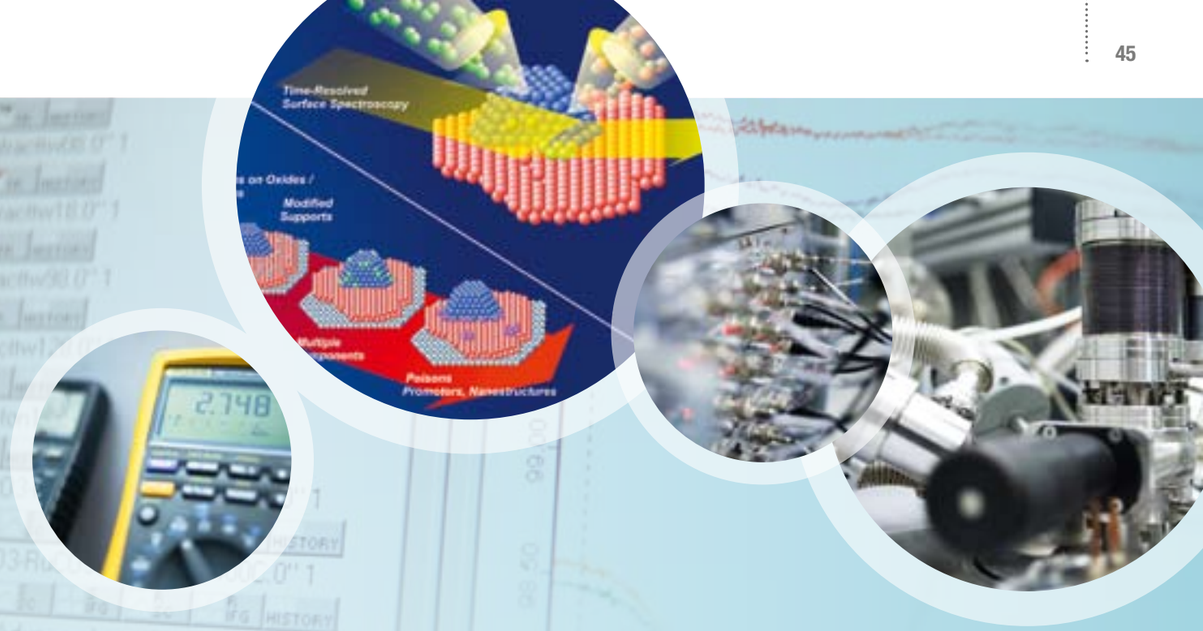
OBJECTIVES

Chemical reactions and physical processes at complex surfaces play a pivotal role in many areas of today's technology. Towards a better understanding of the underlying physical and chemical phenomena at the microscopic level, we develop and investigate complex nanostructured model surfaces. Mechanisms, dynamics, and kinetics of chemical reactions on these models are probed using time-resolved in situ und operando spectroscopies from ultrahigh vacuum up to atmospheric pressure conditions. Thus, our work aims at linking fundamental surface science approaches to applied research.

SCIENTIFIC BACKGROUND

Heterogeneous catalysis, environmental and energy technology, materials science and nanotechnology: these are only few examples of central areas of 21st century technology, where surface and interface reactions play a key role. A brief look at current research on related processes reveals, however, a quite surprising fact: The underlying chemistry is only poorly understood in most cases. This lack of knowledge is not just disappointing from a purely academic point of view. In fact, it also prevents any rational improvement and development in the corresponding fields.

The reasons for the limited insight into 'real life' surface and interface reactions become obvious if we have a closer look at the related chemical systems and environments. As an example, let us focus on the field of heterogeneous catalysis. Catalyst materials are highly complex multi-component mixtures, with chemical properties sensitively depending on their particular nanostructure and composition. In catalyst development, these dependencies are vital, as they allow empirical optimization of catalytic performance. From a fundamental research point of view, however, the materials' complexity is fatal with respect to a microscopic level understanding. Here, our strategy relies on the development of model systems, which allow us to simulate certain complex features of real systems under well-controlled conditions, simultaneously providing a maximum of structural and chemical control. Mechanistic and kinetic information is obtained on these model systems using state-of-the-art surface spectroscopies. This information can then be transferred to the real world application, where it may potentially inspire future improvements.



RESEARCH HIGHLIGHTS

All current projects of our research group are embedded into interdisciplinary cooperations with research groups in chemistry, physics, theory, materials science, chemical engineering, or industry. In a recent project in environmental catalysis we have, for example, investigated the reaction mechanisms involved in the trapping and release of NO_x on so-called nitrogen storage and reduction catalysts (NSR catalysts). Currently, we study CO_2 and methane activation on ceria based model catalysts. Here, we use not only in-house experiments, such as molecular beam techniques and time-resolved surface IR spectroscopy, but also synchrotron-radiation based methods. Strong activities have been developed within the Excellence Cluster Engineering of Advanced Materials. Herein, the focus is on the development of completely novel classes of model systems. For example, we explore the development of ionic liquid film based model catalysts, based on a surface-science type of approach. Such systems may provide insights into the interface properties and the surface reactions occurring in ionic liquid films at an unprecedented level of detail. A second strategy currently explored relies on the use on nanoporous oxide films such as titania nanotubes. Such surfaces can be used as model supports for catalytically active metal particles, providing access to novel catalysts and model catalysts with designable transport properties.

PERSPECTIVES

The group is involved in several new activities, most of them emerging at the interface between fundamental science and engineering. For example, new facilities for time-resolved in situ and operando spectroscopies are currently being set up within the Excellence Cluster Engineering of Advanced Materials. The idea of these so-called operando methods is to combine measurements of catalytic activity with spectroscopic data on the catalyst obtained at the same time. Within the excellence cluster such measurements will be performed not only on real catalysts but also on model catalysts, using the same class of spectroscopy. In a unique fashion, this approach will allow us to directly link scientific results obtained via the model-surface-approach with the real-life catalyst. Thus, the often-cited gaps between the model studies and applied research will be closed.

SELECTED PUBLICATIONS

- M. Sobota, X. Wang, M. Fekete, M. Happel, K. Meyer, P. Wasserscheid, M. Laurin, J. Libuda, *ChemPhysChem* **2010,** 8, 1632 – 1636
- Y. Lykhach, T. Staudt, M. P. A. Lorenz, R. Streber, A. Bayer, H.-P. Steinrück, J. Libuda, *ChemPhysChem* **2010,** 11, 1496 – 1504.
- A. Desikusumastuti, T. Staudt, M. Happel, M. Laurin, J. Libuda, *J. Catal.* **2008,** 260, 315 – 328
- M. Bäumer, H.-J. Freund, J. Libuda, K. M. Neyman, N. Rösch, G. Rupprechter, *Phys. Chem. Chem. Phys.* **2007,** 9, 3541 – 3558
- T. Schalow, B. Brandt, D. E. Starr, M. Laurin, Sh. K. Shaikhutdivov, S. Schauermann, J. Libuda, H.-J. Freund, *Angew. Chem. Int. Ed.* **2006,** 45, 3693 – 3697
- M. Laurin, V. Johanek, A. W. Grant, B. Kasemo, J. Libuda, H.-J. Freund, *J. Chem. Phys.* **2005,** 123, 054701

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- J. Libuda, Molecular Beam Experiments on Model Catalysts: Activity and Selectivity of Specific Reactive Sites on Supported Nanoparticles, *ChemPhysChem* **2004,** 5, 625 – 631
- J. Libuda, H.-J. Freund, Molecular Beam Experiments on Model Catalysts, *Surf. Sci. Reports* **2005,** 57, 157 – 298

SELECTED AWARDS

- Fellow and Referee "Studienstiftung des Deutschen Volkes"
- 1996 Otto-Hahn-Medaille, Max-Planck-Gesellschaft (MPG)

CHAIR OF THEORETICAL CHEMISTRY

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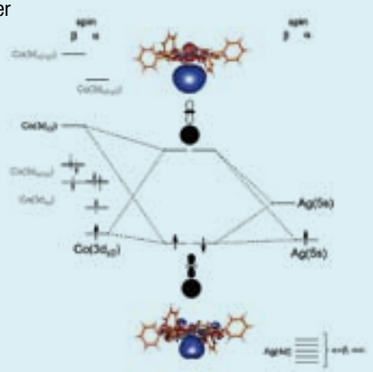
CURRICULUM VITAE

Since 2004	University Full Professor of Theoretical Chemistry and Director of the Computer Chemistry Center (CCC) at the University of Erlangen-Nürnberg, Germany
2003 – 2004	University Professor of Theoretical Chemistry, University of Bonn, Germany
2001 – 2003	Priv. Doz. at the Chair of Theoretical Chemistry, Technische Universität München, Germany
1995 – 2000	Heisenberg Scholar of the Deutsche Forschungsgemeinschaft (DFG), Technische Universität München, Germany
1993 – 1995	Habilitation Scholar of the DFG, Technische Universität München and Tulane University, New Orleans, USA
1991 – 1992	Postdoctoral Fellow, Tulane University, New Orleans, USA
1990	PhD in Chemistry, Technische Universität München (Prof. Rösch), Germany
1986	Diploma in Chemistry, Technische Universität München, Germany



OBJECTIVES

The main topic of the research group of Andreas Görling is the development and application of electronic structure methods to describe structural, electronic, and optical properties of molecules, clusters, surfaces, and solids as well as their reactivity. The focus lies on methods based on density-functional theory both within quantum chemistry and solid state physics. The main goal is the development of generally applicable, efficient methods and their application in close collaboration with experimental groups active in preparative chemistry, spectroscopy, catalysis, surface science, and materials science.

SCIENTIFIC BACKGROUND

Chemistry traditionally has been a science dominated by experiment. However, over the last three decades theory has strongly gained in importance within chemistry. Nowadays it is becoming more and more the rule that articles in originally experimentally oriented chemical journals contain besides experimental results also a section on computations accompanying the experimental work. Also in solid state physics, where theory traditionally plays an important role, the calculation of material properties shows increasing impact. The growing importance of electronic structure calculations results both from the availability of faster and faster computers and the development of more and more powerful electronic structure methods, in particular methods based on or related to density-functional theory. The history of the group of Andreas Görling has to be seen in this context. About ten to five years ago the research activities focused for the most part on the development of formal theory and new methods, including the implementation of the latter. After moving to Erlangen the group grew strongly and the range of activities widened significantly. Now more than half of the group is concerned with applications of various electronic structure methods in joint projects with experimental groups.

A characteristic of the group is that the scientific activities range from “paper and pencil” theory over the development and implementation of electronic structure methods to close collaborations with experimental partners.

RESEARCH HIGHLIGHTS

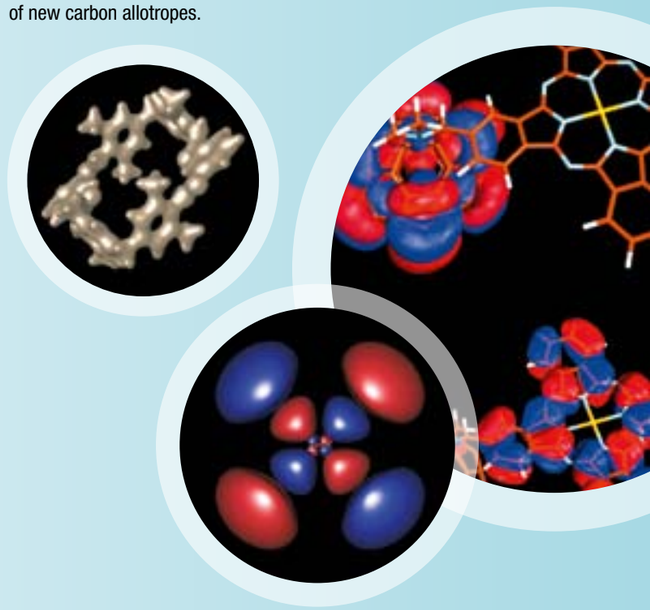
In recent years new density-functional methods employing orbital-dependent functionals were developed. These methods in contrast to conventional density-functional methods do not suffer from shortcomings like the occurrence of unphysical self-interactions and therefore lead to improved band structures in solids and qualitatively correct orbital and eigenvalues spectra in molecules that correspond to the chemical intuition, i.e., contain well-defined bonding and antibonding orbitals or Rydberg series. Density-functional methods with new orbital-dependent correlation functionals are able to treat Van-der-Waals interactions. Within time-dependent density-functional theory new methods that are able to treat charge-transfer excitations were proposed. New magnetization-current density-functional methods enable a unified treatment of magnetic effects, spin-orbit interactions, and noncolinear spin.

Some recent examples of applications in collaboration with experimental groups here in Erlangen comprise the investigation of voltage-dependent chemical fingerprints of adsorbed metallo-porphyrins in scanning tunneling microscopy (STM) together with the group of Hans-Peter Steinrück of Physical Chemistry. Also in collaboration with Physical Chemistry, the groups of Jörg Libuda and Hans-Peter Steinrück, it was demonstrated that supported platinum nanocrystallites can activate methane significantly better than platinum surfaces. Together with the group of Heiko Weber of applied physics vibrational signatures in single molecule current-voltage curves were analysed and related to specific vibrations in chain-like carbyne molecules. In a collaboration with the group of Peter Wasserscheid in chemical reaction technology, new concepts in the catalysis of butene dimerization are investigated.

PERSPECTIVES

In the future the interplay between method development and applications shall become closer. New methods developed in recent years, shall be implemented in efficient programs well-suited for parallel computer architectures. In this way the arsenal of available methods for considering questions in materials science shall be enlarged.

A line of research to be worked on in the future is the real-time propagation of electronic structures in order to accompany experiments with atto-second-lasers by quantum chemistry. On the application side we started recently to consider various aspects of graphene and graphene-like structures and generally of new carbon allotropes.



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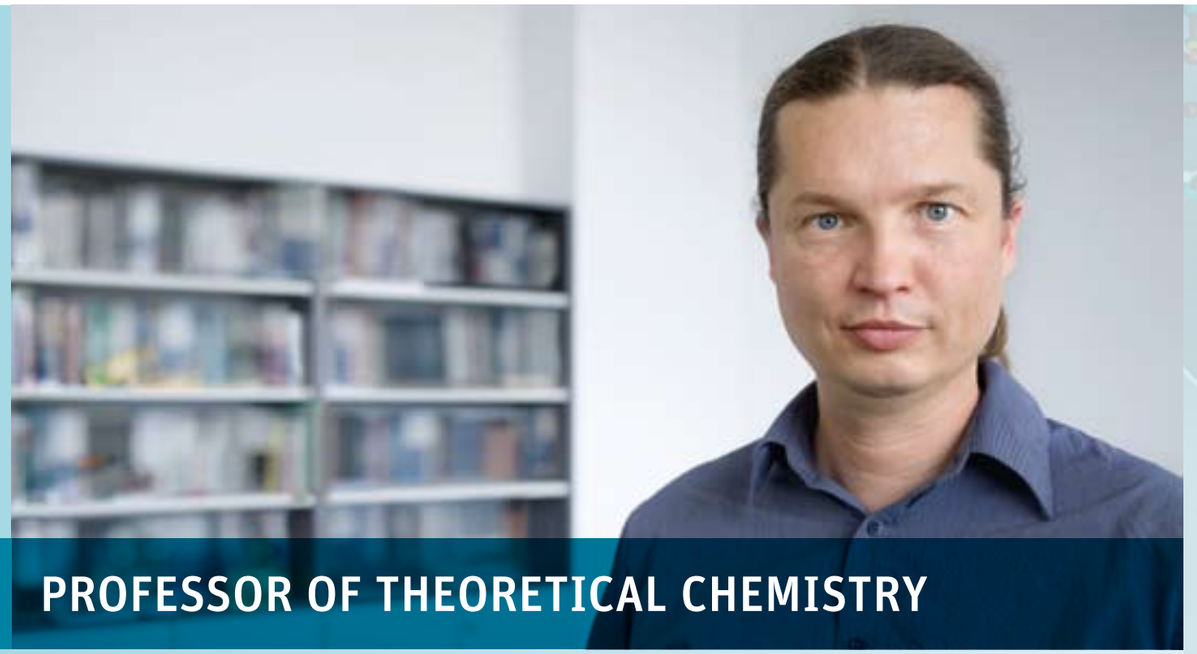
- F. Viñes, Y. Lykhach, T. Staudt, M. P. A. Lorenz, C. Papp, H.-P. Steinrück, J. Libuda, K. M. Neyman, A. Görling, *Chem. A Eur. J.* **2010,** 16, 6530 – 6539
- F. Buchner, K.-G. Warnick, T. Wölfle, A. Görling, H.-P. Steinrück, W. Hieringer, H. Marbach, *J. Phys. Chem.* **2009,** 113, 16450 – 16457
- A. Heßelmann, A. Görling, *Phys. Rev. Lett.* **2009,** 102, 233003
- A. Heßelmann, A. Ipatov, A. Görling, *Phys. Rev. A* **2009,** 80, 012507
- A. Heßelmann, A. W. Götz, F. Della Sala, A. Görling, *J. Chem. Phys.* **2007,** 127, 054102
- S. Rohra, A. Görling, *Phys. Rev. Lett.* **2006,** 97, 013005

SELECTED REVIEWS

- A. Görling, Exact-exchange Methods and Perturbation Theory along the Adiabatic Connection, in: Time Dependent Functional Theory, Ed. M. Marques, C. A. Ullrich, F. Nogueira, A. Rubio, K. Burke, E. K. U. Gross, Lecture Notes in Physics 706, Springer, Heidelberg **2006,** 137
- A. Görling, Orbital- and state-dependent functionals in density-functional theory, *J. Chem. Phys.* **2005,** 123, 062203

SELECTED AWARDS

- 1995 – 2000 Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (DFG)
- 2000 Hans G. A. Hellmann Prize for Theoretical Chemistry



PROFESSOR OF THEORETICAL CHEMISTRY

PROF. DR. DIRK ZAHN

zahn@chemie.uni-erlangen.de / www.chemie.uni-erlangen.de/zahn

CURRICULUM VITAE

Since 2010	University Professor of Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany
2008 – 2010	Heisenberg Fellow, Visiting Professor in Cagliari / Italy and Istanbul, Turkey
2002 – 2008	Habilitation at the Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
2000 – 2002	Postdoctoral Fellow at the Max Planck Institute for Solid State Research, Stuttgart, Germany and the Swiss Federal Institute of Technology (ETH), Zürich, Switzerland
1997 – 2000	PhD in Theoretical Biochemistry at the Technische Universität Darmstadt, Germany

OBJECTIVES

The aim of our group is the development and application of static and molecular dynamics simulations for the investigation of the mechanisms of reactions, nucleation events and self-organization processes. The addressed topics range from materials science, solid state chemistry up to biophysics and general physical chemistry.

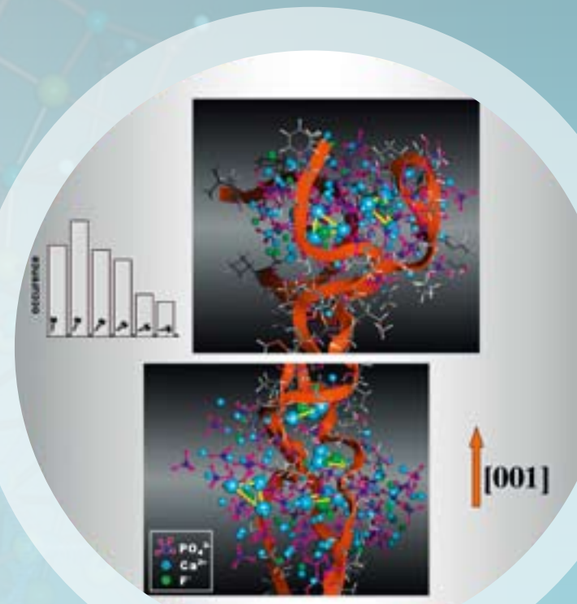
SCIENTIFIC BACKGROUND

The time-length scale problem inherent to complex systems represents the key obstacle to the direct simulation of many interesting processes. By development and application of powerful algorithms to tackle these limitations to atomistic simulations, we paved the road to detailed mechanistic investigations of nucleation, self-organization and reactions. On the basis of realistic simulation scenarios we establish increasingly close connections to the experiments.

RESEARCH HIGHLIGHTS

Using novel molecular dynamics strategies, we uncovered mechanisms of ion aggregation and nanocrystal formation and rationalized the structure and properties of (nano)composite materials. Crystal nucleation and growth is of fundamental interest in physics, chemistry, and materials science, but also in a specific discipline of biology – the investigation of biominerals. While nucleation processes and materials properties are well characterized at the macroscopic and mesoscopic scale by a wealth of experimental evidence, in particular for understanding mechanisms at the atomic level of detail, computer simulations have proven to be a very powerful tool.

An important part of our work is the development of efficient methods to allow the study of realistic crystal nucleation scenarios with a direct relation to solid state and materials chemistry. The aim of our molecular dynamics simulation studies is i) to explore the nucleation mechanisms of nanocrystalline matter. Starting from the association of single ions, accessible insights range from the mechanisms of motif formation, ripening reactions and the self-organization of nanocrystals to interactions with growth-controlling additive molecules and the formation of hybrid materials. On this basis, ii) reliable building rules for scale-up models are derived. By bridging length scales from aggregates counting a few hundreds of ions to models of up to millions of atoms we iii) pave the way to the investigation of materials properties.



On the one hand, our studies address suspensions of nanocrystals with a particular focus on their functionalization by additive molecules. On the other hand, we explore the nucleation of biocomposites. From this, scale-up models mimicking otoconia, enamel, dentine, and bone materials at the 10 nm length scale shall be developed and subjected to detailed studies of mechanical properties and deformation/fracture mechanisms. Thus, by bridging fundamental physical chemistry and materials science, a bottom-to-top approach is pursued to open a new perspective to the profound understanding of complex nanomaterials and the characterization of its peculiar properties from computer simulation.

Moreover, we explore the mechanisms of reactions in solution and in the solid state, the mechanisms of self-organization processes and the nucleation mechanisms of a series of phase transitions and their interplay with phase segregation.

PERSPECTIVES

We wish to boost bottom-to-top strategies for nanomaterial syntheses by mechanistic understanding elaborated from atomistic simulations. Along this line, we explore nanocrystal growth, the self-organization of adsorbate molecules and the formation of composites, particularly biomimetic models to bone and teeth. For the latter class of compounds, we also explore atomic scale processes involved in deformation, fatigue, and fracture.

By further development and application of advanced molecular dynamics simulation methods, we wish to tackle the time-length scale limitations of complex systems. From this, new insights into molecular self-organization and reaction mechanisms are envisaged.

SELECTED PUBLICATIONS

- A. Kawska, P. Duchstein, O. Hochrein, D. Zahn, *Nanoletters* **2008,** 8, 2336 – 2340
- A. Kawska, O. Hochrein, A. Brickmann, R. Kniep, D. Zahn, *Angew. Chem. Int. Ed.* **2008,** 120, 4982 – 4985
- D. Zahn, J. Phys. *Chem. B* **2007,** 111, 12518 – 12523
- D. Zahn, *Phys. Rev. Lett.* **2004,** 93, 227801 – 227804
- D. Zahn, *Phys. Rev. Lett.* **2004,** 92, 40801 – 40805
- D. Zahn, S. Leoni, *Phys. Rev. Lett.* **2004,** 92, 250201 – 250204

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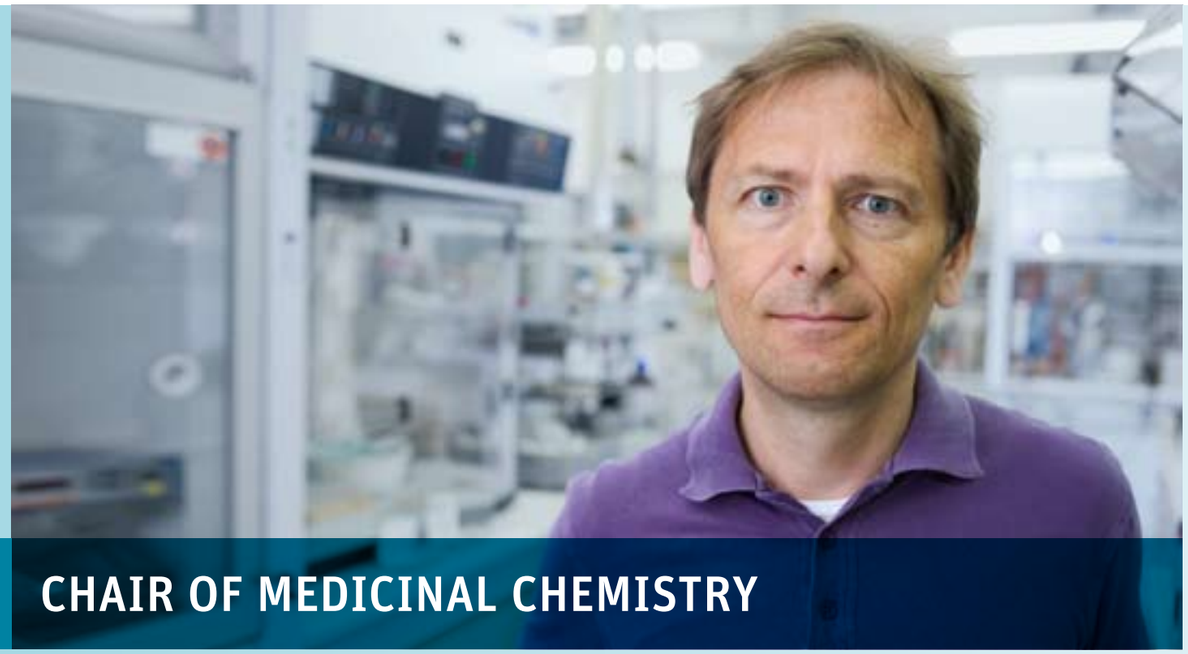
- D. Zahn, On the Role of the Solvent in Biosystems: Atomistic Insights from Computer Simulations, *Front. Biosci.* **2009,** 14, 3586 – 3593
- D. Zahn, O. Hochrein, A. Kawska, J. Brickmann, R. Kniep, Towards an Atomistic Understanding of Apatite-Collagen Biomaterials: Linking Molecular Simulation Studies of Complex-, Crystal- and Composite-Formation to Experimental Findings, *J. Mater. Sci.* **2007,** 42, 8966 – 8973
- D. Zahn, O. Hochrein, A. Kawska, G. Seifert, Y. Grin, R. Kniep, S. Leoni, Extending the Scope of 'In-Silico Experiments': Theoretical Approaches for the Investigation of Reaction Mechanisms, Nucleation Events and Phase Transitions, *Sci. Tech. Adv. Mater.* **2007,** 8, 434 – 441
- D. Zahn, Exploring the Mechanisms of Reactions in Solution from Transition Path Sampling Molecular Dynamics Simulations, *J. Chem. Theo. Comput.* **2006,** 2, 107 – 114

SELECTED AWARDS

- 2008 Heisenberg Fellowship
- 2008 Visiting professorship awards (Italy, Turkey)



CHAIR OF MEDICINAL CHEMISTRY

PROF. DR. PETER GMEINER

gmeiner@medchem.uni-erlangen.de / www.chemie.uni-erlangen.de/gmeiner

CURRICULUM VITAE

Since 1999	University Full Professor, Chair of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany
1994 – 1996	Professor of Pharmaceutical Chemistry at the University of Bonn, Germany
1988 – 1994	Research Associate at the Ludwig-Maximilians-Universität München, Germany
1987 – 1988	Postdoc at the University of California in Berkeley, USA

OBJECTIVES

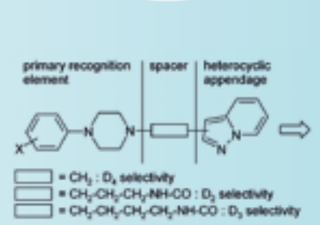
At the aim of discovering molecular probes and drug candidates for allosteric target proteins, Peter Gmeiner's group investigates design, chemical synthesis, and pharmacological properties of subtype-selective GPCR ligands, TetR effectors (SFB 473) and bioactive agents for the treatment of prion-related diseases. In this context, radio-ligand binding studies and functional assays reveal the structural origins of subtype selectivity and intrinsic activity. Within these topics, the Gmeiner laboratory prooves substantial experience regarding design, organic synthesis, and biological investigation of bioactive molecules and contributes to highly attractive developments in CNS-active drugs and gene therapy.

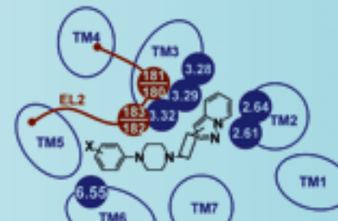
SCIENTIFIC BACKGROUND

Prof. Dr. Peter Gmeiner received his PhD in 1986 from the University of Munich. He was a Postdoc at the University of California in Berkeley, USA. He subsequently returned to Munich as a research associate. In 1992, he was appointed at the University of Bonn as a Professor of Pharmaceutical Chemistry declining an offer for a professorship at the University of Heidelberg, at the same time. Dated of October 1996, he has been chaired Full Professor of Pharmaceutical Chemistry at the University of Erlangen-Nürnberg. In 2008, Peter Gmeiner has been elected as the chairman of the Pharmaceutical / Medicinal Chemistry Section of the German Pharmaceutical Society (DPhG). Peter Gmeiner has a track record of more than 150 publications in peer-reviewed scientific journals including patents and patent applications. He serves as referee for the German Research Foundation (DFG), the Alexander von Humboldt-Foundation and the DAAD and for more than 20 top ranked journals in the fields of Chemistry and Pharmacology. He is an Editorial Board Member of international journals including Bioorganic & Medicinal Chemistry and Bioorganic & Medicinal Chemistry Letters. Peter Gmeiner's research spans the design, organic synthesis and pharmacological investigation of bioactive molecules.

RESEARCH HIGHLIGHTS

G-Protein coupled receptors are of particular interest as pharmaceutical target proteins since pathophysiological dysregulations can be treated by selective GPCR agonists or antagonists. The Gmeiner research group investigates allosterically regulated target proteins including the dopamine receptor subtypes D2long, D2short, D3 and D4 as valuable model systems. On the course of these investigations, we found the first family of receptor ligands that selectively display full (neutral) antagonist properties at the dopamine D4 receptor. Behavioral pharmacological investigations at the ETH Zuerich indicated atypical antipsychotic activities for the azaindole derivative FAUC 213. In collaboration with research laboratories at the University of North Texas and UCSF, molecular origins for the high subtype selectivity have been detected. Heterocyclic carboxamides of the type FAUC 346 and FAUC 365 as analogs of the lead compound BP 897 were developed in the Gmeiner Laboratory as valuable compounds for the treatment of cocaine abuse. In vivo investigations that were performed at the National Institute of Drug Abuse (NIDA) in Bethesda, USA, revealed diagnostic biological properties in animal models. When we explored the binding site crevice of the dopamine receptor, novel atypical arene bioisosteres could be identified, which had not been investigated in drug discovery, yet. Thus, metallocene and paracyclophane derived bioisosteres showed excellent ligand binding properties. Our current investigations involve site-directed mutagenesis studies, to gain further insights into the mechanisms of recognition. Exploiting both solution phase and solid phase supported syntheses, we rationally developed small molecules displaying structure-activity relationships that revealed novel insights into the binding and activation process of the dopamine D4 receptor subtypes. These studies were facilitated by click-chemistry-based functionalized resins.





FUTURE PERSPECTIVE

Based on in-house structure-activity data, the Gmeiner group tries to better understand homo- and heterodimerization of GPCRs. To exploit dimer related phenomena for a better treatment of GPCR mediated diseases, dimer specific receptor ligands are of superior importance. We currently synthesize bivalent GPCR agonists and antagonists and investigate their binding and activation properties in comparison to the respective monomer analogs. For the construction of flexible linker systems we take advantage of click-chemistry. Our research efforts are particularly directed to homo- and heterodimer specific dopamine receptor ligands that could be of special interest for the understanding and the treatment of neurological and psychiatric diseases. A part of our GPCR projects is done in collaboration with Prof. B. Kobilka at the Department of Molecular Physiology / Stanford University and supported by the Bavaria-California technology center (BaCaTec).

SELECTED PUBLICATIONS

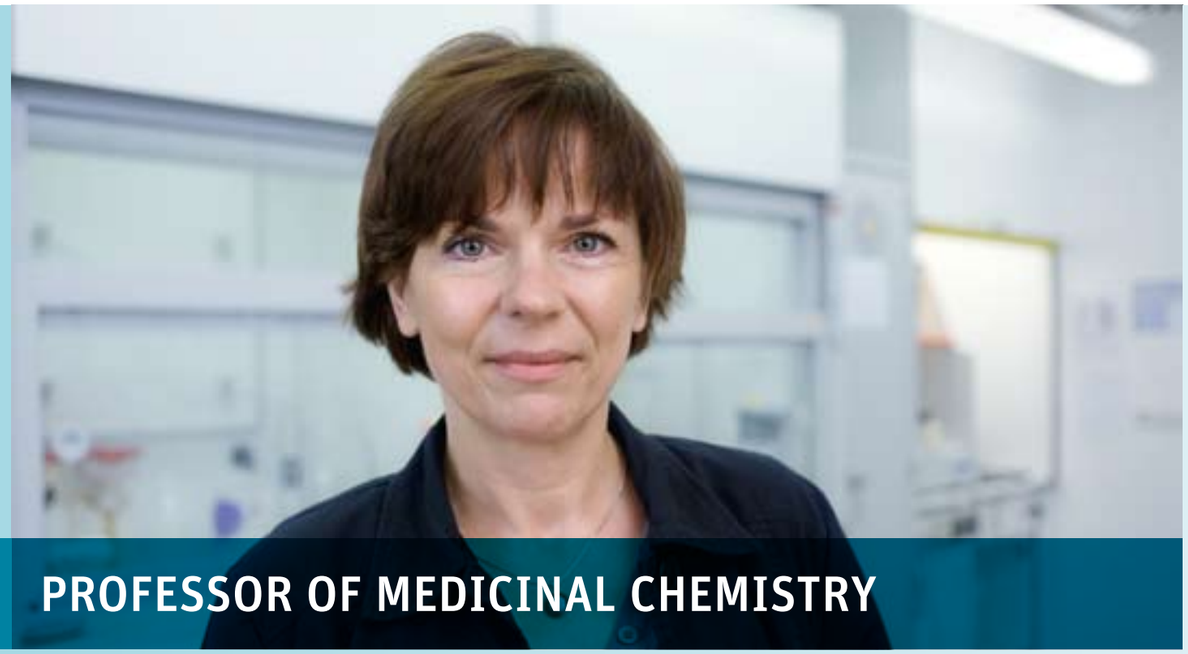
- S. Maschauer, J. Einsiedel, R. Haubner, C. Hocke, M. Ocker, H. Hübner, T. Kuwert, P. Gmeiner, O. Prante, *Angew. Chem. Int. Ed.* **2010,** 49, 976 – 979
- Nuska Tschammer, Miriam Dörfler, Harald Hübner, Peter Gmeiner, *ACS Chemical Neuroscience* **2010,** 1, 25 – 35
- H. Bittermann, F. Böckler, J. Einsiedel, P. Gmeiner, *Chem. Eur. J.* **2006,** 12, 6315 – 6322
- L. Bettinetti, S. Löber, H. Hübner, P. Gmeiner, *J. Comb. Chem.* **2005,** 7, 309
- S. Löber, P. Rodriguez-Loaiza, P. Gmeiner, *Org. Lett.* **2003,** 5, 1753
- L. Bettinetti, K. Schlotter, H. Hübner, P. Gmeiner, *J. Med. Chem.* **2002,** 45, 4594

SELECTED REVIEWS

- Frank M. Boeckler and Peter Gmeiner, Dopamine D3 Receptor Ligands – Recent Advances in the Control of Subtype Selectivity and Intrinsic Activity, Biochimica et Biophysica Acta, *Biomembranes* **2007,** 1768, 871 – 887
- Frank Boeckler and Peter Gmeiner, The Structural Evolution of Dopamine D3 Receptor Ligands – Structure-Activity Relationships and Selected Neuropharmacological Aspects., *Pharmacology & Therapeutics* **2006,** 112, 281 – 333

SELECTED AWARDS

- Johann-Wolfgang-Döbereiner Prize of the DPhG
- Phoenix Pharmazie Wissenschaftspreis



PROFESSOR OF MEDICINAL CHEMISTRY

PROF. DR. JUTTA EICHLER

eichler@medchem.uni-erlangen.de / www.chemie.uni-erlangen.de/eichler

CURRICULUM VITAE

Since 2008	University Professor of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany
2004	Habilitation in Bioorganic Chemistry at Technical University Braunschweig, Germany
2000 – 2008	Group Leader at Helmholtz Centre for Infection Research, Braunschweig, Germany
1991 – 1998	Postdoctoral Fellow, Research Scientist, Assistant Member, Torrey Pines Institute for Molecular Studies, San Diego, USA
1991	PhD at Humboldt-University, Berlin, Germany

OBJECTIVES

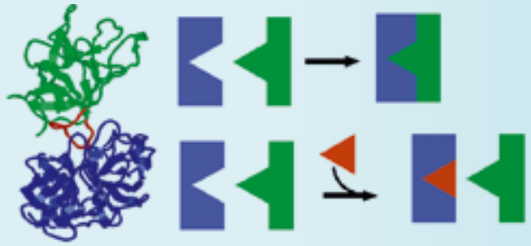
To modulate protein function through controlled interference with the underlying molecular interactions. The focus of our research is on the exploration and inhibition of protein-protein interactions based on synthetic mimicry of protein binding sites.

SCIENTIFIC BACKGROUND

Essentially all biological processes are based on specific binding events, which are initiated by molecular recognition between biomacromolecules. The design and generation of molecules, which can mimic the binding and/or functional sites of proteins, represents a promising strategy for the exploration and understanding of protein structure and function. In addition to this basic significance, such mimetic molecules are also useful tools for a range of biomedical applications, particularly the development of inhibitors of therapeutically relevant protein-protein interactions. Synthetic peptides are a promising type of molecules for protein binding site mimetics, as they can be generated as exact copies of protein fragments, as well as in diverse chemical modification, including the incorporation of building blocks other than the proteinogenic amino acids. These variations not only increase the chemical diversity presented by synthetic peptides, but also their metabolic stability, making them better drug candidates.

RESEARCH HIGHLIGHTS

Despite enormous efforts in basic and clinical research, HIV-1 vaccine development is greatly hampered by the difficulty in eliciting a virus-neutralizing antibody response. Entry of the virus into its host cells is initiated by specific interaction of the HIV-1 exterior envelope glycoprotein gp120 with the receptor CD4 on T-lymphocytes and other CD4-expressing cells. The binding site of gp120 for CD4 (CD4bs) represents a conserved region in this otherwise highly variable protein. Furthermore, the epitope of the broadly neutralizing anti-HIV-1 antibody mAb b12 has been found to overlap the CD4bs, defining this region of gp120 as a potential neutralizing epitope. Based on the crystal structure of a gp120-CD4 complex, we have designed and generated scaffolded peptides, which present the gp120 fragments that constitute its CD4bs. These peptides are able to compete with gp120 for binding to CD4 and mAb b12, respectively. Furthermore, antibodies raised against such a CD4bs mimetic peptide recognize gp120 with a specificity related to that of mAb b12. This peptide now serves as a template for rational immunogen design.



PERSPECTIVE

Questions we will be addressing in our future research include the relationship between functional and structural mimicry, i.e., whether protein binding site mimetics are able to adopt structures that resemble their arrangement within the structural context of the protein they are derived from, and whether such structural analogy correlates with the affinity to the respective ligand. This will be accomplished by structural analysis of binding sites mimetic molecules in complex with the respective ligand. The goal is to understand the structural features that govern the affinity to ligand, which will in turn guide the design of improved mimetic molecules. Furthermore, we want to explore the scope of computational protein design for the optimization of protein binding site mimetics, as well as their utility as vehicles for drug targeting and internalization into cells.

SELECTED PUBLICATIONS

- E. Sudarman, M. Bollati-Fogolin, M. Hafner, W. Müller, J. Scheller, S. Rose-John, J. Eichler, *Chem. Biol. Drug Des.* **2008,** 71, 494 – 500
- U. Strijowski, T. Hirsch, A. Quintilla, W. Wenzel, J. Eichler, *Int. J. Peptide Res. Therap.* **2007,** 13 (1-2), 245 – 250
- R. Franke, T. Hirsch, H. Overwin, J. Eichler, *Angew. Chem. Int. Ed.* **2007,** 46 (8), 2007, 1253 – 1255
- C. Hunke, T. Hirsch, J. Eichler, *ChemBioChem* **2006,** 7 (8), 1258 – 1264
- R. Franke, C. Doll, C. J. Eichler, *Tetrahedron Lett.* **2005,** 46 (26), 4479 – 4482
- R. Franke, C. Doll, V. Wray, J. Eichler, *Org. Biomol. Chem.* **2004,** 2 (19), 2847 – 2851

SELECTED REVIEWS

- K. Möbius, J. Eichler, HIV-derived peptide mimics. Drug Discovery Today: Technologies, DOI: 10.1016/j.ddtec.2009.09.001
- J. Eichler, Peptides as protein binding site mimetics. *Curr. Opin. Chem. Biol.* **2008,** 12, 707 – 713
- J. Eichler, Synthetic Peptide Arrays and Peptide Combinatorial Libraries for the Exploration of Protein-Protein Interactions and the Design of Protein Inhibitors, *Comb. Chem. High Throughput Screen.* **2005,** 8 (2), 135 – 143

SELECTED AWARDS

- 2001 BioFuture Award of the German Federal Department of Education and Research (BMBF)

PROFESSOR OF MEDICINAL CHEMISTRY

PROF. DR. MARKUS HEINRICH

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CURRICULUM VITAE

2009	University Professor of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany
2005 – 2009	Habilitation, Technische Universität München (TUM), Germany
2003 – 2005	Postdoctoral Fellow, Ecole Polytechnique, Palaiseau, France
2000 – 2003	PhD in Chemistry, Ludwig-Maximilians-Universität München (LMU), Germany
1995 – 2000	Diploma in Chemistry, Ludwig-Maximilians-Universität München (LMU), Germany

OBJECTIVES

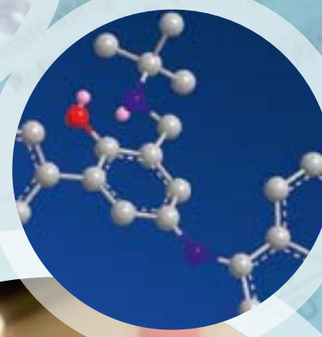
Our group is interested in the development of new radical reactions and their application in the fields of medicinal chemistry, radiochemical labelling and imaging, environmental chemistry, agrochemistry and natural product synthesis.

SCIENTIFIC BACKGROUND

Prof. Dr. Markus Heinrich studied chemistry at the Ludwig-Maximilians-Universität München. With a thesis on the total synthesis of marine alkaloids he received his PhD in 2003. During his postdoctoral stay at the Ecole Polytechnique Markus Heinrich got interested in new developments and opportunities in the field of radical chemistry. Back to Germany in 2005, he started independent research at the TU München and finished his habilitation on new radical reactions for medicinal and radiopharmaceutical purposes in 2009. In the same year, Markus Heinrich was appointed as a Professor of Medicinal Chemistry at the Friedrich-Alexander-Universität Erlangen-Nürnberg.

Concerning his field of research, the general applicability of organic radical chemistry is still restricted by the fact that even newly developed methods often depend on the use of toxic ingredients. In addition, radical chemistry is widely believed to be non-selective and the reaction course to be difficult to control. Not surprisingly, only very few radical reactions can be found among the industrial processes used for the preparation of pharmaceutical substances. Regarding this background the synthetic potential of radical reactions appears to be not yet exploited.

The Heinrich research group therefore focuses on the development of radical reactions that can be conducted under mild and simple reaction conditions with solvents such as water. Low solubilities of either reactants or products can effectively be employed to increase selectivity in radical transformations. To maintain a wide and general applicability, we only use non-toxic metals as initiators or metal-free conditions such as in photochemistry.



RESEARCH HIGHLIGHTS

In the past five years we have been able to show that reactions proceeding via aryl radicals possess a far greater potential in organic synthesis than was known before. The radicals were generated under well-defined reaction conditions which enable them to undergo selective addition reactions to various substrates. In a first step new methodologies for the intermolecular carboamination and carbohydroxylation of olefins could be developed. Later we found that improved protocols where the use of water as solvent plays a key role, even allow the functionalization of aromatic substrates. With these new synthetic opportunities in hands several important products became accessible in fewer steps and far more efficiently than before. Applications include the diagnosis and treatment of Alzheimers disease as well as the synthesis of antimalarials and agrochemicals.

PERSPECTIVES

Our future research is aimed at the discovery of new, ideally metal-free, radical reactions possessing a broad applicability in organic and medicinal chemistry. In addition we are currently investigating the combination of our synthetic methods with the important issue of waste reduction. So far unknown synthetic transformations are going to be evaluated with respect to their potential use in combinatorial syntheses of compound libraries. Finally, biological testing will be performed for the elucidation of structure-activity relationships. In this way we hope to open up new, efficient and environmentally benign ways of access to important chemical products, especially pharmaceuticals.

SELECTED PUBLICATIONS

- A. Wetzel, G. Pratsch, R. Kolb, M. R. Heinrich, *Chem. Eur. J.* **2010,** 18, 2547 – 2556
- A. Wetzel, V. Ehrhardt, M. R. Heinrich, *Angew. Chem. Int. Ed.* **2008,** 47, 9130 – 9133
- M. R. Heinrich, A. Wetzel, M. Kirschstein, *Org. Lett.* **2007,** 9, 3833 – 3835
- M. R. Heinrich, O. Blank, D. Ullrich, M. Kirschstein, *J. Org. Chem.* **2007,** 72, 9609 – 9616
- M. R. Heinrich, O. Blank, S. Wölfel, *Org. Lett.* **2006,** 8, 3323 – 3325

SELECTED REVIEWS

- M. R. Heinrich, Intermolecular olefin functionalizations involving aryl radicals generated from arenediazonium salts, *Chem. Eur. J.* **2009,** 15, 820 – 833

SELECTED AWARDS

- 2008 ADUC Prize of the Year

CHAIR OF FOOD CHEMISTRY

PROF. DR. MONIKA PISCHETSRIEDER

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CURRICULUM VITAE

Since 2004	University Full Professor, Chair of Food Chemistry at the University of Erlangen-Nürnberg, Germany
1999 – 2004	Associate Professor at the University of Erlangen-Nürnberg, Germany
1997 – 2000	Visiting Assistant Professor at the Columbia University, New York, USA
1995 – 1999	Assistant Professor at the Ludwig-Maximilians-Universität, München (LMU), Germany
1994 – 1995	Postdoctoral Fellow at the Case Western University, Cleveland, USA
1994	PhD from the Ludwig-Maximilians-Universität, München (LMU), Germany

OBJECTIVES

The goal of our research is to understand how chemistry and physiology interact in nutrition.

SCIENTIFIC BACKGROUND

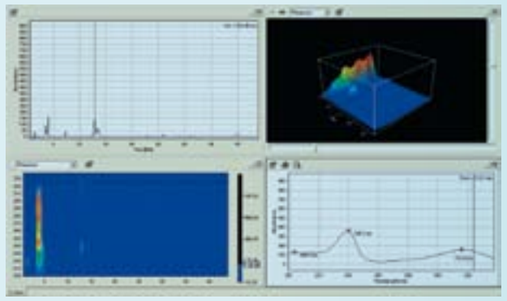
As a food chemist, I am convinced that we need to combine profound knowledge in chemistry as well as physiology in order to understand how food interacts with the human organism. Therefore, I worked in a chemistry lab for my PhD before joining work groups interested in the molecular basis of diseases as postdoctoral fellow and visiting assistant professor. This experience taught me that the major challenge in food chemistry is the complexity arising from the interaction of a diverse and heterogeneous chemical system with a diverse and heterogeneous biological system. As a consequence, systematic approaches are required on the chemical as well as biological interface to understand the diversity of physiological reactions caused by food components. For a food chemist, thermally processed food is particularly fascinating as well as challenging, because the complex natural composition of a food item is considerably multiplied by a network of thermally induced reactions among a multi-component system. In this context, the development and application of novel, highly sensitive analytical techniques is a prerequisite to fully comprehend the chemical composition of a food item. On the long run, the understanding how complex food systems interact with the human organism will catalyze the development of new food products with custom-tailored functionality.

RESEARCH HIGHLIGHTS

There are several approaches to face the challenge of the chemical complexity of food in physiological reactions. In order to evaluate the influence of coffee on the gut health, activity guided fractionation led to the identification of hydrogen peroxide as the cytotoxic component of roasted coffee. Using a synthesized substructure library as an alternative approach, aminoreductones were identified as major immunomodulating compounds in roasted coffee. Bioactive proteins, on the other hand, can neither be mastered by activity guided methods nor by synthesized libraries. Therefore, a method for non-targeted proteome analysis was developed which allowes the systematic mapping of non enzymatic posttranslational modifications (nePTMs) in the milk proteome as well as systematic nePTM mapping in single proteins. Furthermore, non-targeted proteome analysis opened an insight into the low molecular weight peptidome of milk. Consequently, physiological reactions on selected nePTMs, which had been identified before, were studied. Thus, the pro-inflammatory activity of the nePTM carboxymethyllysine was revealed. However, clinical studies in collaboration with the University hospitals indicate that, for example in the group of very young neonates, the exposure to carboxymethyllysine from nutrition is overcompensated by its endogenous formation.

PERSPECTIVES

During the last years, we were able to gain a lot of information on the chemical composition of our nutrition. The major future challenge will be to link this information to the complex physiological and biological consequences. Similar to the chemical interface, novel systematic and non-targeted approaches will be required to understand the diversity of physiological reactions to food.



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- J. Meltretter, C.-M. Becker, M. Pischetsrieder, *J. Agric. Food Chem.* **2008,** 56, 5165 – 5171
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- M. Frischmann, C. Bidmon, J. Angerer, M. Pischetsrieder, *Chem. Res. Toxicol.* **2005,** 18, 1586 – 1592

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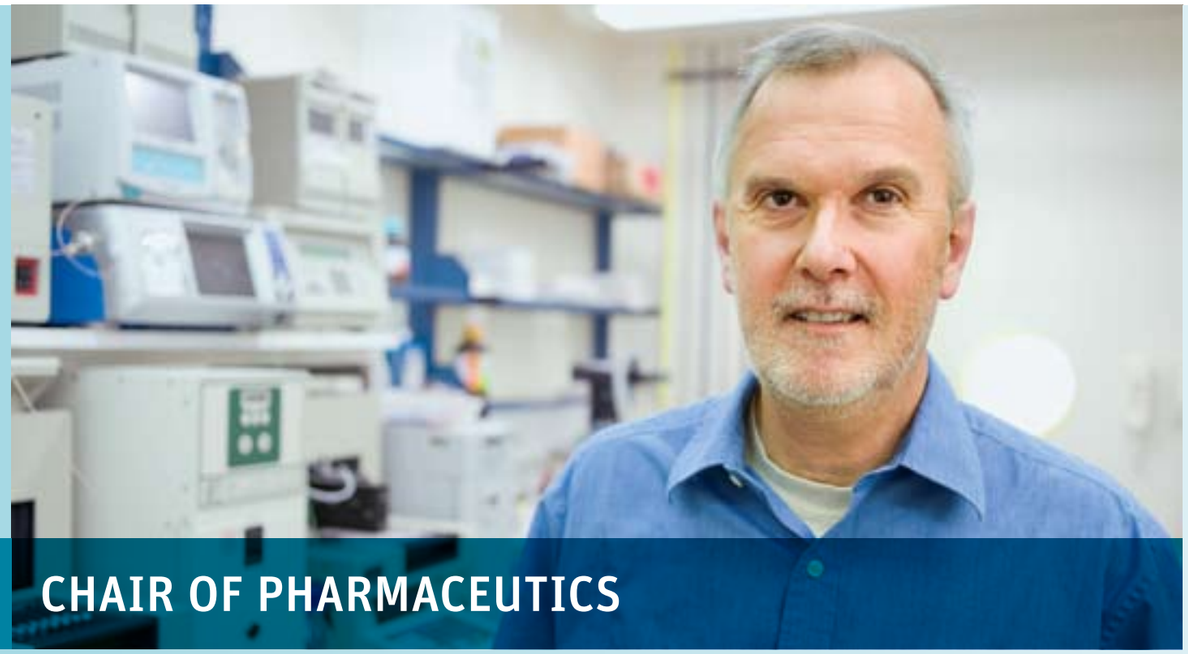
- M. Pischetsrieder, R. Bäuerlein, Proteome research in food science, *Chem. Soc. Rev.* **2009,** 38, 2600 – 2608
- C. Bidmon, M. Frischmann, M. Pischetsrieder, Analysis of DNA-bound advanced glycation end-products by LC and mass spectrometry, *J. Chromatogr. B* **2006,** 55, 51 – 58
- T. Kislinger, A. Humeny, M. Pischetsrieder, Analysis of protein glycation products by matrix-assisted laser desorption ionization time-of-flight mass spectrometry *Curr. Med. Chem.* **2004,** 11, 16, 2185 – 2193

SELECTED AWARDS

- 2007 Forprion Research Award
- 2007 Cofresco Research Prize
- 1996 Bayerischer Habilitationsförderpreis



CHAIR OF PHARMACEUTICS

PROF. DR. GEOFFREY LEE

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CURRICULUM VITAE

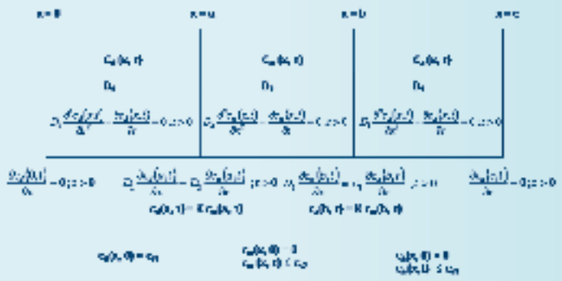
Since 1993	University Full Professor, Chair of Pharmaceutical Technology at the University of Erlangen-Nürnberg, Germany
1986 – 1993	Professor of Pharmaceutical Technoloy at the University of Heidelberg, Germany
1984 – 1986	Assistant Professor, College of Pharmacy, University of Illinois, Chicago, USA
1983 – 1984	Alexander-von-Humboldt Stipendiat, University of Regensburg, Germany
1980 – 1983	Postdoctoral Research Fellow, University of Southern California, Los Angeles and University of North Carolina, Chapel Hill, USA

OBJECTIVES

The ultimate goal in pharmaceutics is easy to declare: let's deliver a drug to its molecular site of action in the right dose at the right time. Achieving this goal is quite another matter. We specialize in all aspects of the development, manufacture, and pharmacokinetic behaviour of classic and more modern drug delivery systems. Our goal is to ensure that they perform as required to give the optimum therapeutic effect.

SCIENTIFIC BACKGROUND

My PhD research work was only marginally related to pharmaceutics – I worked on the colloidal stability of emulsions supervised by Tharwat Tadros in London. It was in Los Angeles that I first became involved in the transdermal delivery of drugs. I gained much expertise in the in vitro measurement of drug permeation rate through excised membranes of human skin. When I started in Heidelberg, I expanded this research area greatly. Our group worked in describing quantitatively the barrier property of human skin and relating permeation rate to the structure of the stratum corneum. This involved lots of work considering molecular orientation of lipid bilayers within the stratum corneum. We also established a number of numerical solutions to the diffusion equation to describe the influence of drug diffusivity and lipophilicity on permeation behaviour. After moving to Erlangen I established a second major research area, namely that of the stabilization of protein drugs for parenteral and pulmonary application. There has been a steady increase in number of approved protein drugs on the market. Their formulation poses, however, quite different problems from that of low molecular weight drugs. This continues to be a central research theme that attracts substantial industrial interest.



RESEARCH HIGHLIGHTS

1. Formulation and Stabilization of Proteins

The major thrust of this project is the use of drying processes such as spray-drying, spray freeze-drying, and freeze-drying, to produce stable solid dosage forms of proteins. Protein conformational stability can be adversely affected by the various technological processes taking place during drying. This needs to be better understood so that rational formulation development can be made to stabilize proteins. Of particular current interest is the use of spray-drying to produce flowable, storage stable protein particles as an alternative to freeze-drying of bulk. This involves understanding the powder properties of stickiness, fusion, and flowability in the amorphous state.

2. Drug Polymer Interactions in Thin Films

Modern transdermal systems comprise a pressure sensitive polymeric adhesive in which the drug is dispersed. The permeation of drugs through the skin out of such a system depends on a combination of drug diffusivity and its partitioning behaviour between the polymer and the skin. The "thermodynamic activity" concept implies that reduced solubility in a polymer film should enhance membrane permeation. The relationship between drug solubility in thin polymer films and also within the skin membrane to its permeation behaviour is under close scrutiny. One particular highlight of this research area was the development of a new transdermal system for aminolevulinic acid that is used in a photodynamic therapy of skin cancer. This idea was developed into a new drug product due to be introduced later in 2010.

PERSPECTIVES

Both protein drugs and transdermal systems are of immense interest to the modern drug product market. Their fascinating properties will remain the main stay of research activities in our group. In the field of transdermal drug delivery we plan to extend our research activities into the field of nanotechnology. Our plans for protein research concentrate on finding alternatives to freeze-drying of bulk, and also improving the parenteral formulation and delivery of sensitive biomolecules.

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- H. Gieseler, G. W. J. Lee, *J. Pharm. Sci.* **2009,** 98, 3447 – 3455
- H. Gieseler, G. W. J. Lee, *Pharm. Devel. Technol.* **2008,** 13, 463 – 472
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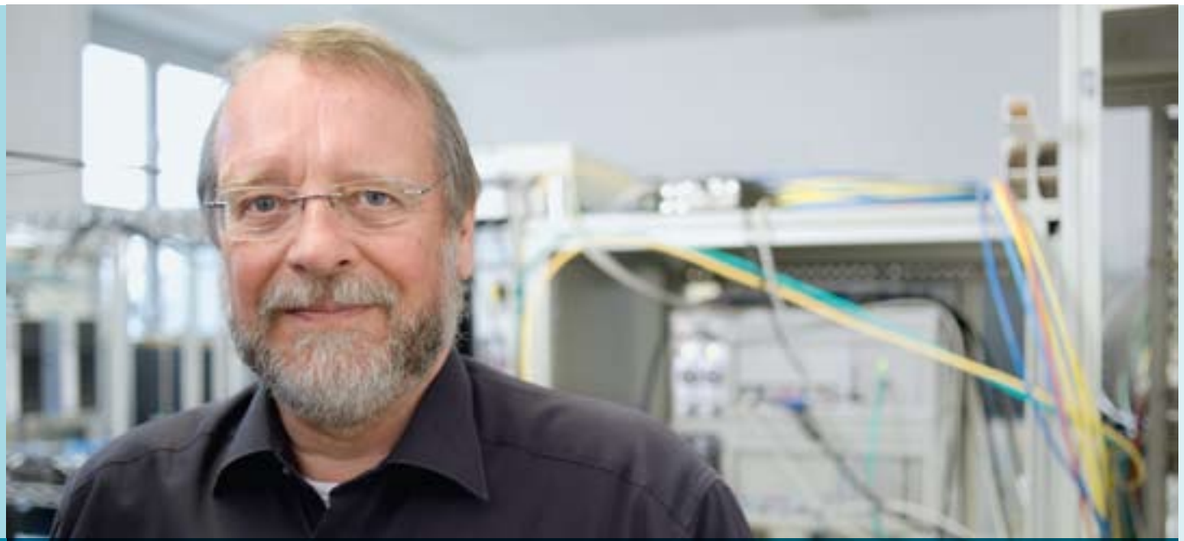

APL. PROFESSOR OF COMPUTATIONAL CHEMISTRY

PROF. DR. TIM CLARK

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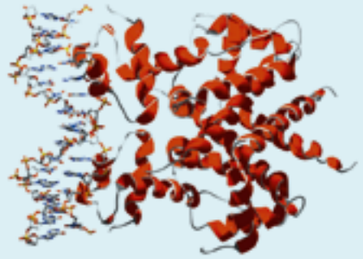
CURRICULUM VITAE

Since 2006	Professor of Computational Chemistry at the University of Portsmouth, UK
Since 1993	Technical Director, Computer Chemistry Center at the University of Erlangen-Nürnberg, Germany
1977 – 1993	Academic Councilor of the Institute of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
1976 – 1977	NATO Fellow at the University of Erlangen-Nürnberg, Germany
1975 – 1976	NATO Fellow at Princeton University, USA
1973 – 1975	Imperial Chemical Industries Fellow at Queen's University, Belfast, UK



OBJECTIVES

Our aim is to develop and use methods to simulate real systems, both technical and biological in order to understand their function and the factors that govern it. To this end, a broad spectrum of theoretical techniques from classical force fields to high-level quantum mechanics is employed. Topics of special interest are biological signaling and control, molecular electronics and the size-dependence of electronic and spectroscopic properties in the size range up to a few tens of nanometers. The methods developed are designed to bridge the gap between classical modeling techniques on the atomistic and mesoscales and to calculating the electronic properties of extremely large (50,000 atom) systems reliably.

SCIENTIFIC BACKGROUND

Computational chemistry, as distinct from the more traditional theoretical chemistry, is primarily concerned with modeling and simulating real systems in order to understand their behavior, calculate data that are not available experimentally and, more recently to predict properties and behavior before experiments are performed. The techniques used range from seemingly simple force fields (mechanical models of molecules) to extremely compute-intensive levels of ab initio molecular orbital (MO) or density functional theory (DFT). As our interest is centered on biological and nanotechnological systems, we usually deal with large, often flexible molecular aggregates. We must therefore consider the dynamics of the system by performing molecular dynamics (MD) simulations at quite "cheap" levels of theory before collecting "snapshots" from the simulations to calculate not only the instantaneous properties of the complex system, but also its macroscopic properties as the sum of those of the individual snapshots. Thus, modeling complex systems of "soft matter" involves not only calculating the properties correctly (the Hamiltonian), but also making sure that the structures calculated are really representative for the macroscopic system at real temperatures (the sampling).

RESEARCH HIGHLIGHTS

Research highlights in computational chemistry almost always involve predictions that are later confirmed by experiment or theoretical models that lead to a better understanding of experimental results. Our recent classical MD simulations of structurally persistent micelles revealed the dominant influence of the alkali metal counterions on the structure and stability of the micelles, which was later observed experimentally, and led to the experimental observation that sodium counterions can lead polycarboxylate dendrimers to organize themselves into "superlattices", even though they are highly negatively charged and should therefore repel each other.

Some predictions take longer to be confirmed. The accelerating effect of lithium counterions on radical additions to olefins was observed experimentally in 2006, twenty years after we first predicted it using *ab initio* MO theory.

Quite generally, the combination of experiment and simulations often proves to provide far more detailed insight than either alone. We have demonstrated this for organic catalysis reaction mechanisms, a variety of synthetic donor-bridge-acceptor photoinduced electron transfer systems and in the rational design of biologically active molecules.

PERSPECTIVES

Computational techniques are limited only by the capacity of the hardware and the imagination of the researcher. Strangely enough, the former is often less limiting than the latter. It is therefore important to recognize the immense power of modern computers and to develop new techniques to use them to the full to investigate chemical and biological questions. Experimentalists are increasingly working with molecules, particles and aggregates than are small enough to be simulated completely, even by quantum mechanical calculations, using a combination of modern hard- and software. The dual aspects of sampling and the Hamiltonian outlined above will play an ever increasing role as modeling and simulation begin to be able to treat complete nanoscale devices. There are already many areas of the chemistry of molecules in which high level quantum mechanical calculations can be considered more accurate than experiment. Extending these areas and developing techniques to treat ever more complex macromolecules, micelles, vesicles, membranes, self-assembled monolayers and even complete photocells or electronic devices is the aim of modern computational chemistry.

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- C. Kormann, I. Pimenta, S. Löber, C. Wimmer, H. Lanig, T. Clark, W. Hillen, P. Gmeiner, *ChemBioChem* **2009,** 10, 2924 – 2933
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- M. Wielopolski, C. Atienza, T. Clark, D. M. Guldi, N. Martin, *Chem. Eur. J.* **2008,** 14, 6379 – 6390
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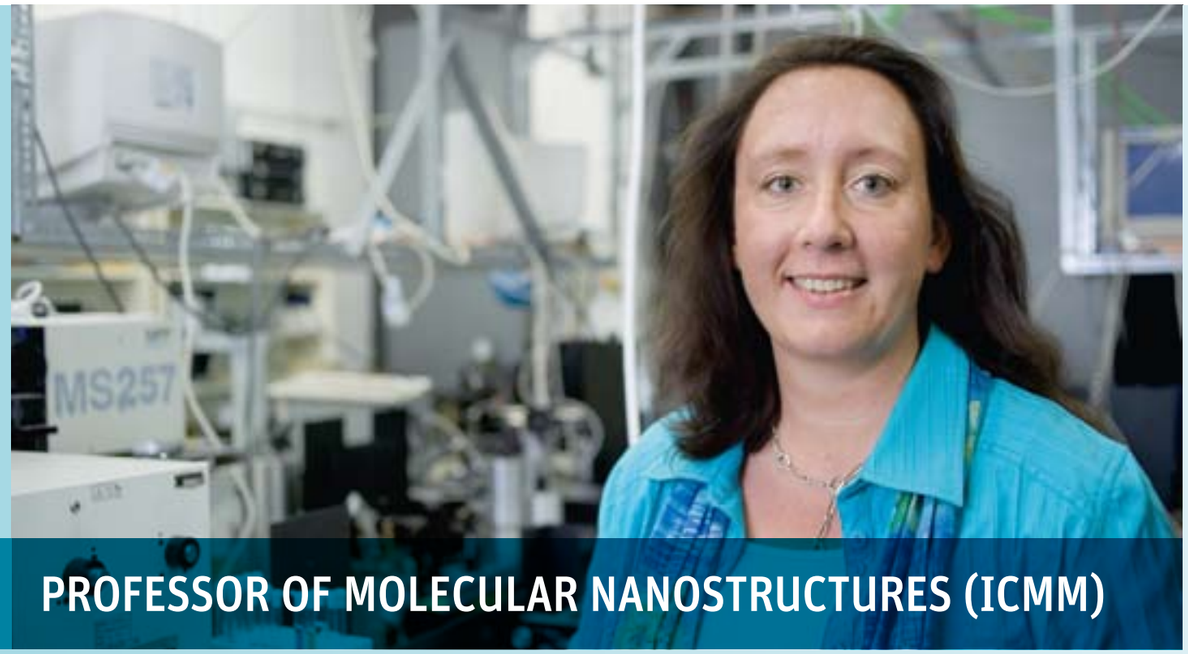
- H. Erras-Hanauer, T. Clark, R. van Eldik, Molecular orbital and DFT studies on water exchange mechanisms of metal ions, *Coordination Chemistry Reviews* **2003,** 238 – 239, 233 – 253
- T. Clark, Quo Vadis, Semiempirical MO-Theory?, *J. Mol. Struct. (THEOCHEM)* **2000,** 530, 1

SELECTED AWARDS

- 2009 Klaus-Wilhelm-von-der-Lieth-Medaille of the Molecular Graphics and Modelling Society



PROFESSOR OF MOLECULAR NANOSTRUCTURES (ICMM)

PROF. DR. FRANZISKA GRÖHN

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Since 2009	University Professor of Molecular Nanostructures at the Interdisciplinary Center for Molecular Materials (ICMM), University of Erlangen-Nürnberg, Germany
2001 – 2009	Group leader at the Max Planck Institute for Polymer Research, Mainz & Institute of Physical Chemistry, University of Mainz, Germany
1998 – 2000	Guest Researcher at National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA
1998	PhD from Max Planck Institute of Colloids and Interfaces, Teltow, and University of Potsdam, Germany

OBJECTIVES

Our goal is to develop new concepts for the design of nanostructures through self-assembly, and to establish routes for the formation of functional and responsive supramolecular nanoparticles and organic-inorganic hybrid materials. In this context, one important aim is to understand physical chemical fundamentals of self-assembly and particle formation.

SCIENTIFIC BACKGROUND

A variety of fascinating structures and functions in natural systems such as cell membranes or DNA-protein complexes is realized by supramolecular structures, that is, the non-covalent connection of building units. Therefore, in my opinion, great potential lies in synthetic structure design through self-assembly. The prospect is a simple way to build complex architectures with tailored properties, and large advantage is the capability for rearrangements, leading to responsive and switchable systems. Exciting potential lies in areas as nanoelectronics, molecular machines or smart drug carriers.

Another "secret" of natural systems is the use of organic-inorganic hybrid nanostructures to optimize material properties, for example sea shells or shark teeth being stable but light. It is thus exciting to investigate the formation of synthetic hybrid structures, for example by polymer templating, which can lead to nanoparticles with special optical, electrical or magnetic properties.

With these inspirations in mind, from my point of view, major key is to develop fundamental understanding of underlying principles of self-assembly and particle formation. This means that organic synthesis of desired building blocks plays a role in our group, while it is also crucial to characterize nanoscale structures by a combination of analytical methods, ranging from microscopy to scattering methods, including instrumental developments.

RESEARCH HIGHLIGHTS

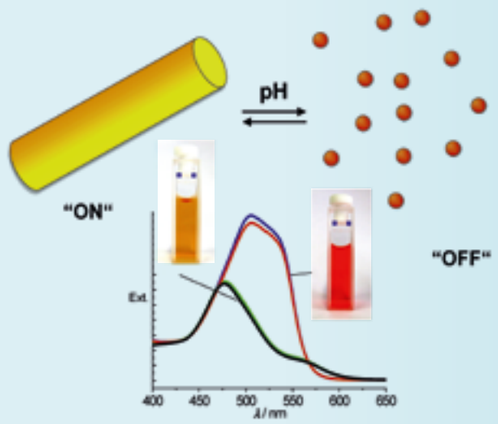
Recently we established a new concept for the formation of supramolecular assemblies with a variety of architectures: electrostatic self-assembly of macroions and organic counterions. Nanoscale spheres, rods, networks, rings, and hollow spheres can be built. The approach is based on the interconnection of polyelectrolytes through structural multivalent organic counterions under secondary interaction effects such as π–π stacking in-between counterions or geometric factors. Nanoassemblies have a narrow size distribution, are stable in aqueous solution and can be deposited on surfaces.

For example, hollow spheres with 250 nm diameter and 20 nm wall thickness spontaneously form from 5 nm sized dendrimeric building blocks and a trivalent dye counterion. Capsules can be filled with a fluorescently labelled peptide that can be released through a pH change.

New types of self-assembled morphologies were created involving porphyrins. A tetravalent cationic porphyrin interconnected anionic cylindrical polyelectrolyte brushes into finite networks of several hundred nanometer size. Individual porphyrin-loaded cylindrical brushes were also built. These may be of interest in molecular electronics, light harvesting systems or medical applications.

Highlights from earlier research include fundamental results on the interaction of polyelectrolytes, proving domain formation due to effective attraction of like charged macroions mediated by counterions. This is important as – despite most natural polymers are polyelectrolytes and they are found in many applications – fundamental questions on interaction effects had been discussed for decades.

Another highlight has been the formation of polyelectrolyte templated inorganic nanoparticles, which is based on a purely hydrophilic precursor assembly for example of gold ions accumulated inside an ionic dendrimer template. The size of the resulting gold colloid is controlled through the number of gold ions added per dendrimer. Thus, again electrostatic interaction involving polyelectrolytes represents a route to design nanoparticles.



PERSPECTIVES

With this concept of electrostatic self-assembly we have opened a route to versatile nanostructures. In future, in particular the potential to build functional and responsive assemblies will be exploited. The advantage of this approach lies in its wide applicability without relying on specific chemical binding motifs. Therefore, a variety of functional building blocks can be introduced either through the polyelectrolyte or the counterion. Examples are conducting polyelectrolytes or catalytically active counterions. Future potential also lies in structures that respond to external triggers, in particular to light. Furthermore, electrostatic self-assembly will be combined with nanotemplating of metal and semiconductor nanoparticles to create complex organic-inorganic hybrid structures. With future perspectives not limited to these examples, it is expected that electrostatic self-assembly will lead to striking novel functional nanoparticles and structures.

SELECTED PUBLICATIONS

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- I. Willerich, H. Ritter, F. Gröhn, *J. Phys. Chem.* **2009,** 113, 3339 – 3354
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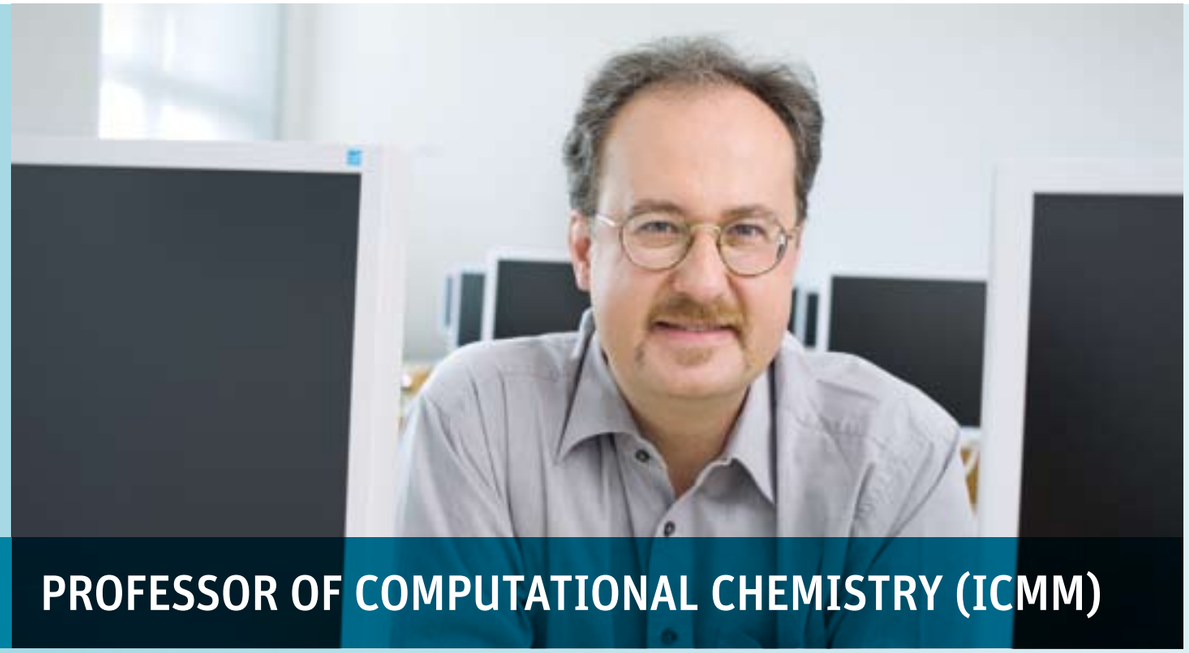
- I. Willerich, F. Gröhn, *Chem. Eur. J.* **2008,** 14, 9083 – 9447
- F. Gröhn, K. Klein, S. Brand, *Chem. Eur. J.* **2008,** 14, 6866 – 6869
- F. Gröhn, B. J. Bauer, E. J. Amis, C. L. Jackson, *Macromolecules* **2000,** 33, 6042 – 6050

SELECTED REVIEWS

- F. Gröhn, Soft Matter Nanoparticles with Various Shapes and Functionalities Can Form through Electrostatic Self-Assembly, *Soft Matter* **2010,** DOI: 10.10039/c0sm00411a
- F. Gröhn, Electrostatic self-assembly as route to supramolecular structures, *Macromol. Chem. Phys.* **2008,** 209, 2295 – 2301

SELECTED AWARDS

- 2006 Invitation to the Transatlantic Frontiers of Chemistry Symposium by ACS, RSC, and GdCh
- 2004 Reimund-Stadler Award, German Chemical Society
- 1989 International Chemistry Olympiad



PROFESSOR OF COMPUTATIONAL CHEMISTRY (ICMM)

PROF. DR. BERND MEYER

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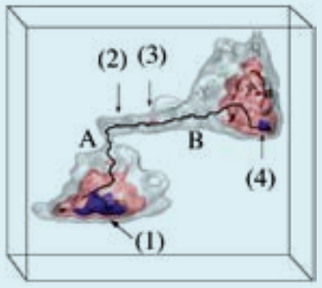
CURRICULUM VITAE

Since 2007	University Professor of Computational Chemistry at the Interdisciplinary Center for Molecular Materials (ICMM) and the Computer Chemistry Center (CCC) at the University of Erlangen-Nürnberg, Germany
2007	Visiting Scientist at the University of Oxford, UK
2006	Habilitation in Theoretical Chemistry
2004 – 2007	Head of a Junior Research Group at the Ruhr-University of Bochum, Germany
2000 – 2004	Research Associate at the Ruhr-University of Bochum, Germany
1999 – 2000	Postdoc at Rutgers University, New Jersey, USA
1998	PhD in Physics at the Max Planck Institute for Metals Research, Stuttgart, Germany



OBJECTIVES

The aim of our research is to achieve a better understanding of chemical processes on solid surfaces. Using atomistic computer simulations we study how molecules interact with surfaces and how their physical and chemical properties are modified by adsorbates. In particular, we focus on identifying relevant surface structures formed under the conditions of chemical processes, and we elucidate mechanisms of chemical reactions on surfaces in order to gain new insights into heterogeneous catalysis and the growth mechanism of adsorbate films, coatings and nanostructures.

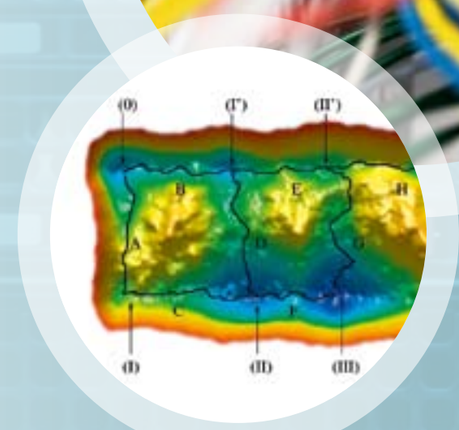
SCIENTIFIC BACKGROUND

Most large-scale chemical processes in industry depend on heterogeneous catalysis. These include synthesis of many bulk chemicals, oil refinement for gasoline, and environmental protection processes such as exhaust gas cleaning. Future technologies for renewable energies will also depend crucially on efficient catalysts for the interconversion of water and carbon dioxide to hydrogen or methanol, both of which may serve as energy carrier. Heterogeneous catalysis is based on the ability of surfaces to form and break chemical bonds to the reactant molecules from the surrounding liquid or gas phase. In many cases adsorbates profoundly modify the structural and electronic properties of surfaces. This is utilized, for example, in sensors, but it also takes place when materials corrode. An understanding of the properties of coatings in order to protect materials or to make them more wear resistant is therefore of fundamental interest. Another area in which the interaction and bonding of molecules to surfaces plays an important role is the functionalization of surfaces, for example, in dye-sensitized solar cells or in molecular electronics.

RESEARCH HIGHLIGHTS

Our recent research has been focused on the investigation of ZnO and Cu/ZnO catalysts which are employed for hydrogenation reactions, for example, in methanol synthesis from syngas. The reducibility of ZnO is the main driving force behind its catalytic activity. Using atomistic total energy calculations in combination with thermodynamic modeling, new insights into the reduction state of ZnO under reaction conditions of catalytic processes could be obtained. In particular, the properties and charge state of surface defects and the origin of the morphological changes of copper particles in Cu/ZnO under the influence of the reducing atmosphere of syngas (a so called 'strong metal-support interaction') was investigated. Subsequent accelerated molecular dynamics simulations revealed a subtle interplay between the reduction state of ZnO, the stability of reaction intermediates, and the activation barrier for the elementary reactions steps, which gives rise to an extensive free energy landscape and a complex reaction network from hydrogen and carbon monoxide to methanol.

Further research projects comprise investigations of the structure and dynamical behavior of the first water layer in contact with ZnO surfaces, the modification of surface reactivity by coadsorbates, surface metallization by hydrogen adsorption and the characterization of surface structures by calculation of scanning tunneling microscopy images. Using kinetic Monte Carlo simulations to study the growth of surface nanostructures, the mechanism and the atomistic processes have been identified which lead to a very unusual growth of one-dimensional Pd nanowires on surfaces of tin oxide.



PERSPECTIVES

First-principles-based atomistic calculations and molecular dynamics simulations are restricted to system sizes of one or two hundred atoms due to the high computational cost. To be able to study larger systems we are currently developing a more approximate, semiempirical method which is based on a parametrization of the electronic structure problem (density-functional-based tight-binding). This parametrization, however, will be fully derived from first-principles calculations. In the future the new method will be applied to study the interaction of large organic molecules with oxide surfaces, to elucidate the mechanism of the growth and self-assembly of molecular monolayers, and to simulate the growth of ZnO nanoparticles from solution. Special attention will be given to interface properties in dye-sensitized solar cells and tailored adsorbate films for molecular electronics.

SELECTED PUBLICATIONS

- J. Kiss, A. Witt, B. Meyer, D. Marx, *J. Chem. Phys.* **2009,** 130, 184706 – 184714
- Y. Umeno, C. Elsässer, B. Meyer, P. Gumbsch, J. Weissmüller, *Europhys. Lett.* **2008,** 84, 13002/1-6
- R. Kovacik, B. Meyer, D. Marx, *Angew. Chem. Int. Ed.* **2007,** 46, 4894 – 4897
- K. Katsiev, M. Batzill, U. Diebold, A. Urban, B. Meyer, *Phys. Rev. Lett.* **2007,** 98, 186102
- Y. Wang, X. Xia, A. Urban, H. Qiu, J. Strunk, B. Meyer, Ch. Wöll, M. Muhler, *Angew. Chem. Int. Ed.* **2007,** 46, 7315 – 7318
- Y. Wang, B. Meyer, X. Yin, M. Kunat, D. Langenberg, F. Traeger, A. Birkner, Ch. Wöll, *Phys. Rev. Lett.* **2005,** 95, 266104
- O. Dulub, B. Meyer, U. Diebold, *Phys. Rev. Lett.* **2005,** 95, 136101
- B. Meyer, D. Marx, O. Dulub, U. Diebold, M. Kunat, D. Langenberg, Ch. Wöll, *Angew. Chem. Int. Ed.* **2004,** 43, 6641 – 6645

FOOD CHEMISTRY

PD DR. ANDREA BÜTTNER

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www.chemie.uni-erlangen.de/buettner

CURRICULUM VITAE

Since 2007	Assistant Professor (PD), Food Chemistry and Head of the 'Physiological and Psychological Effects of Odorants on Humans' Junior Research Group (BMBF) at the University of Erlangen-Nürnberg, Germany
Since 2007	Research Scientist and Head of the "Sensory Analytics" group at Fraunhofer IVV, Freising, Germany
2006	Habilitation at the Technische Universtität München (TUM) (Prof. Schieberle), Germany
2002 – 2006	Internship for Excellent Junior Researchers (HWP II) at the TUM, Germany and of the German Research Community at the German Research Center for Food Chemistry, Garching, Germany
1999 – 2002	Postdoctoral Fellow at the German Research Center for Food Chemistry, Garching, Germany and the Institute for Food Chemistry, TUM, Germany
1999	PhD in Food Chemistry at the TUM (Prof. Schieberle), Germany

RESEARCH HIGHLIGHTS

In our research group we investigate physiological and psychological effects of odorants on humans, specifically in relation to foods. Recent studies deal with the characterization of odorants by sensory and chemo analytical techniques such as high resolution gas chromatography-mass spectrometry/olfactometry and stable isotope dilution assays. Characterization of uptake and metabolism processes within the human body is realized by in vivo as well as in vitro studies. Of special interest is the transfer of human-specific but also dietary odorants and their metabolites into human milk, e.g. originating from maternal food intake. In these studies, we evaluate the potential influence of odorants on neonates with regard to physiological but also behavioural effects. These are monitored, for example, by biofeedback methodologies (EEG, heart rate, breathing patterns) as well as mimic analysis. We have shown that the chemosensory skills of neonates differ drastically from those of adult humans and that they can react to substances that some adults do not smell.

Uptake and metabolism data are the basis to investigate other physiological effects of odorants in vivo and in vitro such as the activation of brain receptor systems involved in sedative and anxiolytic processes.

One final goal is to understand modification of food acceptance or preference due to odorant exposure and to characterize and develop optimized food aroma systems that support beneficial nourishment.

FUTURE PERSPECTIVE

Issues of research will be:

- Characterization of odorants of relevance to human food and the environment
- Resorption, transfer and metabolism processes of odorants in humans
- Physiological and psychological/behavioural action of humans resulting from odorant exposure

SELECTED PUBLICATIONS

- J. Beauchamp, J. Frasnelli, A. Buettner, M. Scheibe, A. Hansel, T. Hummel, *Meas. Sci. Technol.* **2010,** DOI: 10.1088/0957-0233/21/2/025801
- J. Spitzer, A. Buettner, *Food Chem.* **2010,** 120, 240 – 246
- A. Strube, H. Guth, A. Buettner, *Water Res.* **2009,** 43, 5216 – 5224
- A. Strube, A. Buettner, C. Groetzinger. *Water Sci. Technol.: Water Supply—WSTWS* **2009,** 9, 299 – 309
- A. Buettner, S. Otto, A. Beer, M. Mestres, P. Schieberle, T. Hummel, *Food Chem.* **2008,** 108, 1234 – 1246
- A. Buettner, *Flav. Fragr. J.* **2007,** 22, 465 – 473

SELECTED REVIEWS

- A. Buettner, J. Beauchamp, Chemical input – sensory output: diverse modes of physiology-flavour interaction. *Food Qual. Pref.* **2010,** DOI: 10.1016/j.foodqual.2010.01.008
- M. Mertens, E. Kirchhoff, A. Buettner. The volatile constituents of frankincense – a review. *Flavour Fragr. J.* **2009,** 24, 279 – 300

SELECTED AWARDS

- 2004 Firmenich Flavor and Fragrance Science Award
- 2001 Joseph-Schormüller-Award for the research internship in the group of Prof. Paolo Pelosi, University of Pisa
- 1999 Weurman Flavour Research Award

PHYSICAL CHEMISTRY

PD DR. MICHAEL GOTTFRIED

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CURRICULUM VITAE

Since 2010	Assistant Professor (PD), Physical Chemistry at the University of Erlangen-Nürnberg, Germany
2010	Habilitation in Physical Chemistry at the University of Erlangen-Nürnberg (Prof. Steinrück), Germany
2009	Visiting Scientist at the University of Science and Technology of China, Hefei, P. R. China
2005 – 2008	Visiting Scientist at the University of Washington, Seattle, USA
2004 – 2009	Habilitation, University of Erlangen-Nürnberg (Prof. Steinrück), Germany
2003 – 2004	Postdoctoral Fellow, Department of Chemistry, University of Washington (Prof. Campbell), USA
2003	PhD in Physical Chemistry, Freie Universität Berlin (Prof. Christmann), Germany
1999	Diploma Degree in Chemistry, Freie Universität Berlin, Germany
1995	Research project with C. Glidewell, Organometallic Chemistry, University of St Andrews, UK

RESEARCH HIGHLIGHTS

Our research focuses on reactivity, structure and electronic properties of chemically complex surfaces and interfaces. Examples are (a) surfaces functionalized with metal complexes, (b) metal/polymer interfaces, (c) model catalysts and (d) surfaces of ionic liquids. We study surface-confined coordination reactions of porphyrins and other planar metal complexes and investigate the nature of the surface coordinative bond using photoelectron spectroscopy and other techniques. In addition, we measure adsorbate-substrate bond lengths using X-ray standing waves (XSW). We are developing a surface nanojoule calorimeter for the direct measurement of adsorbate-substrate bond energies on well-defined surfaces of single crystals, polymers, and molecular films. Our catalysis-related studies focus on surface chemistry of catalysis by gold, where we use in situ photoelectron spectroscopy to investigate a range of model systems with increasing structural and chemical complexity: gold single crystals, nanoporous gold foams, planar gold/oxide model catalysts, and powder catalysts. In collaboration with groups in chemical engineering, we also study the properties novel catalysts designed for industrial applications. We collaborate with research groups in USA, France, China, Poland and other countries, which gives our students the opportunity to do parts of their projects abroad.

FUTURE PERSPECTIVE

We will further develop our expertise on synthesis, reactivity and structure of complex solid and liquid surfaces as well as on gas/solid and liquid/solid interfaces.

Our future main research fields will include:

- Nanostructured molecular materials with novel surface properties
- Mechanisms of complex surface reactions
- Development of experimental techniques for surface and interface chemistry

SELECTED PUBLICATIONS

- F. Bebensee, J. F. Zhu, J. H. Baricuatro, J. A. Farmer, Y. Bai, H.-P. Steinrück, C. T. Campbell, J. M. Gottfried, *Langmuir* **2010,** 26, 9632 – 9639
- J. Zhu, F. Bebensee, W. Hieringer, W. Zhao, J. H. Baricuatro, J. A. Farmer, Y. Bai, H.-P. Steinrück, J. M. Gottfried, *J. Am. Chem. Soc.* **2009,** 131, 13498
- F. Buchner, K. Flechtner, Y. Bai, E. Zillner, I. Kellner, H.-P. Steinrück, H. Marbach, J. M. Gottfried, *J. Phys. Chem.* **2008,** C 112, 15458–15465
- K. Flechtner, A. Kretschmann, H.-P. Steinrück, J. M. Gottfried, *J. Am. Chem. Soc.* **2007,** 129, 12110 – 12111
- T. E. Shubina, H. Marbach, K. Flechtner, A. Kretschmann, N. Jux, F. Buchner, H.-P. Steinrück, T. Clark, J. M. Gottfried, *J. Am. Chem. Soc.* **2007,** 129, 9476 – 9483
- J. M. Gottfried, K. Flechtner, A. Kretschmann, T. Lukasczyk, H.-P. Steinrück, *J. Am. Chem. Soc.* **2006,** 128, 5644 – 5645

SELECTED REVIEWS

- J. M. Gottfried, H. Marbach, Surface-confined coordination chemistry with porphyrins and phthalocyanines: Aspects of formation, electronic structure, and reactivity, *Z. Phys. Chem.* **2009,** 223, 53 – 74

SELECTED AWARDS

- 2004 Feodor-Lynen Fellowship of the Alexander von Humboldt Foundation

THEORETICAL CHEMISTRY

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CURRICULUM VITAE

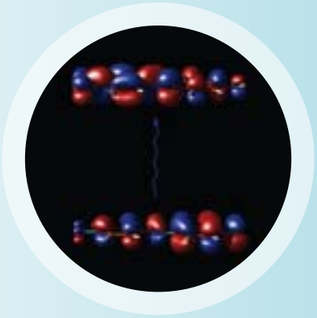
Since 2010	Assistant Professor (PD), Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany
2010	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Görling), Germany
2004 – 2010	Habilitand, Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Görling), Germany
2003 – 2004	Postdoctoral Fellow, Theoretical Chemistry at the Technische Universität München (TUM), Germany
2002 – 2003	Postdoctoral Fellow, Theoretical Chemistry at the Universität Bonn, Germany
2000 – 2002	Postdoctoral Fellow, Theoretical Chemistry at the Vrije Universiteit Amsterdam (Prof. Baerends), NL
2000	PhD in Inorganic Chemistry, Technische Universität München (Prof. W. A. Herrmann), Germany
1997	Diploma Degree in Chemistry, Technische Universität München, Germany

RESEARCH HIGHLIGHTS

In our research we use density-functional methods to theoretically study complex problems in materials science, catalysis, and chemical bonding theory, with a special focus on systems containing transition metals. Recent examples deal with the electronic structure, spectroscopy, and scanning tunnelling microscopy simulations of metalloporphyrin adsorption on surfaces, the theoretical study of the photophysical properties of charge-transfer diads for solar-energy conversion, and investigations concerning the transport of electronic charge through single molecules embedded between gold contacts. Very recently, we have developed new density-functional methods to both accurately and efficiently describe excitations of core-electrons in large adsorbate systems.

FUTURE PERSPECTIVE

Our focus will be on the further development of density-functional methods into a practical and reliable tool to study to complex problems in chemistry and materials science. The greatest challenge here is to develop new density-functional methods which are at the same time reliable, accurate, and efficient enough to make predictions about the properties of complex systems. Current projects comprise, among other things, the development of new model kernels for time-dependent density functional theory for application in photoactive systems, the simulation of catalytic processes in ionic liquid environments, and the theoretical description of nonlinear optical effects on structured surfaces.



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- N. Schmidt, R. Fink, W. Hieringer, *J. Chem. Phys.* **2010,** 133, DOI: 10.1063/1.3435349
- F. Buchner, K.-G. Warnick, T. Wölfle, A. Görling, H.-P. Steinrück, W. Hieringer, H. Marbach, *J. Phys. Chem.* **2009,** 113, 16450 – 16457
- M. Quintiliani, A. Kahnt, T. Wölfle, W. Hieringer, P. Vázquez, A. Görling, D. M. Guldi, T. Torres, *Chem. Eur. J.* **2008,** 14, 3765 – 3775
- W. Hieringer, E. J. Baerends, *J. Phys. Chem.* **2006,** 110, 1014 – 1021
- W. Hieringer, F. Della Sala, A. Görling, *Chem. Phys. Lett.* **2004,** 383, 115 – 121
- W. Hieringer, J. Eppinger, R. Anwander, W. A. Herrmann, *J. Am. Chem. Soc.* **2000,** 122, 11983 – 11994

SELECTED REVIEWS

- W. Hieringer, Palladium-catalyzed C-C coupling reactions: The Heck reaction by in Applied Homogeneous Catalysis with Organometallic Compounds, Eds. B. Cornils, W. A. Herrmann, Wiley-VCH, Weinheim, **2002**

SELECTED AWARDS

- 2003 Marie Curie Reintegration Grant of the European Commission
- 2000 Marie Curie Individual Fellowship of the European Commission

ORGANIC CHEMISTRY

PD DR. NORBERT JUX

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CURRICULUM VITAE

Since 2007	Assistant Professor (PD), Organic Chemistry at the University of Erlangen-Nürnberg, Germany
2006	Habilitation in Organic Chemistry at the University of Erlangen-Nürnberg (Prof. A. Hirsch), Germany
1997 – 2006	Research Group leader in Organic Chemistry, University of Erlangen-Nürnberg, Germany
1995 – 1996	Postdoctoral Fellow, Department of Chemistry & Biochemistry, University of California, Los Angeles (Prof. Y. Rubin), USA
1994	PhD (Dr. rer nat.) University of Cologne (Prof. E. Vogel), Germany
1990	Diploma Degree in Chemistry, University of Cologne, Germany

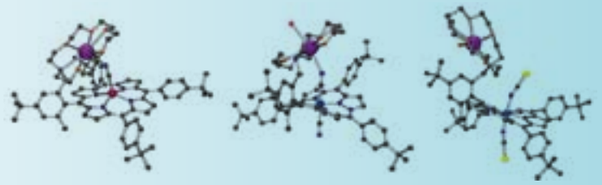
RESEARCH HIGHLIGHTS

Our research focuses on synthesis and functionalization of novel porphyrin and porphyrinoid materials. We are particularly interested in water-soluble systems as this solvents plays not only the dominant role in all natural processes but allows also for easy manipulation via electrostatic interactions. Our work aims at (a) photovoltaic devices based on layer-by-layer deposition of dyes generating a redox gradient, (b) understanding fundamental processes like the activation of dioxygen and related species by porphyrin metal complexes, (c) generating novel porphyrinoids and carbon-rich materials based on porphyrins, (d) preparing novel photosensitizers and carrier systems for the Photodynamic Therapy of Tumors, and, (e) applying and developing reactions to modify porphyrins making new materials. Employing powerful methods of porphyrin synthesis, we have prepared series of highly functionalized systems which carry up to eight bromomethyl groups. Thus, nucleophilic substitution reactions allow for easy functionalization. We are strongly cooperating with groups in Erlangen within the Cooperative Research Center 583 – Redox-active metal centers – but have also good contacts to groups worldwide.

FUTURE PERSPECTIVE

Taking advantage of our expertise in porphyrin chemistry, we will develop and explore novel materials which address the following topics:

- photovoltaic devices and energy-related issues
- complex photosensitizer systems with enhanced tumor selectivity
- novel porphyrin-based compounds with high carbon content



SELECTED PUBLICATIONS

- T. E. Shubina, H. Marbach, K. Flechtner, A. Kretschmann, N. Jux, F. Buchner, H.-P. Steinrück, T. Clark, J. M. Gottfried, *J. Am. Chem. Soc.* **2007,** 129, 9476 – 9483
- K. Dürr, B. P. Macpherson, R. Warratz, F. Hampel, F. Tuczek, M. Helmreich, N. Jux, I. Ivanović-Burmazovića, *J. Am. Chem. Soc.* **2007,** 129, 4217 – 4228
- J.-E. Jee, S. Eigler, N. Jux, A. Zahl, R. van Eldik, *Inorg. Chem.* **2007,** 46, 3336 – 3352
- F. Rancan, M. Helmreich, A. Mölich, E. A. Ermilov, N. Jux, B. Röder, A. Hirsch, F. Böhm, *Bioconjugate Chem.* **2007,** 18, 1078 – 1086
- D. M. Guldi, G. M. A. Rahman, N. Jux, D. Balbinot, U. Hartnagel, N. Tagmatarchis, M. Prato, *J. Am. Chem. Soc.* **2005,** 127, 9830 – 9838
- M. Helmreich, E. A. Ermilov, M. Meyer, N. Jux, A. Hirsch, B. Röder, *J. Am. Chem. Soc.* **2005,** 127, 8376 – 8385
- N. Jux, *Org. Lett.* **2000,** 2, 2129 – 2132

SELECTED REVIEWS

- N. Jux, B. Röder, Targeting Strategies for Tetrapyrrole-based Photodynamic Therapy, *Handbook of Porphyrin Science* (eds.: K. M. Kadish, K. M. Smith, R. Guilard), vol. 4, Phototherapy, Radioimmunotherapy and Imaging, World Scientific Publishing Co. Pte. Ltd **2010,** 325 – 400

SELECTED AWARDS

- 1997 Liebig-Fellowship for Habilitation, Funds of the Chemical Industry

PHYSICAL CHEMISTRY

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CURRICULUM VITAE

Since 2010	Assistant Professor (PD), Physical Chemistry at the University of Erlangen-Nürnberg, Germany
2010	Habilitation in Physical Chemistry at the University of Erlangen-Nürnberg (Prof. Steinrück), Germany
2004 – 2009	Postdoctoral Fellow, Physical Chemistry at the University of Erlangen-Nürnberg (Prof. Steinrück), Germany
2002 – 2004	Postdoctoral Fellow at the Surface Science Center, University of Pittsburgh (Prof. Yates, Prof. Levy), PA/USA
2002	PhD in Physical Chemistry and Electrochemistry, University of Hannover (Prof. Imbihl), Germany
1997	Diploma Degree in Physics, University of Dortmund, Germany

RESEARCH HIGHLIGHTS

The generation and investigation of nanostructures on surfaces is in the center of my current research activities. In my working group we follow different routes to fabricate tailor-made nano-scaled structures. The first (bottom-up) approach is based on the self-assembly of molecules or atoms on surfaces. In this context the geometric and electronic structure of porphyrin derivatives as prototype examples for functional molecules has been intensively studied on different substrates. In our second (top-down) approach a highly focused electron beam is used to locally dissociate adsorbed precursor molecules (electron beam induced deposition, EBID) or to directly modify the properties of the substrate with lithographical control. For both projects we target the understanding of the fundamental physical and chemical processes on an atomic level based on microscopic and spectromicroscopic investigations. Our main methods are scanning tunneling microscopy and spectroscopy, scanning electron microscopy, local Auger electron spectroscopy and atomic force microscopy in an ultra high vacuum environment.

FUTURE PERSPECTIVE

In the future we will target the combination of the two projects described above. Structures fabricated with the electron beam techniques will serve as templates for the local anchoring and/or functionalization of large organic molecules, i.e. in particular porphyrins.

Other future research activities will include:

- further investigation of fundamental aspects of electron induced processes
- instrumental development of EBID attachments to further explore in particular the lithographic process
- further exploration to switch the conformation of certain molecules at or close to room temperature

SELECTED PUBLICATIONS

- M.-M. Walz, M. Schirmer, F. Vollnhals, T. Lukasczyk, H.-P. Steinrück, H. Marbach, *Angew. Chem. Int. Ed.* **2010,** 49, 4669 – 4673
- F. Buchner, K. Seufert, W. Auwärter, D. Heim, J. V. Barth, K. Flechtner, J. M. Gottfried, H.-P. Steinrück, H. Marbach,. *ACS Nano* **2009,** 3, 1789 – 1794
- T. Lukasczyk, M. Schirmer, H.-P. Steinrück, H. Marbach, *Small* **2008,** 4, 841 – 844
- T. E. Shubina, H. Marbach, K. Flechtner, A. Kretschmann, N. Jux, F. Buchner, H.-P. Steinrück, T. Clark, J. M. Gottfried, *J. Am. Chem. So.* **2007,** 129, 9476 – 9483
- F. Buchner, V. Schwald, K. Comanici, H.-P. Steinrück, H. Marbach, *ChemPhysChem* **2007,** 8, 241 – 243
- H. Marbach, S. Günther, B. Lüerßen, L. Gregoratti, M. Kiskinova, R. Imbihl, *Catalysis Letters* **2002,** 83, 161 – 164

SELECTED REVIEWS

- J. M. Gottfried, H. Marbach, Surface-confined coordination chemistry with porphyrins and phthalocyanines: Aspects of formation, electronic structure and reactivity, *Z. Phys. Chem.* **2009,** 223, 53 – 74

SELECTED AWARDS

- 2010 PCCP Hot Topic Price, Bunsen Tagung, Bielefeld
- 2008 PCCP Hot Topic Price, Bunsen Tagung, Saarbrücken

THEORETICAL CHEMISTRY

PD DR. MARÍA BELÉN RUIZ

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CURRICULUM VITAE

2010	Habilitation in Theoretical Chemistry at the University of Erlangen-Nürnberg (Prof. Görling), Germany
2009	Visiting Professor at Autonoma University of Madrid, Spain
1996	Visiting Researcher at the University of Hiroshima, Japan
1995 – 2004	Postdoctoral Fellow, Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany
1994	PhD in Theoretical Chemistry at the Spanish National Research Council, Madrid, Spain
1993 – 1994	Graduate Assistant at the University of Erlangen-Nürnberg, Germany
1993	Graduate Assistant at the Hungarian Academy of Sciences, Budapest, Hungary

RESEARCH HIGHLIGHTS

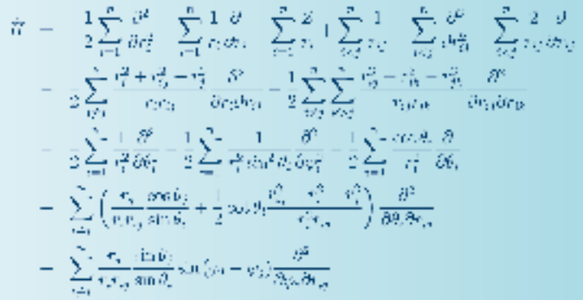
First to Hylleraas-Configuration Interaction calculations on boron atom. An analytical method for the evaluation of two-, three- and four-electron integrals and development of the corresponding computer programs. Derivation of the Hamiltonian in Hylleraas coordinates for atoms and molecules. New formulas for integrals with negative powers, orbital rotation and recursion relations. Contribution to the extension of the Hy-CI method to atoms with five or more electrons.

FUTURE PERSPECTIVE

The highly accurate (exact for physical and chemical purposes) calculation of energy and properties of atoms and molecules has multiple applications, like to give reference values for testing other methods, study the electronic structure of atoms and molecules under confinement conditions, excitations during beta decay processes, final state probabilities in nuclear reactions, especially the Boron Neutron Capture Therapy, a promising therapy for head, neck and many cancers.

Next projects are to write a Hylleraas-CI program code for C, N and O atoms to study nuclear reactions and neutron damage in DNA; to study the changes of the energy levels of confined helium atom, what is important for the conductivity in microelectronics.

A future project is the extension of the method to molecules to study week intermolecular interactions, variation of the electron density under electric and magnetic fields.



SELECTED PUBLICATIONS

- M. B. Ruiz, M. Rojas, G. Chicón, P. Otto, *Int. J. Quantum Chem.* **2010**
- M. B. Ruiz, *J. Math. Chem.* **2009,** 46, 1322 – 1355
- M. B. Ruiz, *J. Math. Chem.* **2009,** 46, 24 – 64
- S. Ragot, M. B. Ruiz, *J. Chem. Phys.* **2008,** 129, 124117
- M. B. Ruiz, R. Schumann, *Chem. Phys. Lett.* **2005,** 406, 1 – 9
- M. B. Ruiz, *Int. J. Quantum Chem.* **2005,** 101, 261 – 273
- M. B. Ruiz, *Int. J. Quantum Chem.* **2005,** 101, 246 – 260

SELECTED REVIEWS

- M. B. Ruiz, K. Peuker, Mathematical Techniques in molecular calculations using Slater orbitals, in: *Recent Advances in Computational Chemistry: Molecular Integrals over Slater orbitals*, Eds. T. Özdogan, M. B. Ruiz **2008,** 2008, 99 – 144
- P. E. Hoggan, M. B. Ruiz, T. Özdogan, Molecular Integrals over Slater orbitals. From pioneers to recent progress, in: *Quantum Frontiers of Atoms and Molecules*, Ed. Mihai V. Putz **2010,** 63 – 90

SELECTED AWARDS

- Member of the American Chemical Society
- Grant for excellent young women academics from the University of Erlangen-Nürnberg
- Grants from Spanish Ministry of Education
- Grant from the Hungarian Exterior Ministry

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CURRICULUM VITAE

Since 2006	Postdoctoral Fellow, Pharmaceutical Technology, University of Erlangen-Nürnberg, Germany, Head of the "Freeze Drying Focus Group"
2004 – 2006	Postdoctoral Fellow, School of Pharmacy, University of Connecticut (Prof. Pikal), Storrs, CT, USA
2001 – 2004	Graduate student, Pharmaceutical Technology, University of Erlangen-Nürnberg (Prof. Lee), Germany
2000	Licensed pharmacist, Germany
1995 – 1999	Undergraduate student, School of Pharmacy, University of Würzburg, Germany

OBJECTIVES AND PERSPECTIVES

The objective of the present research is to extend the knowledge space in the field of pharmaceutical freeze-drying (formulation and process) and to establish a scientific approach to product and process development (Quality-by-Design, QbD) in this field of interest.

Focus on new technologies in the field of pharmaceutical freeze-drying to further shorten cycle time while maintaining the same quality level of the final product. Moreover, focus on defining and standardizing "quality" of a freeze-dried pharmaceutical product.

SELECTED PUBLICATIONS AND REVIEWS

- H. Gieseler, G. Lee, *J. Pharm. Sci.* **2009,** 98, 3447 – 3455
- S. Schneid, H. Gieseler, W. Kessler, M.-J. Pikal, *J. Pharm. Sci.* **2009,** 98, 3406 – 3418
- M. Meister, H. Gieseler, *J. Pharm. Sci.* **2009,** 98, 3072 – 3087
- R.-E. Johnson, H. Gieseler, D.-L.Teagarden, L.-M. Lewis, *Am. Pharm. Rev.* **2009,** 4, 54 – 60
- S. Schneid, H. Gieseler, *PharmSciTech* **2008,** 9, 729 – 739
- H. Gieseler, T. Kramer, M.-J. Pikal, *J. Pharm. Sci.* **2007,** 96, 3402 – 3418
- H. Gieseler, *Eur. Pharm. Rev.* **2007,** 12, 62 – 67

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CURRICULUM VITAE

Since 2006	Postdoctoral Fellow, Theoretical Chemistry, University of Erlangen-Nürnberg, Germany
2005	Postdoctoral Fellow, University of Århus (Prof. Jørgensen), Denmark
2004	Postdoctoral Fellow, University of Duisburg-Essen (Prof. Jansen), Germany
2003	PhD, Theoretical Chemistry, Heinrich Heine University of Düsseldorf, Germany

OBJECTIVES AND PERSPECTIVES

We are working on the development of generally applicable new density functionals that are based on wave-function methods but in which the favourable scaling behaviour of standard DFT is conserved. This will require the combination of the method with fast numerical algorithms to extend the applicability to large systems. A first step in this direction has already been made by introducing a new orbital-dependent exchange-correlation functional derived from the fluctuation-dissipation formula with exact Kohn-Sham exchange.

SELECTED PUBLICATIONS AND REVIEWS

- A. Heßelmann, A. Görling, *Mol. Phys.* **2010,** 108, 359 – 372
- A. Heßelmann, A. Görling, *Phys. Rev. Lett.* **2009,** 102, 233003
- A. Heßelmann, *J. Chem. Phys.* **2008,** 128, 144112
- A. Heßelmann, A. Götz, F. Della Sala, A. Görling, *J. Chem. Phys.* **2007,** 127, 054102
- A. Heßelmann, G. Jansen, M. Schütz, *J. Am. Chem. Soc.* **2006,** 128, 11730
- A. Heßelmann, G. Jansen, M. Schütz, *J. Chem. Phys.* **2005,** 122, 014103

AWARDS

- 2004 Gottschalk-Diederich-Baedeker Award

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CURRICULUM VITAE

Since 2005	Postdoctoral Fellow, Medicinal Chemistry, University of Erlangen-Nürnberg, Germany
2000 – 2005	Research Assistant, Pharmacy and Food Chemistry, University of Erlangen-Nürnberg, Germany
1995 – 1999	Postdoctoral Fellow, Organic Chemistry, Computer Chemistry Center, University of Erlangen-Nürnberg, Germany
1994	PhD, Physical Chemistry, University of Würzburg, Germany

OBJECTIVES AND PERSPECTIVES

My general interest focuses on the exploration of structure and dynamics of proteins and DNA with classical simulation methods. I am applying Molecular Dynamics and Homology Modeling techniques to understand how chemical signals are processed, transduced, and converted into protein structural changes. Future work will concentrate on nucleotide-binding proteins and interleukins with their receptors. Especially the latter systems allow the prediction and control of selective protein-protein interactions as a test case for successful synergy between theory and experiment.

SELECTED PUBLICATIONS AND REVIEWS

- F. Haberl, H. Lanig, T. Clark, *Proteins* **2010,** 77, 857 – 866
- U. Böiers, H. Lanig, B. Sehnert, R. Holmdahl, H. Burkhardt, *Eur. J. Immunol.* **2008,** 38, 2784 – 2795
- K. von der Mark, H. von der Mark, E. Pöschl, H. Lanig, T. Sasaki, R. Deutzmann, *J. Mol. Biol.* **2007,** 371, 1188 – 1203
- F. Boeckler, H. Lanig, P. Gmeiner, *J. Med. Chem.* **2005,** 48, 694 – 709
- H. Lanig, H. Bradl, H.-M. Jäck, *Mol. Immunol.* **2004,** 40, 1263 – 1272
- H. Lanig, T. Clark, in: Systems Chemistry, M. G. Hicks, C. Kettner, Eds., Proceedings of the International Beilstein Workshop 2008

AWARDS

- Member of the DPhG and RSC
- Chairman of the MGMS, German Section
- Grants from BMBF, Fonds der Chemischen Industrie and Bavarian Ministry of Science and Research

DR. RALPH PUCHTA

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CURRICULUM VITAE

Since 2004	Postdoctoral Fellow, Inorganic and Analytic Chemistry, University of Erlangen-Nürnberg, Germany
2003 – 2004	Postdoctoral Fellow, Computer Chemistry Center and Theoretical Chemistry, University of Erlangen-Nürnberg, Germany
2003	PhD, Organic Chemistry, Computer Chemistry Center, University of Erlangen-Nürnberg, Germany

OBJECTIVES AND PERSPECTIVES

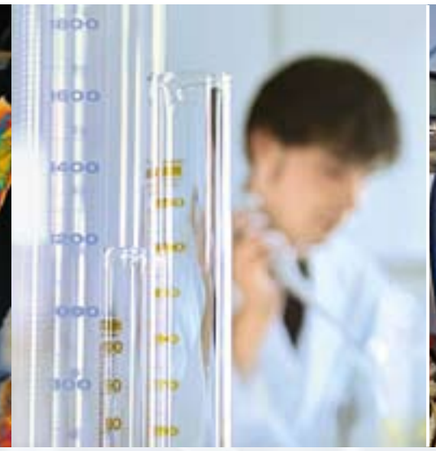
Our goal is to apply the knowledge gained from model reactions at metal ion centers to metal ions in a bioinorganic environment and to investigate the reaction mechanisms in the real surrounding in order to specifically manipulate them afterwards. We therefore need detailed knowledge about the factors that influence the energetic aspects of reactions and the reaction mechanisms.

For the (metallo)supramolecular systems, we want to design by quantum chemical calculations, systems with specific properties like pKa values or selective complexation abilities to ions and molecules.

SELECTED PUBLICATIONS AND REVIEWS

- B. M. Alzoubi, R. Puchta, R. van Eldik, *Aust. J. Chem.* **2010,** 63, 236 – 244
- R. Puchta, A. Scheurer, *Z. Naturforsch.* **2010,** 65b, 231 – 237
- R. W. Saalfrank, H. Maid, A. Scheurer, R. Puchta, W. Bauer, *Eur. J. Inorg. Chem.* **2010,** 2903 – 2906
- R. Puchta, E. Pasgreta, R. van Eldik, *Adv. Inorg. Chem.* **2009,** 61, 523 – 571
- B. Neumüller, K. Dehnicke, R. Puchta, *Z. Anorg. Allg. Chem.* **2008,** 634, 1473 – 1476
- R. Puchta, R. van Eldik, *Eur. J. Inorg. Chem.* **2007,** 1120 – 1127
- R. Puchta, N. van Eikema Hommes, R. Meier, R. van Eldik, *Dalton Trans.* **2006,** 3392 – 3395
- Z. Chen, C. S. Wannere, C. Corminbœuf, R. Puchta, P. von Ragué Schleyer, *Chem. Rev.* **2005,** 105, 3842 – 3888



EMIL FISCHER GRADUATE SCHOOL OF PHARMACEUTICAL SCIENCES AND MOLECULAR MEDICINE

Training future generations of scientists to discover promising new drugs and target proteins in novel ways:
The Emil Fischer Graduate School in Pharmaceutical Sciences & Molecular Medicine (EFS) leads to a Dr. rer. nat. degree in one of the most dynamic and expanding fields of current science. The program aims to educate students to address the major questions in pharmaceutical sciences and molecular medicine, teach students the basic sciences needed to answer these questions, and create an environment where students can develop into independent and creative scientists. The program is multidisciplinary and has a dual focus: Pharmaceutical Sciences & Molecular Medicine.

CONTACT

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GRADUATE SCHOOL ADVANCED MATERIALS AND PROCESSES

Particles and people – Innovation occurs at the interfaces
The Graduate School Advanced Materials and Processes (GS AMP) acts as a common platform for all doctoral researchers in the Cluster of Excellence Engineering of Advanced Materials (EAM). In EAM, researchers from science and engineering work on innovative nanoelectronic, catalytic, optic and photonic, as well as lightweight materials. Their common research approach is to develop and optimize advanced materials along the entire process chain, from the molecular level to their application in products. Important aspects of the Cluster are its interdisciplinary research approach and its international and industrial cross-links. Working in such an environment is tremendously inspiring and creates vast opportunities and new challenges. GS AMP members get in contact with scientists from other disciplines, look beyond the perimeter of their projects and build up an international network. GS AMP offers continual support to its members. The graduate school program is based on an intensive mentoring system and strong networking. It ensures that the doctoral projects are effectively organized and that the researchers are integrated into an interdisciplinary and international community. In addition to research in an inspiring environment, GS AMP provides special training for doctoral researchers through courses for advanced scientific qualification as well as personal and leadership skills development.

CONTACT

Coordinator: *Prof. Dr.-Ing. Wolfgang Peukert*
Program manager: *Dr. Carsten Schür*
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GRADUATE SCHOOL MOLECULAR SCIENCE

Molecular organization and transformations form the basis for life on earth. Research on structures and properties of molecules and the ability to synthesize specific target molecules are two of the most important foundations of the progress made in medicine and technology in the last century and will gain even more importance in the future. We are living in the “age of the molecule”. The demand for adequate food, energy, pharmaceuticals, medical care and the development of new, high-performance materials can only be satisfied by cooperative, interdisciplinary research designed to develop and understand new molecular concepts.

In order to satisfy these demands, we must strengthen academic training in interdisciplinary techniques that have molecules as their common theme. The University of Erlangen-Nürnberg (FAU) has already made the first step in this direction by establishing the consecutive B.Sc./M.Sc. degree course *Molecular Science* in 2001. The extraordinary success of this degree course and the large number of applications from all over Germany underline the importance of this concept. As a logical consequence and given the experience we obtained within the last years of this course, we have founded in 2008 the Graduate School Molecular Science at the FAU, with support of the Bavarian initiative “Bayern excellent”. Supervised by excellent researchers, elite students from Chemistry, Physics, Biology, Pharmacy, Chemical and Bioengineering, Materials Science, Molecular Science, and related fields, are trained to solve molecular problems in industrial and academic research successfully by tailored training in interdisciplinary research and techniques to enhance communication between disciplines.

The basis of the *GSMS,* molecules, is a clearly defined and homogenous training and research area despite the broadness of the various research fields. The experimental and theoretical techniques used in the individual disciplines are complementary. Our experience so far has shown that this concept works exceptionally well and gives great stimulus to research. Newly conceived teaching concepts in frontier areas provide important impetus which already led to a large series of seminal publications in first-class journals. Thus, we have prepared the ideal environment for the *GSMS* to develop into a world-leading centre for academic education in Molecular Science.

Currently, 40 students are enlisted in the GSMS program with 21 academic teachers as members. With a lecture program hosting nationally and internationally recognized leaders in their research fields, a winter school and access to all training courses of the university for soft skills development, languages, and others, the *GSMS* actively promotes the personal and scientific development of its graduate students.

The *GSMS* is strongly connected and scientifically linked to three research centers at the FAU. The Interdisciplinary Center for Molecular Materials (ICMM) at the FAU serves as a platform for interdisciplinary research projects in the fields of Molecular Materials and Nanotechnology. The Erlangen Catalysis Resource Center (ECRC) merges scientists from chemical engineering and synthetic organic and inorganic chemistry, supplemented with expertise from physical and theoretical chemistry. The Computer Chemistry Center (CCC) offers excellent experience and capability in modeling molecules, supramolecules, and materials.

CONTACT

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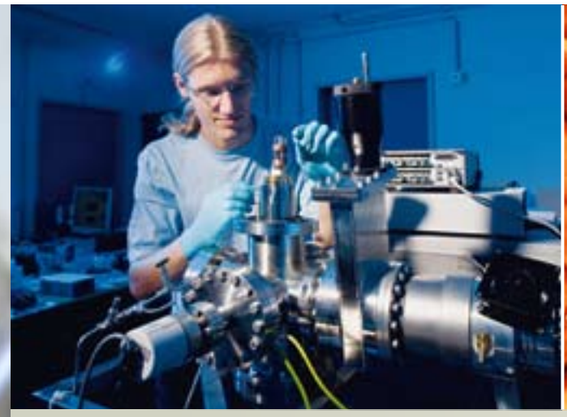


ENGINEERING OF ADVANCED MATERIALS (EAM)

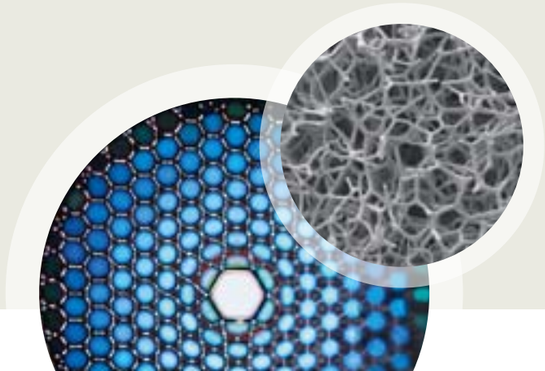
ENGINEERING OF ADVANCED MATERIALS

FROM MOLECULES TO MATERIALS

Advanced materials with properties tailored on the molecular scale and mesoscale are expected to stimulate evolutionary advances and revolutionary breakthroughs in emerging key technologies such as information and communications technology, catalysis, energy, and transportation. The Cluster of Excellence "Engineering of Advanced Materials – Hierarchical Structure Formation for Functional Devices" – or EAM – is the only interdisciplinary research collaboration of its type in Germany to focus on materials science and processes.

The vision of the Cluster is to bridge the gap between fundamental research and real-world applications of modern high-performance materials in key scientific and engineering areas. Bridging the gap between materials design at the molecular level and macroscopic properties ("from molecules to materials to functions") requires novel forms of interdisciplinary cooperation.

At the Cluster 200 researchers from 8 disciplines (Applied Mathematics, Chemical Engineering, Chemistry, Computer Science, Electrical Engineering, Materials Science and Engineering, Mechanical Engineering, and Physics) collaborate in more than 70 projects, from basic research in physics and chemistry as well as many areas of applications such as chemical and electrical engineering and materials science.



RESEARCH AREAS

Cross-sectional topics are explored in three interdisciplinary centers:

- Functional Particle Systems
- Nanoanalysis and Electron Microscopy
- Multiscale Modeling and Simulation

EAM focuses on four fields of application which are organized in value chains that represent hierarchical material classes with increasing complexity:

- Engineering of nanoelectronic materials
- Engineering of photonic and optical materials
- Engineering of catalytic materials
- Engineering of lightweight materials

INTERDISCIPLINARY NETWORK OF PARTNERS

The Cluster of Excellence was established at the University Erlangen-Nürnberg in November 2007 within the framework of the Excellence Initiative. The funding by DFG amounts to 40 million Euros for five years with additional substantial support by the University and the State of Bavaria. The EAM is based on existing and visible excellences within the University of Erlangen-Nürnberg as well as on the expertise of the Max Planck Institute for the Science of Light, the Fraunhofer Institute for Integrated Circuits (IIS) and Fraunhofer Institute for Integrated Systems and Device Technology (IISB), the New Materials Fürth GmbH, the Bavarian Laser Center and other notable academic and industrial research partners.

CONTACT

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Cluster Co-Coordinator: *Prof. Dr. Peter Wasserscheid*
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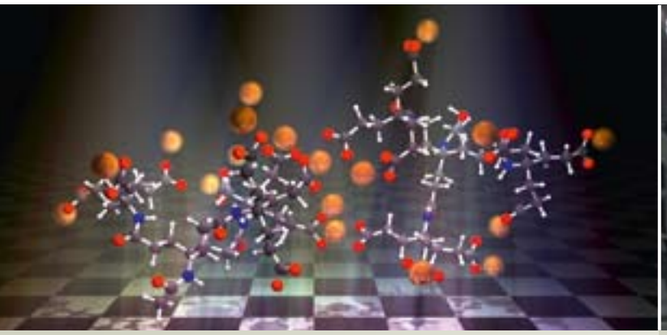

COMPUTER CHEMISTRY CENTER (CCC)

The Computer Chemistry Center (CCC) was founded in 1993 as a central facility of the Faculty of Natural Sciences II (Chemistry, Pharmacy and Biology) and was later integrated into the Department of Chemistry and Pharmacy. CCC houses three research groups, those of Profs Tim Clark (CCC/Organic Chemistry), Bernd Meyer (Interdisciplinary Center for Molecular Materials, ICMM) and Dirk Zahn (Theoretical Chemistry) with a total of approximately 50 researchers. Prof. (emeritus) Paul von Ragué Schleyer also spends part of each year in CCC. The research topics treated in CCC range from protein and DNA simulations and computational drug design to simulation and design of new materials. Together, the three groups in CCC use a spectrum of calculational techniques from classical molecular dynamics and semiempirical molecular orbital theory to density-functional theory and high level ab initio calculations. Groups from CCC are involved in both SFB583 and the Excellence Cluster Engineering of Advanced Materials. CCC offers teaching in modeling and simulation and computational drug design as well as more traditional subjects. Prof. Andreas Görling is the Chairman of the Kollegiale Leitung of CCC and Prof. Tim Clark is its Technical Director.

CONTACT

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EMIL FISCHER CENTER (EFC)

The Emil Fischer Center serves as a platform for interdisciplinary research between work groups from pharmaceutical sciences, food chemistry, chemistry, and molecular medicine.

The goal of the Emil Fischer Center is to focus, to crosslink and to support the scientific work on bioactive molecules, target proteins, and bioanalytics. The main topics are the identification of target proteins, target protein formulation and modulation, ligand-protein interactions and target proteins in signal transduction. The intention behind this research is to bridge chemistry and biomedical sciences leading to the development of novel therapeutic strategies. For this purpose, it is crucial to understand the interaction of new bioactive small molecules with their target proteins and resulting cellular reactions.

The Emil Fischer Center operates the Core Unit for Bioanalytics, where the scientific and technical competence on targeted and non-targeted metabolome analysis as well as targeted proteome analysis is focused. The bioanalytical expertise covers further techniques of molecular biology and functional assays.

Furthermore, the Emil Fischer Center coordinates the interdisciplinary education of students in the field of pharmacy, food chemistry, and molecular medicine. Excellent post graduates are trained by the Emil Fischer Graduate School, which is operated by the Emil Fischer Center.

Research at the Emil Fischer Center and the Emil Fischer Graduate School is supported by several organizations and research collaborations, such as the collaborative research centers SFB 423, SFB 583, SFB 796, the DFG graduate program 1071, BMBF, EU, the Elite Network of Bavaria, and the Bayerische Forschungsstiftung.

CONTACT

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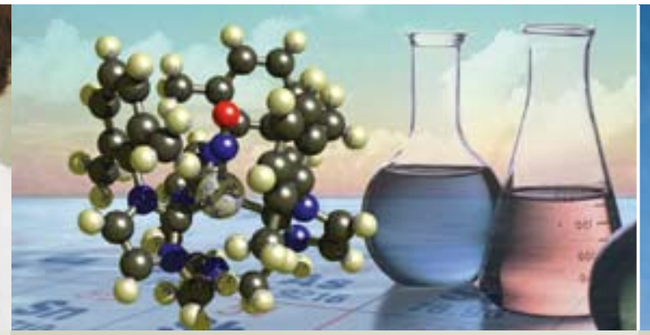

ERLANGEN CATALYSIS RESOURCE CENTER (ECRC)

The Erlangen Catalysis Resource Center was established in 2008 as one of the Interdisciplinary Centers of the University Erlangen-Nürnberg. With the inauguration of the ECRC, the University established the new and unique curriculum “catalysis” which brings together scientists from chemical engineering, synthetic organic and inorganic chemistry supplemented with expertise from physical and theoretical chemistry. Fourteen research groups from the Department of Chemistry and Pharmacy (DCP) and the Department of Chemical and Biological Engineering (CBI) participate in the center representing an active and highly interdisciplinary community of chemists and engineers working in the fields of homogenous, heterogeneous and biocatalysis as well as chemical reaction engineering. Research within the ECRC aiming at the integration of catalyst, reactor and process design is currently focusing on:

- the design of novel catalysts for sustainable processes and energy applications,
- the use of a large number of spectroscopic techniques to study catalysts under working conditions,
- the development of new reactor concepts,
- process intensification.

Moreover, the Erlangen Catalysis Resource Center is part of the interdisciplinary undergraduate and graduate education in catalysis. Particular emphasis is placed on the integration of (undergraduate) students into state-of-the-art catalysis research at an early stage of their education.

The ECRC is managed by an executive board elected by the members of the Center which presently consists of two scientists from the CBI (Prof. P. Wasserscheid, Speaker, and Prof. K. E. Wirth) and two scientists from the DCP (Prof. K. Meyer and Prof. J. Libuda) and the Professor of Catalysis within the ECRC (Prof. M. Hartmann) as a permanent member.

CONTACT

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INSTITUTE OF ADVANCED MATERIALS AND PROCESSES (ZMP)

The Institute of Advanced Materials and Processes (ZMP) is an interdisciplinary research center of the University of Erlangen-Nürnberg with more than 80 coworkers originating from chemistry, materials sciences and engineering. In June 2006 no more than 20 persons moved into the friendly and innovative environment at the “Uferstadt Fürth” and step by step breathed life into the concept of interdisciplinary research of 4 chairs from the school of engineering (WW1 – General Materials Processes, WTM – Science and Technology of Metals, WW3 – Glass and Ceramics, LFT – Manufactoring Technology) and one chair of the Department of Chemistry and Pharmacy (Organic Chemistry II). The ZMP is administered by a cooperative headship formed by the five professors involved (Prof. Singer, Prof. Greil, Prof. Göken, Prof. Hirsch and Prof. Schmidt) and an executive board (Dipl.-Ing. Kellermann and Dr. Hauke).

The research goal is the construction of revolutionary light weight materials and includes the fundamental investigation of novel substance classes, the development of visonary concepts and processes as well as the application of the insights gained for the construction of prototypes. The contribution from the Department of Chemistry and Pharmacy is thus the synthesis and characterization of innovative, functional carbon allotropes based on carbon nanotubes and graphene under the supervision of Prof. A. Hirsch and Dr. F. Hauke.

The interdisciplinarity is further reflected by the joint efforts of researchers also involved in other research centers of the FAU such as the Cluster of Excellence Engineering of Advanced Materials (EAM), the Interdisciplinary Center for Molecular Materials (ICMM) and the Graduate School Molecular Science (GSMS).

CONTACT

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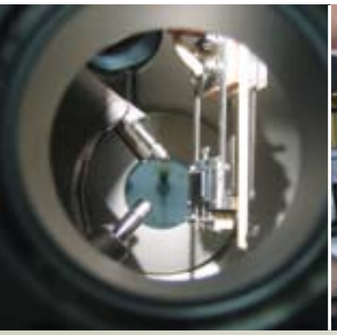

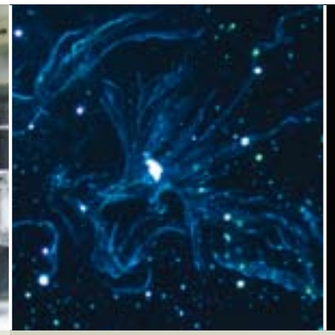

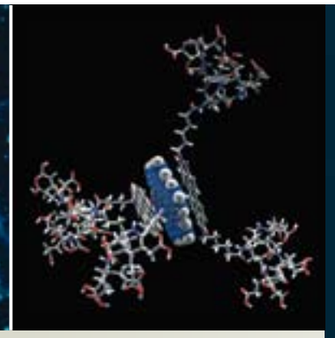

INTERDISCIPLINARY CENTER FOR INTERFACE-CONTROLLED PROCESSES (ICICP)

The ICICP was founded in 2004 with the idea to coordinate and strengthen cooperation between research groups in the field of surfaces, interfaces, and nanostructured materials. Today, around twenty groups from the Department of Physics, Chemistry and Pharmacy, Chemical and Biological Engineering, and Materials Science and Engineering actively participate. The research of these groups is focusing on three areas: (i) the preparation and characterization of interface-modified geometric structures, (ii) theoretical and experimental investigation of structure-property relationships in interface-modified structures and their applications, (iii) interfaces of particulate systems and interface-stabilized nanoparticles.

The intrinsic strength of the center is the excellent but complementary expertise of the participating groups. Bundling this know-how, the ICICP has contributed to the evolution of a lively and interdisciplinary research environment, in which numerous cooperation activities have been initiated.

Interdisciplinary graduate and undergraduate education is the second focus of the ICICP's activities. Offering lab-courses and contributing to the Master program in Chemistry, it aims at integrating excellent students into cutting-edge research at an early level of their studies. In terms of graduate education, the ICICP is organizing a scientific seminar program and, most importantly, a 4-term Interdisciplinary Graduate Course (IGC). These activities provide a thorough basis of interdisciplinary education in state-of-the-art research and foster direct scientific exchange between the PhD students.

The ICICP is managed by an executive board elected by the members of the center (Prof. Dr. Jörg Libuda, Department of Chemistry and Pharmacy (Speaker); Prof. Dr. M. Alexander Schneider, Department of Physics; Prof. Dr. Oliver Diwald, Department of Chemical and Biological Engineering).

CONTACT

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INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS (ICMM)

Molecular materials represent a fundamental and interdisciplinary research area at the interface between Chemistry, Physics, and Materials Science. At the same time they provide the basis for a variety of future technologies. Materials based on defined molecular building blocks are characterized by tuneable performance, which is of great importance for high end applications in nanoelectronics, medicine and energy conversion technology. The ICMM at the Friedrich-Alexander-University of Erlangen-Nürnberg serves as a platform for interdisciplinary research projects in the field of Molecular Materials and Nanotechnology. Currently, the ICMM houses 20 groups from the Chemistry and Physics Departments of the FAU (http://www.chemie.uni-erlangen.de/icmm/). Their complementary research expertise spans from the synthesis and the supramolecular oganization of new molecular architectures including fullerenes, carbon nanotubes, polyynes, porpyhrins and dendrimers to the development of opto-electronic devices. Next to molecules also nanoparticles, ultrathin layers and interfaces are investigated. Physical characterization is achieved, for example, by single-molecule conductivity measurements, by time resolved photophysical investigations and modern microscopy techniques including TEM, STM and AFM. The research at the ICMM is supported by a variety of organizations such as DFG, BMBF, EU and the Bayerische Forschungsstiftung.

In addition close scientific collaboration with industrial laboratories serves as a major stimulus for developing new applications for molecular materials. Modern student training programs in particular the subject Molecular Science which was recently established at the FAU as a consecutive Bachelor/Master curriculum as well as recruitment of excellent international graduates and Post-Docs guarantees a continuous supply of highly qualified researches for the ICMM.

CONTACT

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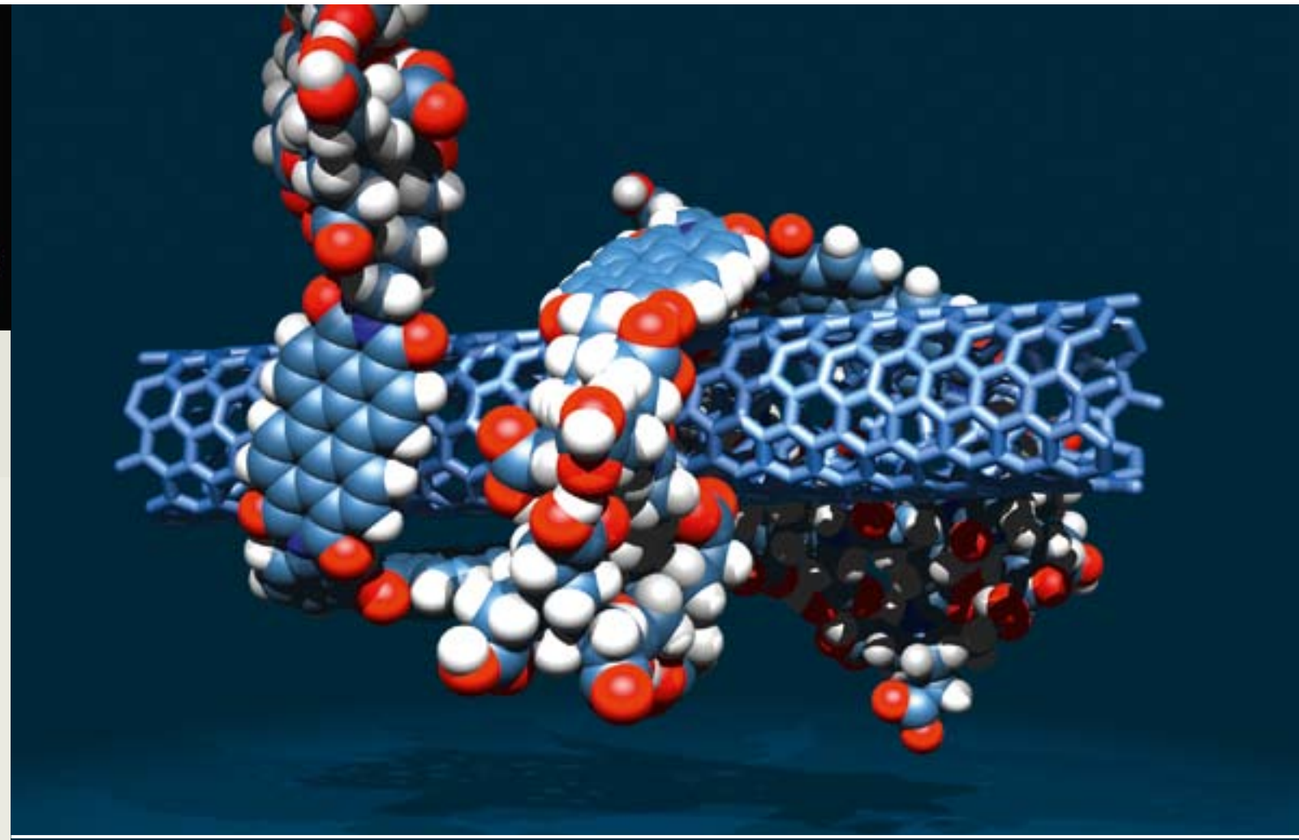

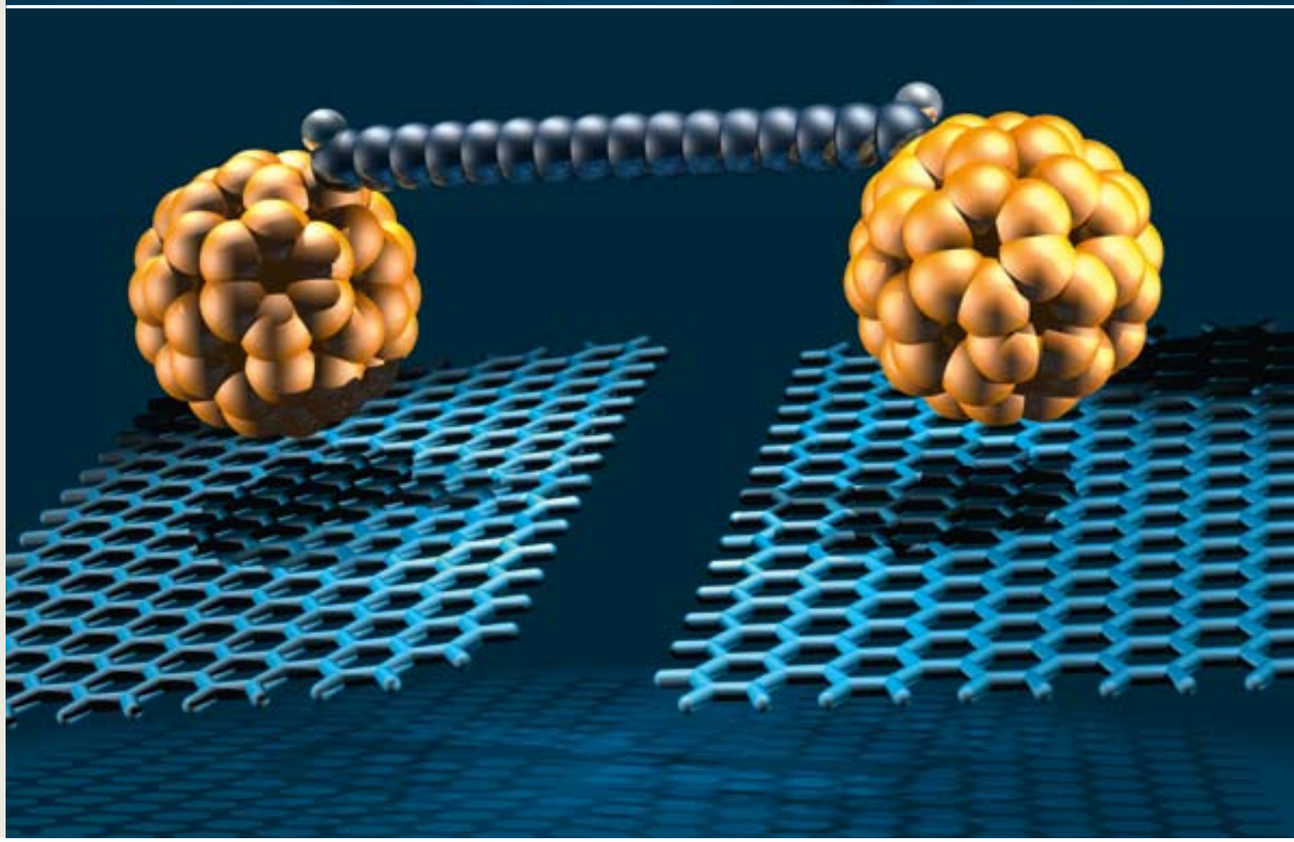




QUALIFYING FOR THE FUTURE: OUR DEGREE PROGRAMS

The University of Erlangen-Nürnberg is part of an extended international network and maintains close ties with 500 partner universities in 62 countries. Researchers from Erlangen and Nürnberg work closely with leading universities throughout the world in more than 130 research collaborations. The University of Erlangen-Nürnberg is one of the most attractive German universities for visiting academics from abroad. Every year more and more Humboldt scholars and prize-winning researchers choose this Northern Bavarian university as their research base.

The main focus of the University of Erlangen-Nürnberg in research and teaching is to be found at the interface between Natural Sciences, Engineering, and Medicine in close cooperation with the classical university disciplines Law, Theology, and the Humanities. Economics, Social and Educational Sciences complete the range of subjects offered.

The University offers an enormous variety of subjects in > 140 different degree courses. Even at undergraduate level the students have many opportunities to experience advanced levels of research which enable them to benefit from the interdisciplinary, international and practically-oriented range of courses on offer.

The **Department of Chemistry and Pharmacy** offers the following study courses

CHEMISTRY
Bachelor of Science (B.Sc.) / Master of Science (M.Sc.)

MOLECULAR SCIENCE
Bachelor of Science (B.Sc.) / Master of Science (M.Sc.)

CHEMISTRY TEACHER'S DEGREE
Gymnasium / Realschule / Hauptschule / Grundschule

PHARMACY – State Examination

FOOD CHEMISTRY – State Examination

More than 1,500 students are educated and trained in the aforementioned programs. In addition, the Department of Chemistry and Pharmacy is involved in the chemistry education of twelve other B.Sc. / M.Sc. or diploma programs ranging from medical to engineering sciences: every year more than 1,600 students from other programs attend classes and lab-courses in the various fields of chemistry.

In close collaboration with the Department of Didactics (Didactics of Chemistry) we train future school teachers for different school levels, from primary school to upper school.



CHEMISTRY (B.Sc. / M.Sc.)

The established study course is based on a wide-ranging basic and advanced education in the key subjects of chemistry. Substantiated chemical basic knowledge will be taught in all parts of this Natural Science.

Chemistry includes the core disciplines of Inorganic and General Chemistry, Organic Chemistry, Physical Chemistry, and Theoretical / Computational Chemistry. The substantial education is performed by lectures and seminars and through intense experimental work. Lab-courses allow direct insight into the basic and application oriented chemical research and support the lecture series.

Our consecutive *Chemistry* program is divided into a three-year Bachelor (B.Sc.) plus a two-year Master (M.Sc.) program. During the Bachelor program basic principles in Chemistry are addressed to prepare the students for graduate studies in chemical and related sciences. The Master program focuses on various subjects in chemical core disciplines. In addition, various subjects can be chosen to provide deeper insight into specific topics related to chemistry or interdisciplinary aspects. The Master Phase also includes a 6-month research project (Master Thesis) which usually concludes the course of study.

Our students studying Chemistry today will have best career opportunities tomorrow!

Chemical expertise is relevant in many different ways particularly with regard to important issues in the fields of energy, nutrition, health, mobility, and communication. Therefore there is a widespread task for educated chemists: Chemical and pharmaceutical industry, research institutes, universities and the public sector are only a few employers who offer interesting job opportunities.

The Bachelor's degree program in Chemistry is admission free.

CONTACT

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MOLECULAR SCIENCE (B.Sc. / M.Sc.)

The current Molecular Science is an interdisciplinary science and technology oriented course program including Biochemistry, Molecular Biology, Medicine and Pharmacy. In contrast to the Chemistry program, admission for the Molecular Science program is restricted.

The consecutive interdisciplinary Bachelor / Master program *Molecular Science* was successfully started at the Department of Chemistry and Pharmacy in 2001.

The Bachelor program of six semesters consists of basic studies (which are related to the chemistry program) followed by a specialization in either Molecular Nano Science or Molecular Life Science.

In both tracks, Molecular Life Science and Molecular Nano Science, the molecular aspects are the main issues differing in the relevant applications, i.e., life science or material science oriented. These aspects also serve as focus in the obligatory modules of the master program Drug Discovery and Nano Science, respectively.

Molecular Science goes far beyond the general understanding of Chemistry. The implementation of a Master-level program in Molecular Science at the University of Erlangen-Nürnberg tackles new scientific and technological developments with emphasis on the smallest relevant units: the molecules. However, the stronger topical focus within the individual tracks reduces the M.Sc. program to a total of 3 semesters (1 ½ years).

The combination of knowledge in synthesis chemistry with a solid microbiological education is in demand in Life Science industry (e.g. biotechnology, bioengineering, drug discovery). In Nanotechnology various job prospects are in modern material science orientated branches of technology (e.g. nanotechnology, microelectronics, energy research). With regard to the growing demand in molecular well-trained graduates in chemical and pharmaceutical companies, the job opportunities are excellent.

CONTACT

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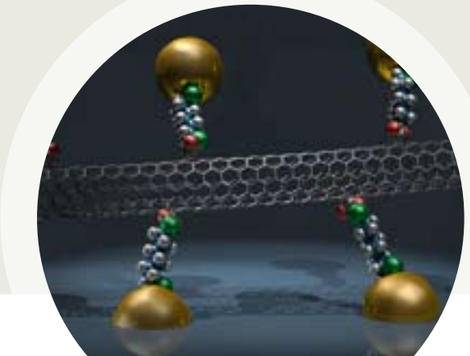

PHARMACY

Pharmacy is a scientific discipline at the interface of chemistry, biology, and medicine. Pharmaceutical sciences are focused on all aspects of bioactive compounds used as drugs, including the development, synthesis, quality control, preparation, and storage of pharmaceuticals, as well as their biological effects and safe application.

Our four-year Pharmacy curriculum includes lectures, seminars, tutorials, as well as a range of intensive laboratory courses in which state-of-the art scientific and instrumental methods are presented and used. Reflecting the interdisciplinary character of Pharmacy, subjects that are taught in the first two years include physics, inorganic, organic and analytical chemistry, as well as biochemistry, physiology, and microbiology. The first section of the Pharmaceutical Examination concludes this first, basic part of the curriculum. In the third and fourth year, the curriculum focuses on specific pharmaceutical disciplines, including Medicinal Chemistry, Pharmaceutical Biology, Pharmaceutical Technology/Biopharmacy, Pharmacology/Toxicology, as well as Clinical Pharmacy. Upon passing the second section of the Pharmaceutical Examination, graduates are required to perform a 12 months pharmaceutical internship before they can take the third and final section of the Pharmaceutical Examination, and, subsequently, apply for the state licensure as a Pharmacist.

While the majority of Pharmacy graduates take up positions at drug stores or hospital pharmacies, professional opportunities also include teaching and research at universities and other research institutes, the pharmaceutical industry, as well as public health agencies and testing laboratories.

Pharmacy graduates are also eligible to enter a PhD program at one of the Graduate Schools at our university.

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FOOD CHEMISTRY

Food chemists are experts in the field of the chemical composition, analysis, and product design of foods and cosmetics. Moreover, they understand how food constituents affect the human organism and have a basic knowledge about the industrial processing of foodstuffs, the respective juridical evaluation, and of the role of microorganisms in food production and spoilage.

Traditionally, food chemists work in the food industry, for the food control authorities, or in commercial laboratories. However, they are also well in demand when analytic expertise is needed, for example, in forensics or in the pharmaceutical and cosmetics industry.

Especially in the second (main) study period, food chemistry courses in Erlangen are characterized by a small number of students in the respective groups and project-oriented learning. Theory lectures are mostly enlarged by practical courses. During the first four terms, students attain the scientific basics in mathematics, physics, biology, chemistry, and biochemistry. This knowledge is vital for the subsequent food chemistry courses during the following terms. During the main study period, the students concentrate on issues of food chemistry. Several extensive lab-courses offer the opportunity to practice elementary analytical methods as well as to apply modern bio-analytical and instrumental techniques. The food chemistry courses are completed by lectures in nutritional physiology, food technology, microbiology, food law, toxicology, forensic analysis, quality management, and the chemistry and analytics of cosmetics.

A state examination finishes university education, usually after nine terms. Subsequently, graduates can add one year of further professional training to qualify as certified food chemists ("staatlich geprüfte Lebensmittelchemiker") and/or can do their PhD in various natural sciences or medicine.

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DIDACTICS OF CHEMISTRY

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CURRICULUM VITAE

Since 2009	Head of Department, Department of Didactics
Since 2009	Vice Dean, School of Humanities and Social Sciences
Since 2005	University Full Professor, Professor of Chemistry Teaching at the University of Erlangen-Nürnberg, Germany
2002 – 2005	Scientific assistant in Didactics of Chemistry, Oldenburg University, Germany
1989 – 2002	Scientific assistant in Didactics of Chemistry, Halle University, Germany
1985 – 1989	Secundary school teacher and class teacher, Hoyerswerda, Germany

Chemical education, especially didactics of chemistry, is a very important part of the education and advanced training for chemistry teachers. It comprises both theory and practice of how to teach chemistry topics and how students learn chemistry.

Chemistry education includes lectures such as the basics of chemistry education, seminars, and laboratory practice. Laboratory practice includes "school experiments in chemistry", which the students have to pass and also contains instruction such as how to set-up experiments in chemistry classes. These courses address multiple education levels: elementary school, secondary general school, intermediate secondary school, and grammar school. Experience in planning lessons and lessons learned from first-year teachers are taught during practical training at the schools, in conjunction with the university chemistry education courses.

In addition to training students, the didactics of chemistry also provides scientific in-service-training to teachers. The work of the in-service Training Centre, supported by GDCh, is guided by the three principles: "competence – cooperation – authenticity". Development of scientific teaching, application of didactic research to practical teaching, actual assistance in teaching classes, and assistance with creating new syllabi are the program's aims. Approximately 70 courses of various chemistry topics and their classroom implementation are offered for different education levels annually.

Practical experience is necessary when teaching science. Therefore the NESSI-Lab, a chemical lab for children, was founded in 2005. Once a week, students between first and sixth grade can visit the University to gain experience in chemistry applications. Chemistry education students assist the children to conduct experiments about water, air, fire, and earth. The lab experiments efficiently correlate experiments with real world concepts and materials that are relevant to students.

While these experiments could be easily constructed in class, setting up the experiments in a separate, student's laboratory adds the benefits of an extracurricular learning place.

Opening the NESSI-Lab for special education schools and higher school grades are current research projects at the chair of chemistry education. To orient the experiments to the special needs of children with hearing and learning disabilities, the experiments and their instruction have to be adapted. The combination of E-Learning and practical experiments within the framework of a business game offers a context-based method for classes from 7th to 12th grades. Both projects are accompanied with studies.

Another focus of research is Microscale Chemistry and its implementation at schools. Microscale is an environmentally safe, pollution prevention method of performing chemical processes. Without compromising the quality and standard of chemical applications in education, even small quantities of chemicals are used for Microscale experiments. Reduced costs, shorter experiment times, and reduced storages requirements are examples of the benefits for the application at schools. Other fields of research content "chemistry in context" as well as "media and experiments".

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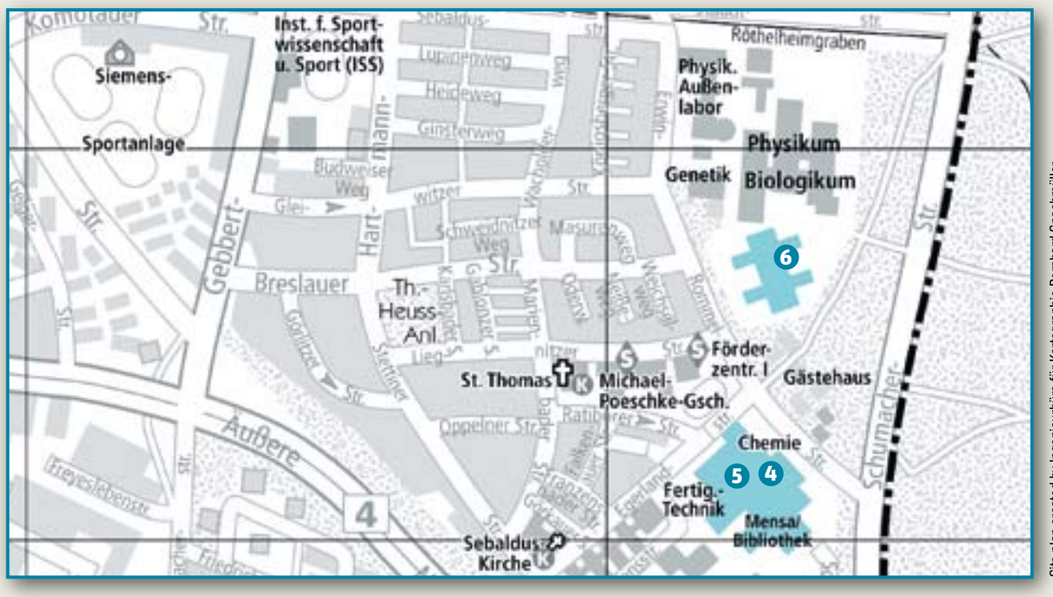
3 **Computer Chemistry Center,** Nägelsbachstr. 25, 91052 Erlangen
4 **Inorganic Chemistry,** Egerlandstr. 1, 91058 Erlangen
5 **Physical / Theoretical Chemistry,** Egerlandstr. 3, 91058 Erlangen
6 **"Chemikum",** under construction

ERLANGEN CITY

SOUTH CAMPUS



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